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3  ! "The role of chemistry in the oscillating combustion of hydrocarbons:
4  ! an experimental and theoretical study"
5  ! A. Stagni, Y. Song, L.A. Vandewalle, K.M. Van Geem,
6  ! G.B. Marin, O. Herbinet, F. Battin-Leclerc, T. Faravelli
7  !
8  ! Submitted to Chemical Engineering Journal (March 2019)
9  !
10 !
11 ! Thermodynamic properties
12 ! CHEMKIN format
13 !
14 !VERSION: 17_03
15 !AUTHORS: C1-C3 Burcat
16 !NOTE: SPECIES RE-ARRANGED AS THE SAME ORDER IN MECH
17 !
18 !VERSION: 17_05
19 !Following species are updated from Burcat's Database:Kik
20 ! C6H5CHCH3 FLUORENE C5H6 INDENYL C14H19 C12H7 C12H9
21 ! C6H5CH2C6H5 C10H7 CH3C6H4 C6H5C2H C6H5O C6H5C2H3 C10H7CH3
22 ! C10H7CHO RXYLENE C10H7CH2 XYLENE C6H2 Toluene C6H5OH
23 ! C14H10 C6H5C2H4C6H5 C4H2 C16H10 MCPTD C7H7 BENZYNE
24 ! C6H5C2H2 C12H8 C6H5C2H5 C10H7O BENZENE C4H4 INDENE
25 ! C5H5 C10H6CH3 C6H5 C10H8 FULVENE BIPHENYL C6H4C2H
26 !Following species are updated from ATcT's Database:Ghobad
27 ! H H2 O O2 HE
28 ! OH H2O N2 HO2 HCO
29 ! H2O2 AR CO CO2
30
31 THERMO
32 300. 1000. 4000.
33 C6H4O C 6H 4O 1 G 300.00 4000.00 1000.00 1 !
Biradicale da guaiacolo rivedeer sono quelle di C6H5O
34 .137221720E+02 .174688771E-01-.635504520E-05 .103492308E-08-.623410504E-13 2
35 15.2872748E+03-.488181680E+02-.466204455E+00 .413443975E-01 .132412991E-04 3
36 -.572872769E-07 .289763707E-10 1.97785839E+04 .276990274E+02 4
37 RPHENPH C 6H 5O 1 G 300 3500 1000 1
38 7.48628748E+00 3.11726354E-02-1.63674822E-05 4.10796074E-09-3.98797024E-13 2
39 1.49961514E+04-1.26543728E+01-8.11677970E+00 9.35849042E-02-1.09985886E-04 3
40 6.65202295E-08-1.60018642E-11 1.81167649E+04 6.26214070E+01 4
41 RCATEPH C 6H 5O 2 G 300 3500 1000 1
42 1.18218904E+01 2.70911132E-02-1.34162451E-05 3.08575091E-09-2.72411991E-13 2
43 -7.82412443E+03-3.10506043E+01-7.41421113E+00 1.04035520E-01-1.28832855E-04 3
44 8.00301573E-08-1.95085136E-11-3.97690414E+03 6.17524664E+01 4
45 C6H4C2H3 T12/07C 8.H 7. 0. 0.G 200.000 6000.000 1000.00 1
46 1.57334515E+01 2.38965492E-02-8.60829763E-06 1.39223384E-09-8.35065775E-14 2
47 4.08827573E+04-5.82476667E+01 1.17830774E+00 3.40765502E-02 5.85065530E-05 3
48 -1.10953244E-07 4.95222636E-11 4.61414992E+04 2.36053284E+01 4.83284254E+04 4
49 C7H6O3 C 7H 6O 3 G 300 3500 1000 1
50 9.6100307E+00 4.6312670E-02 -2.4985466E-05 6.2313178E-09 -5.9678291E-13 2
51 -5.2881308E+04 -1.4662558E+01 -7.0701097E+00 1.1303323E-01 -1.2506631E-04 3
52 7.2951879E-08 -1.7276923E-11 -4.9545280E+04 6.5809478E+01 4
53 RC7H5O3 C 7H 5O 3 G 300 3500 1000 1
54 1.03519980E+01 4.06949717E-02-2.16398081E-05 5.16863129E-09-4.69580170E-13 2
55 -3.48541024E+04-1.78724727E+01-6.94106227E+00 1.09867214E-01-1.25398170E-04 3
56 7.43408724E-08-1.77626405E-11-3.13954904E+04 6.55565469E+01 4
57 C8H6O3 C 8H 6O 3 G 300 3500 1000 1
58 4.593105E+00 6.232992E-02 -3.473750E-05 8.749391E-09 -8.397915E-13 2
59 -4.481918E+04 1.511354E+01 -8.470549E+00 1.145845E-01 -1.131194E-04 3
60 6.100401E-08 -1.390345E-11 -4.220645E+04 7.813812E+01 4
61 RGUAIPH C 7H 7O 2 G 300 3500 1000 1
62 1.0328870E+01 4.1581495E-02 -2.2022073E-05 5.3914934E-09 -5.0157294E-13 2
63 -4.9145545E+03 -2.2004822E+01 -7.2388396E+00 1.1185234E-01 -1.2742833E-04 3
64 7.5662334E-08 -1.8069283E-11 -1.4010125E+03 6.2749224E+01 4
65 RSALICPH C 7H 5O 2 G 300 3500 1000 1
66 6.006532E+00 4.553370E-02 -2.518536E-05 6.391630E-09 -6.195741E-13 2
67 4.679999E+02 2.823677E+00 -8.006329E+00 1.015851E-01 -1.092625E-04 3
68 6.244307E-08 -1.463244E-11 3.270572E+03 7.042763E+01 4
69 RANISPH C 7H 7O 1 G 300 3500 1000 1
70 6.1403860E+00 4.5274166E-02 -2.4649522E-05 6.3063297E-09 -6.1560301E-13 2
71 1.7881392E+04 -4.3538799E+00 -8.0284207E+00 1.0194939E-01 -1.0966236E-04 3
72 6.2981557E-08 -1.4784410E-11 2.0715154E+04 6.4002422E+01 4

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73 CATECHOL C 6H 60 2 G 300.00 3500.00 1150.00 1
74 1.43499796e+01 2.44086040e-02-1.04210961e-05 2.01938934e-09-1.47232776e-13 2
75 -3.94515398e+04-4.76262851e+01-5.49815264e+00 9.34455856e-02-1.00469333e-04 3
76 5.42212658e-08-1.14954668e-11-3.48864694e+04 5.09034930e+01 4
77 RCATEC C 6H 50 2 G 300.00 3500.00 1140.00 1
78 1.40810368e+01 2.16036559e-02-9.34848731e-06 1.81734390e-09-1.31737736e-13 2
79 -2.57458617e+04-4.55416672e+01-4.82568614e+00 8.79430347e-02-9.66371436e-05 3
80 5.28633417e-08-1.13260355e-11-2.14351289e+04 4.81496570e+01 4
81 GUAIACOL C 7H 80 2 G 300.00 3500.00 1000.00 1
82 9.99301751e+00 4.50609491e-02-2.36180835e-05 5.74985960e-09-5.33615080e-13 2
83 -3.55531886e+04-2.30989118e+01-7.52910597e+00 1.15149443e-01-1.28750824e-04 3
84 7.58383535e-08 -1.80557386e-11-3.20487639e+04 6.14352053e+01 4
85 SALICALD C 7H 60 2 G 300.00 3500.00 1000.00 1
86 1.64419508E+01 2.56565170E-02-9.29837990E-06 1.30953013E-09-5.02395383E-14 2
87 -3.38514104E+04-5.63974383E+01-4.36490575E-01 5.47073717E-02-7.07267500E-07 3
88 -3.69175398E-08 1.74133046E-11-2.82980420E+04 3.52247637E+01 4
89 VANILLIN C 8H 80 3 G 300.00 3500.00 1260.00 1
90 1.36544650e+01 4.84143232e-02-2.42641798e-05 5.50487829e-09-4.76001947e-13 2
91 -5.18855416e+04-3.54575728e+01-4.86637458e+00 1.07210639e-01-9.42597942e-05 3
92 4.25395949e-08-7.82416000e-12-4.72182900e+04 5.81751551e+01 4
93 ! -----ARAMCO 2.0 -----
94 C3H6 8/12/15 C 3H 6 0 OG 298.000 6000.000 1000.000 01
95 6.59032304E+00 1.52592866E-02-5.30369441E-06 8.35510888E-10-4.91215549E-14 2
96 -2.47481113E+02-1.15748238E+01-1.54606737E+00 4.36553128E-02-5.61392417E-05 3
97 4.98421927E-08-1.84798923E-11 2.07056233E+03 2.99232495E+01 4
98 C3H5-A 8/12/15 C 3H 5 0 OG 298.000 6000.000 1000.000 01
99 7.37604097E+00 1.23449782E-02-4.26463882E-06 6.69045835E-10-3.92202554E-14 2
100 1.77332960E+04-1.61758204E+01-3.32899442E+00 5.38423469E-02-7.65500752E-05 3
101 6.35512285E-08-2.14283003E-11 2.03420628E+04 3.68038362E+01 4
102 C3H5-S 8/12/15 C 3H 5 0 OG 300.000 5000.000 1390.000 11
103 7.95954498E+00 1.11163183E-02-3.75197834E-06 5.77246260E-10-3.32768957E-14 2
104 2.80567891E+04-1.79800372E+01 1.61793372E+00 2.44803904E-02-1.41856503E-05 3
105 4.16402233E-09-4.90904795E-13 3.04291037E+04 1.66341443E+01 4
106 C3H5-T 8/12/15 C 3H 5 0 OG 300.000 5000.000 1376.000 11
107 7.69949212E+00 1.17803985E-02-4.07791749E-06 6.38119222E-10-3.72229675E-14 2
108 2.61747145E+04-1.68305890E+01 2.29256998E+00 1.98527646E-02-6.42635654E-06 3
109 -5.90016395E-10 5.05491095E-13 2.85773377E+04 1.39407124E+01 4
110 ! ----- end ARAMCO 2.0 -----
111 LC5H8 C 5H 8 G 300.00 4000.00 1000.00 1
112 .797205310E+01 .268614160E-01-.956546320E-05 .113079120E-08 .000000000E+00 2
113 .510466811E+04-.185090870E+02 .176636500E+01 .432678800E-01-.237613290E-04 3
114 .512588110E-08 .000000000E+00 .684030700E+04 .137180600E+02 4
115 CYC5H8 C 5H 8 G 300.00 4000.00 1000.00 1
116 .772447728E+01 .283223160E-01-.115452360E-04 .215408150E-08-.150541780E-12 2
117 -.782614232E+03-.197696844E+02 .268981400E+01 .209545500E-02 .113036870E-03 3
118 -.154080700E-06 .627636580E-10 .231396630E+04 .152940560E+02 4
119 CYC6H8 C 6H 8 G 300.00 4000.00 1384.00 1
120 .167797183E+02 .200748305E-01-.710732570E-05 .112925397E-08-.665827513E-13 2
121 .222453062E+04-.729120687E+02-.719572313E+01 .780676798E-01-.620002183E-04 3
122 .253310854E-07-.423684696E-11 .104082650E+05 .552451233E+02 4
123 CYC6H10 C 6H 10 G 300.00 4000.00 1388.00 1
124 .164687940E+02 .250464584E-01-.873323457E-05 .137353265E-08-.804138942E-13 2
125 -.977694533E+04-.696690108E+02-.607599781E+01 .751138370E-01-.506516889E-04 3
126 .171683701E-07-.235089637E-11-.166592755E+04 .523699408E+02 4
127 DIALLYL C 6H 10 G 300.00 4000.00 1413.00 1
128 .160456030E+02 .234774145E-01-.785797929E-05 .120200542E-08-.690100029E-13 2
129 .211899382E+04-.588452460E+02-.101375402E+01 .638242808E-01-.440653860E-04 3
130 .158295163E-07-.230830701E-11 .794033696E+04 .325056094E+02 4
131 C5H7 C 5H 7 G 300.00 4000.00 1000.00 1
132 .671323690E+01 .274278890E-01-.994311090E-05 .119373240E-08 .000000000E+00 2
133 .235116384E+05-.112735252E+02 .759315300E+00 .432678800E-01-.237613290E-04 3
134 .512588110E-08 .000000000E+00 .251686000E+05 .196131100E+02 4
135 RC6H9A C 6H 9 G 300.00 4000.00 1400.00 1
136 .170842767E+02 .208842788E-01-.714529004E-05 .110943563E-08-.643676989E-13 2
137 .201040204E+05-.639326012E+02-.266715213E+01 .726196475E-01-.605323920E-04 3
138 .266000571E-07-.474613408E-11 .264415017E+05 .402220332E+02 4
139 RCYC6H9 C 6H 9 G 300.00 4000.00 1381.00 1
140 .166730638E+02 .227088190E-01-.801509353E-05 .127088484E-08-.748275111E-13 2
141 .698387216E+04-.723601536E+02-.631908086E+01 .726795534E-01-.484456826E-04 3
142 .157628084E-07-.202092558E-11 .153574632E+05 .524769640E+02 4
143 !HE HE 1 G 300.00 4000.00 1000.00 1
144 ! .250000000E+01 .000000000E+00 .000000000E+00 .000000000E+00 .000000000E+00 2
145 !-.745375000E+03 .928723974E+00 .250000000E+01 .000000000E+00 .000000000E+00 3

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146 ! .000000000E+00 .000000000E+00-.745375000E+03 .928723974E+00 4
147 HE ATcT3EHe 1 0 0 OG 200.00 6000.00 1000.00 1
! [Ghobad] He <g> ATcT ver. 1.122, DHf298 = 0.000 \B1 0.000 kJ/mol - fit MAR17
148 2.49985609E+00 2.19365392E-07-1.07525085E-10 2.07198041E-14-1.39358612E-18 2
149 -7.45309155E+02 9.29535014E-01 2.49976293E+00 1.01013432E-06-8.24578465E-10 3
150 -6.85983306E-13 7.24751856E-16-7.45340917E+02 9.29800315E-01 0.00000000E+00 4
151 !AR AR 1 G 300.00 4000.00 1000.00 1
152 ! .250000000E+01 .000000000E+00 .000000000E+00 .000000000E+00 .000000000E+00 2
153 !-.745375000E+03 .437967491E+01 .250000000E+01 .000000000E+00 .000000000E+00 3
154 ! .000000000E+00 .000000000E+00-.745375000E+03 .437967491E+01 4
155 AR ATcT3EAr 1 0 0 OG 200.00 6000.00 1000.00 1
! [Ghobad] Ar <g> ATcT ver. 1.122, DHf298 = 0.000 \B1 0.000 kJ/mol - fit MAR17
156 2.49989176E+00 1.56134837E-07-7.76108557E-11 1.52928085E-14-1.05304493E-18 2
157 -7.45328403E+02 4.38029835E+00 2.49988611E+00 2.13037960E-07 8.97320772E-10 3
158 -2.31395752E-12 1.30201393E-15-7.45354481E+02 4.38024367E+00 0.00000000E+00 4
159 !N2 N 2 G 300.00 4000.00 1000.00 1
160 ! .295257637E+01 .139690040E-02-.492631603E-06 .786010195E-10-.460755204E-14 2
161 !-.923948688E+03 .587188762E+01 .353100528E+01-.123660988E-03-.502999433E-06 3
162 ! .243530612E-08-.140881235E-11-.104697628E+04 .296747038E+01 4
163 N2 ATcT3EN 2 0 0 OG 200.00 6000.00 1000.00 1
! [Ghobad] N2 <g> ATcT ver. 1.122, DHf298 = 0.000 \B1 0.000 kJ/mol - fit MAR17
164 2.93802970E+00 1.41838030E-03-5.03281045E-07 8.07555464E-11-4.76064275E-15 2
165 -9.17180990E+02 5.95521985E+00 3.53603521E+00-1.58270944E-04-4.26984251E-07 3
166 2.37542590E-09-1.39708206E-12-1.04749645E+03 2.94603724E+00 0.00000000E+00 4
167 !O2 O 2 G 300.00 4000.00 1000.00 1
168 ! .366096065E+01 .656365811E-03-.141149627E-06 .205797935E-10-.129913436E-14 2
169 !-.121597718E+04 .341536279E+01 .378245636E+01-.299673416E-02 .984730201E-05 3
170 !-.968129509E-08 .324372837E-11-.106394356E+04 .365767573E+01 4
171 O2 ATcT3EO 2 0 0 OG 200.00 6000.00 1000.00 1
! [Ghobad] O2 <g> ATcT ver. 1.122, DHf298 = 0.000 \B1 0.000 kJ/mol - fit MAR17
172 3.65980488E+00 6.59877372E-04-1.44158172E-07 2.14656037E-11-1.36503784E-15 2
173 -1.21603048E+03 3.42074148E+00 3.78498258E+00-3.02002233E-03 9.92029171E-06 3
174 -9.77840434E-09 3.28877702E-12-1.06413589E+03 3.64780709E+00 0.00000000E+00 4
175 !H2 H 2 G 300.00 4000.00 700.00 1
176 ! .122006198E+01-.697178276E-02 .149395345E-04-.735836941E-08 .107706311E-11 2
177 ! .964756277E+03 .127210129E+02 .000000000E+00 .000000000E+00 .000000000E+00 3
178 ! .686975867E-08-.400441121E-11 .113556495E+04 .181719411E+02 4
179 H2 ATcT3EH 2 0 0 OG 200.00 6000.00 1000.00 1
! [Ghobad] H2 <g> ATcT ver. 1.122, DHf298 = 0.000 \B1 0.000 kJ/mol - fit MAR17
180 2.90207649E+00 8.68992581E-04-1.65864430E-07 1.90851899E-11-9.31121789E-16 2
181 -7.97948726E+02-8.45591320E-01 2.37694204E+00 7.73916922E-03-1.88735073E-05 3
182 1.95517114E-08-7.17095663E-12-9.21173081E+02 5.47184736E-01 0.00000000E+00 4
183 !H2O H 2O 1 G 300.00 4000.00 1000.00 1
184 ! .267703890E+01 .297318160E-02-.773768890E-06 .944335140E-10-.426899910E-14 2
185 !-.298858940E+05 .688255000E+01 .419863520E+01-.203640170E-02 .652034160E-05 3
186 !-.548792690E-08 .177196800E-11-.302937260E+05-.849009010E+00 4
187 H2O ATcT3EH 2O 1 0 OG 200.00 6000.00 1000.00 1
! [Ghobad] H2O <g> ATcT ver. 1.122, DHf298 = -241.833 \B1 0.027 kJ/mol - fit MAR17
188 2.73117512E+00 2.95136995E-03-8.35359785E-07 1.26088593E-10-8.40531676E-15 2
189 -2.99169082E+04 6.55183000E+00 4.20147551E+00-2.05583546E-03 6.56547207E-06 3
190 -5.52906960E-09 1.78282605E-12-3.02950066E+04-8.60610906E-01-2.90858262E+04 4
191 !H2O2 H 2O 2 G 300.00 4000.00 1000.00 1
192 ! .457977305E+01 .405326003E-02-.129844730E-05 .198211400E-09-.113968792E-13 2
193 !-.180071775E+05 .664970694E+00 .431515149E+01-.847390622E-03 .176404323E-04 3
194 !-.226762944E-07 .908950158E-11-.177067437E+05 .327373319E+01 4
195 H2O2 ATcT3EH 2O 2 0 OG 200.00 6000.00 1000.00 1
! [Ghobad] H2O2 <g> ATcT ver. 1.122, DHf298 = -135.457 \B1 0.064 kJ/mol - fit MAR17
196 4.54017480E+00 4.15970971E-03-1.30876777E-06 2.00823615E-10-1.15509243E-14 2
197 -1.79514029E+04 8.55881745E-01 4.23854160E+00-2.49610911E-04 1.59857901E-05 3
198 -2.06919945E-08 8.29766320E-12-1.76486003E+04 3.58850097E+00-1.62917334E+04 4
199 !CO C 1O 1 G 300.00 4000.00 1000.00 1
200 ! .304848590E+01 .135172810E-02-.485794050E-06 .788536440E-10-.469807460E-14 2
201 !-.142661170E+05 .601709770E+01 .357953350E+01-.610353690E-03 .101681430E-05 3
202 ! .907005860E-09-.904424490E-12-.143440860E+05 .350840930E+01 4
203 CO ATcT3EC 1O 1 0 OG 200.00 6000.00 1000.00 1
! [Ghobad] CO <g> ATcT ver. 1.122, DHf298 = -110.523 \B1 0.026 kJ/mol - fit MAR17
204 3.03397274E+00 1.37328118E-03-4.96445087E-07 8.10281447E-11-4.85331749E-15 2
205 -1.42586044E+04 6.10076092E+00 3.59508377E+00-7.21196937E-04 1.28238234E-06 3
206 6.52429293E-10-8.21714806E-13-1.43448968E+04 3.44355598E+00-1.32928623E+04 4
207 !CO2 C 1O 2 G 300.00 4000.00 1000.00 1
208 ! .463651110E+01 .274145690E-02-.995897590E-06 .160386660E-09-.916198570E-14 2
209 !-.490249040E+05-.193489550E+01 .235681300E+01 .898412990E-02-.712206320E-05 3
210 ! .245730080E-08-.142885480E-12-.483719710E+05 .990090350E+01 4

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211	CO2	ATcT3EC	10	2	0	OG	200.00	6000.00	1000.00	1	
	! [Ghobad] CO2 <g> ATcT ver. 1.122, Dhf298 = -393.475 \B1 0.015 kJ/mol - fit MAR17										
212							4.63537470E+00	2.74559459E-03	-9.98282389E-07	1.61013606E-10	2
213							-4.90203677E+04	-1.92887630E+00	2.20664321E+00	1.00970086E-02	3
214							5.47155623E-09	-1.27733965E-12	-4.83529864E+04	1.05261943E+01	4
215	CH2O	C	1H	2O	1	G	300.00	4000.00	1000.00	1	
216							.316952665E+01	.619320560E-02	-.225056366E-05	.365975660E-09	2
217							-.145486831E+05	.604207898E+01	.479372312E+01	-.990833322E-02	3
218							-.379285237E-07	.131772641E-10	-.143791953E+05	.602798058E+00	4
219	HCOOH	C	1H	2O	2	G	300.00	4000.00	1000.00	1	
220							.461383160E+01	.644963640E-02	-.229082510E-05	.367160470E-09	2
221							-.453303180E+05	.847883830E+00	.389836160E+01	-.355877950E-02	3
222							-.438499590E-07	.171077690E-10	-.467785744E+05	.734953970E+01	4
223	HCO3H	C	1H	2O	3	G	300.00	4000.00	1378.00	1	
224							.987503581E+01	.464663708E-02	-.167230522E-05	.268624413E-09	2
225							-.380502456E+05	-.224938942E+02	.242464726E+01	.219706380E-01	3
226							.625612194E-08	-.911645843E-12	-.354828006E+05	.175027796E+02	4
227	CH4	C	1H	4		G	300.00	4000.00	1000.00	1	
228							.165326226E+01	.100263099E-01	-.331661238E-05	.536483138E-09	2
229							-.100095936E+05	.990506283E+01	.514911468E+01	-.136622009E-01	3
230							-.484246767E-07	.166603441E-10	-.102465983E+05	-.463848842E+01	4
231	CH3OH	C	1H	4O	1	G	300.00	4000.00	1000.00	1	
232							.352726795E+01	.103178783E-01	-.362892944E-05	.577448016E-09	2
233							-.260028834E+05	.516758693E+01	.565851051E+01	-.162983419E-01	3
234							-.758372926E-07	.280427550E-10	-.256119736E+05	-.897330508E+00	4
235	CH3O2H	C	1H	4O	2	G	300.00	4000.00	1000.00	1	
236							.776538058E+01	.861499712E-02	-.298006935E-05	.468638071E-09	2
237							-.182979984E+05	-.143992663E+02	.290540897E+01	.174994735E-01	3
238							-.252827275E-07	.134368212E-10	-.168894632E+05	.113741987E+02	4
239	C2H2	C	2H	2		G	300.00	4000.00	1000.00	1	
240							.465878489E+01	.488396667E-02	-.160828888E-05	.246974544E-09	2
241							.257594042E+05	-.399838194E+01	.808679682E+00	.233615762E-01	3
242							.280152958E-07	-.850075165E-11	.264289808E+05	.139396761E+02	4
243	CH2CO	C	2H	2O	1	G	300.00	4000.00	1000.00	1	
244							.575871449E+01	.635124053E-02	-.225955361E-05	.362321512E-09	2
245							-.808533464E+04	-.496490444E+01	.213241136E+01	.181319455E-01	3
246							.935336040E-08	-.201724844E-11	.714808520E+04	.133807969E+02	4
247	CHOCHO	C	2H	2O	2	G	300.00	4000.00	1000.00	1	
248							.872506895E+01	.633096819E-02	-.235574814E-05	.389782853E-09	2
249							-.291024131E+05	-.203903909E+02	.468412461E+01	.478012819E-03	3
250							-.579018239E-07	.231669328E-10	-.271985007E+05	.451187184E+01	4
251	C2H4	C	2H	4		G	300.00	4000.00	1000.00	1	
252							.399182724E+01	.104833908E-01	-.371721342E-05	.594628366E-09	2
253							.426865851E+04	-.269081762E+00	.395920063E+01	-.757051373E-02	3
254							-.691588352E-07	.269884190E-10	.508977598E+04	.409730213E+01	4
255	CH3CHO	C	2H	4O	1	G	300.00	4000.00	1000.00	1	
256							.540411080E+01	.117230590E-01	-.422631370E-05	.683724510E-09	2
257							-.225931220E+05	-.348079170E+01	.472945950E+01	-.319328580E-02	3
258							-.574586110E-07	.219311120E-10	-.215728780E+05	.410301590E+01	4
259	C2H4O1-2	C	2H	4O	1	G	300.00	4000.00	1000.00	1	
260							.548876410E+01	.120461900E-01	-.433369310E-05	.700283110E-09	2
261							-.918042510E+04	-.707996050E+01	.375905320E+01	-.944121800E-02	3
262							-.100807880E-06	.400399210E-10	-.756081430E+04	.784974750E+01	4
263	CH3CO2H	C	2H	4O	2	G	300.00	4000.00	1000.00	1	
264							.767084601E+01	.135152602E-01	-.525874333E-05	.893184479E-09	2
265							-.557560970E+05	-.154677315E+02	.278950201E+01	.999941719E-02	3
266							-.509031329E-07	.206222185E-10	-.534752488E+05	.141053123E+02	4
267	CH3OCHO	C	2H	4O	2	G	300.00	4000.00	700.00	1	
268							.502910660E+01	-.287377520E-01	.615808971E-04	-.298073518E-07	2
269							-.407046731E+05	.182412180E+02	.000000000E+00	.000000000E+00	3
270							.288411216E-07	-.166481354E-10	-.400005982E+05	.407099939E+02	4
271	CH2OHCHO	C	2H	4O	2	G	300.00	4000.00	1000.00	1	
272							.691088832E+01	.123280849E-01	-.438373062E-05	.703055164E-09	2
273							-.400211587E+05	-.696132551E+01	.614926095E+01	-.596828114E-02	3
274							-.716663578E-07	.274014411E-10	-.388356849E+05	.186644598E+01	4
275	C2-OQOOH	C	2H	4O	3	G	300.00	4000.00	1000.00	1	
276							.127662941E+02	.102143437E-01	-.363547001E-05	.583491588E-09	2
277							-.753528536E+05	-.396511752E+02	.280443702E+01	.210851644E-01	3
278							-.702669107E-07	.326849274E-10	-.720649998E+05	.151180675E+02	4
279	CH3CO3H	C	2H	4O	3	G	300.00	4000.00	1000.00	1	
280							.127662941E+02	.102143437E-01	-.363547001E-05	.583491588E-09	2
281							-.753528536E+05	-.396511752E+02	.280443702E+01	.210851644E-01	3
282							-.702669107E-07	.326849274E-10	-.720649998E+05	.151180675E+02	4

283	DME-OQOOH	C	2H	40	4	G	300.00	4000.00	1000.00	1
284	.114777196E+02 .831667150E-02-.185084560E-05 .103274160E-09 .000000000E+00									2
285	-.451075908E+05-.290204723E+02 .484746000E+01 .218580610E-01-.904284660E-05									3
286	.384145300E-09 .000000000E+00-.429209100E+05 .674072600E+01									4
287	C2H6	C	2H	6		G	300.00	4000.00	1000.00	1
288	.404666411E+01 .153538802E-01-.547039485E-05 .877826544E-09-.523167531E-13									2
289	-.124473499E+05-.968698313E+00 .429142572E+01-.550154901E-02 .599438458E-04									3
290	-.708466469E-07 .268685836E-10-.115222056E+05 .266678994E+01									4
291	CH3OCH3	C	2H	60	1	G	300.00	4000.00	1000.00	1
292	.564844274E+01 .163381875E-01-.586802189E-05 .946836384E-09-.566504295E-13									2
293	-.250864216E+05-.596267354E+01 .530562273E+01-.214253958E-02 .530873092E-04									3
294	-.623146897E-07 .230730916E-10-.239655820E+05 .713244569E+00									4
295	C2H5OH	C	2H	60	1	G	300.00	4000.00	1000.00	1
296	.656243650E+01 .152042220E-01-.538967950E-05 .862250110E-09-.512897870E-13									2
297	-.315256210E+05-.947302020E+01 .485869570E+01-.374017260E-02 .695553780E-04									3
298	-.886547960E-07 .351688350E-10-.299961320E+05 .480185450E+01									4
299	C2H5O2H	C	2H	60	2	G	300.00	4000.00	1000.00	1
300	.958691079E+01 .148603589E-01-.529787964E-05 .847317148E-09-.503436325E-13									2
301	-.238367900E+05-.228310676E+02 .414672004E+01 .978668137E-02 .491492257E-04									3
302	-.742532076E-07 .311169441E-10-.214671219E+05 .984024999E+01									4
303	CH2OHCH2OH	C	2H	60	2	G	300.00	4000.00	1000.00	1
304	.791471937E+01 .158415156E-01-.553486929E-05 .873346629E-09-.514003705E-13									2
305	-.506036554E+05-.123696999E+02 .612883088E+01-.772943096E-02 .865891028E-04									3
306	-.109211943E-06 .432667518E-10-.488825925E+05 .334129960E+01									4
307	C3H4-P	C	3H	4		G	300.00	4000.00	1000.00	1
308	.602524000E+01 .113365420E-01-.402233910E-05 .643760630E-09-.382996350E-13									2
309	.196209420E+05-.860437850E+01 .268038690E+01 .157996510E-01 .250705960E-05									3
310	-.136576230E-07 .661542850E-11 .208023740E+05 .987693510E+01									4
311	C3H4-A	C	3H	4		G	300.00	4000.00	1000.07	1
312	.631687220E+01 .111337280E-01-.396293780E-05 .635642380E-09-.378755400E-13									2
313	.201174950E+05-.109957660E+02 .261304450E+01 .121225750E-01 .185398800E-04									3
314	-.345251490E-07 .153350790E-10 .215415670E+05 .102261390E+02									4
315	C2H3CHO	C	3H	40	1	G	300.00	4000.00	1000.00	1
316	.820654919E+01 .128492916E-01-.464285331E-05 .751738738E-09-.451298116E-13									2
317	-.118838341E+05-.149881933E+02 .469868861E+01 .499965957E-02 .438587397E-04									3
318	-.612883900E-07 .248508985E-10-.100875286E+05 .729812046E+01									4
319	CHOCH2CHO	C	3H	40	2	G	300.00	4000.00	1000.00	1
320	.104962923E+02 .120559957E-01-.434149310E-05 .699425892E-09-.418003976E-13									2
321	-.437332461E+05-.275425657E+02 .124227207E+01 .300698605E-01-.148206586E-05									3
322	-.242738150E-07 .133121686E-10-.408667843E+05 .219242842E+02									4
323	CH3COCHO	C	3H	40	2	G	300.00	4000.00	1000.00	1
324	.104962923E+02 .120559957E-01-.434149310E-05 .699425892E-09-.418003976E-13									2
325	-.437332461E+05-.275425657E+02 .124227207E+01 .300698605E-01-.148206586E-05									3
326	-.242738150E-07 .133121686E-10-.408667843E+05 .219242842E+02									4
327	C3H4O3	C	3H	40	3	G	300.00	4000.00	1388.00	1
328	.137530675E+02 .108054207E-01-.364230159E-05 .560730953E-09-.323659923E-13									2
329	-.577839662E+05-.401019465E+02 .208981535E+01 .383715226E-01-.282590499E-04									3
330	.104299134E-07-.153140407E-11-.538199819E+05 .223338530E+02									4
331	KEA3BG	C	3H	40	4	G	300.00	4000.00	1387.00	1
332	.188513241E+02 .920926912E-02-.331625639E-05 .532903065E-09-.316697392E-13									2
333	-.488407829E+05-.672981510E+02 .114193480E+01 .543367117E-01-.478232702E-04									3
334	.206439596E-07-.352353283E-11-.431220565E+05 .263898462E+02									4
335	C3H6	C	3H	6		G	300.00	4000.00	1000.00	1
336	.603870234E+01 .162963931E-01-.582130800E-05 .935936829E-09-.558603143E-13									2
337	-.741715057E+03-.843825992E+01 .383464468E+01 .329078952E-02 .505228001E-04									3
338	-.666251176E-07 .263707473E-10 .788717123E+03 .753408013E+01									4
339	C3H5OH	C	3H	60	1	G	300.00	4000.00	1000.00	1
340	.811285474E+01 .171952419E-01-.606427393E-05 .967014746E-09-.573968013E-13									2
341	-.214419954E+05-.172623867E+02 .511393563E+01 .469115954E-02 .542574797E-04									3
342	-.729774751E-07 .290683409E-10-.196373114E+05 .316334698E+01									4
343	C2H5CHO	C	3H	60	1	G	300.00	4000.00	1000.00	1
344	.744085690E+01 .177301764E-01-.634081568E-05 .102040803E-08-.609461714E-13									2
345	-.260055814E+05-.144195446E+02 .424529681E+01 .668296706E-02 .493337933E-04									3
346	-.671986124E-07 .267262347E-10-.241473007E+05 .690738560E+01									4
347	CH3COCH3	C	3H	60	1	G	300.00	4000.00	1000.00	1
348	.729796974E+01 .175656913E-01-.631678065E-05 .102025553E-08-.610903592E-13									2
349	-.295368927E+05-.127591704E+02 .555638920E+01-.283863547E-02 .705722951E-04									3
350	-.878130984E-07 .340290951E-10-.278325393E+05 .231960221E+01									4
351	C3H6O	C	3H	60	1	G	300.00	4000.00	1000.00	1
352	.801491079E+01 .173919953E-01-.626027968E-05 .101188256E-08-.606239111E-13									2
353	-.151980838E+05-.188279964E+02 .342806676E+01 .625176642E-02 .613196311E-04									3
354	-.860387185E-07 .351371393E-10-.128446646E+05 .104244994E+02									4
355	C3H5OOH	C	3H	60	2	G	300.00	4000.00	1382.00	1

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356 .139268456E+02 .135384067E-01-.474335693E-05 .748389157E-09-.439105886E-13 2
357 -.132537727E+05-.456757848E+02 .221491505E+01 .390935107E-01-.258809564E-04 3
358 .870894601E-08-.120793929E-11-.896037969E+04 .179425329E+02 4
359 CH2OHCOCH3 C 3H 60 2 G 300.00 4000.00 1000.00 1
360 .110374327E+02 .169177041E-01-.598872959E-05 .957507054E-09-.569424407E-13 2
361 -.479270048E+05-.288076231E+02 .352624872E+01 .266034923E-01 .115090267E-04 3
362 -.353751170E-07 .166033210E-10-.453401970E+05 .125889401E+02 4
363 CH2OHCH2CHO C 3H 60 2 G 300.00 4000.00 1382.00 1
364 .118936666E+02 .144153203E-01-.477525443E-05 .726036430E-09-.415285995E-13 2
365 -.459271652E+05-.327285750E+02 .266613285E+01 .346302298E-01-.214380719E-04 3
366 .690469334E-08-.916939105E-12-.425706030E+05 .173358364E+02 4
367 C3-OQOOH C 3H 60 3 G 300.00 4000.00 1391.00 1
368 .170285271E+02 .130716784E-01-.459310856E-05 .726135156E-09-.426658337E-13 2
369 -.416334217E+05-.592513577E+02 .768933034E+00 .546905880E-01-.465072405E-04 3
370 .203159585E-07-.358398999E-11-.363238861E+05 .268291637E+02 4
371 C3H8 C 3H 8 G 300.00 4000.00 1000.00 1
372 .666919760E+01 .206108751E-01-.736512349E-05 .118434262E-08-.706914630E-13 2
373 -.162754066E+05-.131943379E+02 .421093013E+01 .170886504E-02 .706530164E-04 3
374 -.920060565E-07 .364618453E-10-.143810883E+05 .561004451E+01 4
375 NC3H7OH C 3H 80 1 OG 300.000 5000.000 1400.000 31
! \AUTHOR: CR/KPS ! \REF: GA ! \COMMENT: FITTED WITH THERM ON 11_08_2016_20_43_11
376 1.14717073E+01 1.71812521E-02-5.78165901E-06 8.87786623E-10-5.11116063E-14 2
377 -3.65788256E+04-3.49774412E+01-1.28694006E-01 4.25920996E-02-2.62946409E-05 3
378 8.07203568E-09-9.57756657E-13-3.24028755E+04 2.78855895E+01 4
379 IC3H7OH C 3H 80 1 G 300.00 4000.00 1000.00 1
380 .964183701E+01 .200230715E-01-.711967189E-05 .114138950E-08-.679935249E-13 2
381 -.374835623E+05-.256288343E+02 .430755345E+01 .102582798E-01 .619565411E-04 3
382 -.902973802E-07 .373936384E-10-.349249212E+05 .755995822E+01 4
383 C3H7OOH C 3H 80 2 G 300.00 4000.00 1000.00 1
384 .104115631E+02 .213763889E-01-.755819870E-05 .120207180E-08-.711798090E-13 2
385 -.268935445E+05-.235428789E+02 .708977756E+01-.486163264E-02 .103253531E-03 3
386 -.133200956E-06 .530799252E-10-.244194556E+05 .174859215E+01 4
387 GLYCEROL C 3H 80 3 G 300.00 4000.00 1000.00 1
388 .143043899E+02 .198820797E-01-.705141811E-05 .112196047E-08-.663290455E-13 2
389 -.753417115E+05-.407500023E+02 .129036739E+01 .687295831E-01-.824160146E-04 3
390 .568196772E-07-.162329302E-10-.723210175E+05 .234582202E+02 4
391 !C4H2 C 4H 2 G 300.00 4000.00 1000.00 1
!polimi
392 !.903147468E+01 .604725210E-02-.194878790E-05 .275486300E-09-.138560800E-13 2
393 !.529472934E+05-.238511290E+02 .400519100E+01 .198100000E-01-.986587660E-05 3
394 !-.663515820E-08 .607741290E-11 .542406400E+05 .184573600E+01 4
395 C4H2 C 4H 2 G 300.00 4000.00 1000.00 1
!Burcat kik
396 8.65615648E+00 6.74465042E-03-2.36868410E-06 3.76553454E-10-2.22995205E-14 2
397 5.22459295E+04-2.18462806E+01-5.02389168E-01 5.25164044E-02-9.29945578E-05 3
398 8.17206506E-08-2.73537313E-11 5.38574848E+04 2.06780532E+01 5.53688672E+04 4
399 !C4H4 C 4H 4 G 300.00 4000.00 1000.00 1
!ARAMCO
400 !.665080310E+01 .161294300E-01-.719388700E-05 .149817800E-08-.118641100E-12 2
401 !.311958636E+05-.979559836E+01-.191524700E+01 .527508700E-01-.716559400E-04 3
402 !.550724200E-07-.172862200E-10 .329785000E+05 .314199800E+02 4
403 C4H4 C 4H 4 G 300.00 4000.00 1000.00 1
!Burcat kik
404 7.98456038E+00 1.20558816E-02-4.23587475E-06 6.73646140E-10-3.99059864E-14 2
405 3.11993029E+04-1.67958975E+01 1.37368786E+00 2.88801256E-02-1.46863874E-05 3
406 -3.91045446E-09 4.78133572E-12 3.30633344E+04 1.75941274E+01 3.46213066E+04 4
407 FURAN C 4H 40 1 G 300.00 4000.00 1000.00 1
408 .135912211E+02 .987450910E-02-.345325238E-05 .544429808E-09-.319349896E-13 2
409 -.115639534E+05-.542513644E+02-.750030326E+01 .699899868E-01-.695485649E-04 3
410 .333968809E-07-.619467883E-11-.541634292E+04 .550218432E+02 4
411 CH2CCHCHO C 4H 40 1 G 300.00 4000.00 1000.00 1
412 .929991052E+01 .152201510E-01-.615883937E-05 .112678366E-08-.769359137E-13 2
413 .368009609E+04-.220663746E+02 .123852148E+01 .356054647E-01-.236786887E-04 3
414 .592234361E-08 .282885884E-12 .610569242E+04 .202911558E+02 4
415 C4H6 1,3-butadienT05/04C 4.H 6. 0. 0.G 200.000 6000.000 1000. 1
!Burcat MP
416 7.62637466E+00 1.72523403E-02-6.09184911E-06 9.70800102E-10-5.76169721E-14 2
417 9.55306395E+03-1.48325259E+01 4.10599669E+00 5.05575563E-03 5.83885454E-05 3
418 -8.05950198E-08 3.27447711E-11 1.15092468E+04 8.42978067E+00 1.33302095E+04 4
419 IC3H5CHO C 4H 60 1 G 300.00 4000.00 1396.00 1
420 .136175682E+02 .137917192E-01-.473370118E-05 .736655226E-09-.420097974E-13 2
421 -.199994281E+05-.472987367E+02 .627183793E+00 .466780254E-01-.374430631E-04 3
422 .158330542E-07-.273952155E-11-.157203117E+05 .216034294E+02 4

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423	C3H5CHO	C	4H	60	1	G	300.00	4000.00	1394.00	1
424	.121670926E+02	.150749706E-01-	.518640017E-05	.808302587E-09-	.470194864E-13					2
425	-.156762389E+05-	.365095664E+02-	.227554121E-01	.441176181E-01-	.322046234E-04					3
426	.124986163E-07-	.202269249E-11-	.114618192E+05	.288193193E+02						4
427	ETIBALDGB	C	4H	60	2	G	300.00	4000.00	1000.00	1
428	.130577477E+02	.906905120E-02-	.308189261E-05	.476481380E-09-	.275669277E-13					2
429	-.369274825E+05-	.425273740E+02	.147485987E+00	.464706296E-01-	.451901760E-04					3
430	.219641008E-07-	.416219125E-11-	.331809255E+05	.242182934E+02						4
431	ETALD4X	C	4H	60	2	G	300.00	4000.00	1000.00	1
432	.130577477E+02	.906905120E-02-	.308189261E-05	.476481380E-09-	.275669277E-13					2
433	-.369274825E+05-	.425273740E+02	.147485987E+00	.464706296E-01-	.451901760E-04					3
434	.219641008E-07-	.416219125E-11-	.331809255E+05	.242182934E+02						4
435	ETIBALDGG	C	4H	60	2	G	300.00	4000.00	1000.00	1
436	.130577477E+02	.906905120E-02-	.308189261E-05	.476481380E-09-	.275669277E-13					2
437	-.369274825E+05-	.425273740E+02	.147485987E+00	.464706296E-01-	.451901760E-04					3
438	.219641008E-07-	.416219125E-11-	.331809255E+05	.242182934E+02						4
439	C4H6O2	C	4H	60	2	G	300.00	4000.00	1375.00	1
440	.135393551E+02	.168328392E-01-	.587873230E-05	.925553795E-09-	.542254877E-13					2
441	-.462482008E+05-	.437360830E+02	.182538964E+01	.377978336E-01-	.172044878E-04					3
442	.195698878E-08	.398612932E-12-	.415126261E+05	.214925508E+02						4
443	MACRIL	C	4H	60	2	G	300.00	4000.00	1000.00	1
444	.962595080E+01	.202069860E-01-	.684948550E-05	.109063620E-08-	.671284990E-13					2
445	-.414857110E+05-	.177414250E+02-	.929250120E+00	.565245670E-01-	.531143270E-04					3
446	.263405850E-07-	.484636380E-11-	.390243280E+05	.347643170E+02						4
447	KEA4X	C	4H	60	4	G	300.00	4000.00	1000.00	1
448	.844721220E+01	.279565620E-01-	.931325210E-05	.146601490E-08-	.895812420E-13					2
449	-.149523750E+05-	.219017790E+01	.170003960E+01	.665491220E-01-	.743515920E-04					3
450	.459831110E-07-	.114108380E-10-	.146870580E+05	.263355290E+02						4
451	KIA4G3	C	4H	60	4	G	300.00	4000.00	1000.00	1
452	.308381600E+02-	.332377100E-02	.408622100E-05-	.107259400E-08	.893684300E-13					2
453	-.609320200E+05-	.128876900E+03	.279202700E+01	.460692000E-01-	.161793100E-04					3
454	-.299433100E-08	.105548900E-11-	.505399900E+05	.259977500E+02						4
455	KIA4G2	C	4H	60	4	G	300.00	4000.00	1000.00	1
456	.252315400E+02-	.400599800E-02	.411576000E-05-	.101225600E-08	.821198700E-13					2
457	-.541802300E+05-	.106393200E+03	.276106400E+01	.360555700E-01-	.139183000E-04					3
458	-.578268000E-09	.202447700E-12-	.458617500E+05	.176080200E+02						4
459	C4H8-1	C	4H	8		G	300.00	4000.00	1392.00	1
460	.113508668E+02	.180617877E-01-	.616093029E-05	.954652959E-09-	.553089641E-13					2
461	-.597871038E+04-	.364369438E+02-	.831372089E+00	.452580978E-01-	.293658559E-04					3
462	.100220436E-07-	.143191680E-11-	.157875035E+04	.295084236E+02						4
463	IC4H8	C	4H	8		G	300.00	4000.00	1388.00	1
464	.112258330E+02	.181795798E-01-	.620348592E-05	.961444458E-09-	.557088057E-13					2
465	-.769983777E+04-	.373306704E+02	.938433173E+00	.390547287E-01-	.216437148E-04					3
466	.587267077E-08-	.614435479E-12-	.374817891E+04	.191442985E+02						4
467	C4H8O	C	4H	80	1	G	300.00	4000.00	1371.00	1
468	.154228514E+02	.170211052E-01-	.606347951E-05	.967354762E-09-	.571992419E-13					2
469	-.220196123E+05-	.613882135E+02-	.253690104E+01	.543995707E-01-	.343390305E-04					3
470	.101079922E-07-	.110262736E-11-	.152980680E+05	.367400719E+02						4
471	MEK	C	4H	80	1	G	300.00	4000.00	1000.00	1
472	.929655016E+01	.229172746E-01-	.822048591E-05	.132404838E-08-	.791751980E-13					2
473	-.334442311E+05-	.204993263E+02	.661978185E+01	.851847835E-02	.510322077E-04					3
474	-.658433042E-07	.249110484E-10-	.315251691E+05-	.109485469E+01						4
475	C3H7CHO	C	4H	80	1	G	300.00	4000.00	1460.00	1
476	.177916692E+02	.160697035E-01-	.578626200E-05	.929729307E-09-	.552476040E-13					2
477	-.343943030E+05-	.708794705E+02	.269734263E+01	.347742121E-01-	.145911329E-05					3
478	-.117722414E-07	.392653613E-11-	.276350928E+05	.158339562E+02						4
479	IC3H7CHO	C	4H	80	1	G	300.00	4000.00	1391.00	1
480	.137503148E+02	.183126722E-01-	.628572629E-05	.978250756E-09-	.568538653E-13					2
481	-.326938845E+05-	.477281342E+02-	.273021382E+00	.489696307E-01-	.312770049E-04					3
482	.100052945E-07-	.127512074E-11-	.276054737E+05	.283451139E+02						4
483	C4H7OH	C	4H	80	1	G	300.00	4000.00	1000.00	1
484	.863167950E+01	.241150480E-01-	.832957180E-05	.134433130E-08-	.835340300E-13					2
485	-.230779140E+05-	.163015210E+02	.173864090E+01	.369849060E-01-	.680297030E-05					3
486	-.128647340E-07	.662652570E-11-	.209184180E+05	.207395880E+02						4
487	ALDC6	C	6H	120	1	G	300.00	4000.00	1000.00	1
488	.198891043E+02	.271869340E-01-	.927391515E-05	.143744158E-08-	.833090761E-13					2
489	-.397523444E+05-	.760741671E+02	.137517192E+01	.665669689E-01-	.404423050E-04					3
490	.123836270E-07-	.152905857E-11-	.328740986E+05	.248343934E+02						4
491	ETC3H4O2	C	3H	40	2	G	300.00	4000.00	1404.00	1
492	.130577477E+02	.906905120E-02-	.308189261E-05	.476481380E-09-	.275669277E-13					2
493	-.369274825E+05-	.425273740E+02	.147485987E+00	.464706296E-01-	.451901760E-04					3
494	.219641008E-07-	.416219125E-11-	.331809255E+05	.242182934E+02						4
495	RALD6XOO	C	6H	110	3	G	300.00	3500.00	1240.00	1

496	5.00092571e+01-5.34134237e-02	6.46290118e-05-2.28766994e-08	2.64030350e-12	2
497	-4.06673528e+04-2.20829565e+02-1.12640289e+01	1.44242337e-01-1.74470699e-04		3
498	1.05671532e-07-2.32766787e-11-2.54715779e+04	8.79592018e+01		4
499	RALD6X	C 6H 110 1 G	300.00 4000.00 1378.00	1
500	1.32757019E+01 3.87287541E-02-1.48883385E-05	2.46746786E-09-1.48880472E-13		2
501	-1.81757665E+04-4.13894477E+01 3.91575795E+00	5.06035891E-02-1.65881567E-05		3
502	-1.45714100E-10 6.94235310E-13-1.35519690E+04	1.30373730E+01		4
503	QA6X	C 6H 110 3 G	300.00 3500.00 1020.00	1
504	3.16179272e+01-1.36493906e-02 3.39152683e-05-1.31900640e-08	1.56959129e-12		2
505	-3.26152699e+04-1.14322463e+02-3.56697724e+00	1.24330627e-01-1.68996522e-04		3
506	1.19432021e-07-3.09358218e-11-2.54375494e+04	5.61211162e+01		4
507	ZA6X	C 6H 110 5 G	300.00 3500.00 1030.00	1
508	4.82844919e+01-4.15707488e-02 6.14657190e-05-2.30375151e-08	2.73823914e-12		2
509	-5.69207575e+04-1.98450743e+02-1.56034002e+01	2.06537570e-01-2.99857075e-04		3
510	2.10828371e-07-5.40253255e-11-4.37598517e+04	1.11659856e+02		4
511	KEA6X	C 6H 100 4 G	300.00 3500.00 890.00	1
512	2.81159858e+01-1.51101039e-02 3.53666265e-05-1.35086152e-08	1.59169636e-12		2
513	3.74972700e+04-9.42664402e+01 2.11579046e-01	1.10302960e-01-1.76003706e-04		3
514	1.44821222e-07-4.28829769e-11 4.24642543e+04	3.71043849e+01		4
515	ETALD6X	C 6H 100 2 G	300.00 4000.00 1000.00	1
516	1.30577477E+01 9.06905120E-03-3.08189261E-06	4.76481380E-10-2.75669277E-14		2
517	-3.69274825E+04-4.25273740E+01 1.47485987E-01	4.64706296E-02-4.51901760E-05		3
518	2.19641008E-08-4.16219125E-12-3.31809255E+04	2.42182934E+01		4
519	C5H9CHO	C 6H 100 1 G	300.00 4000.00 1000.00	1
520	.555649280E+01 .338399710E-01-.129908190E-04	.225842790E-08-.147803790E-12		2
521	-.155583360E+05 .376697540E+01 .117554640E+01	.506138280E-01-.305173360E-04		3
522	.629100420E-08 .920183740E-12-.149438880E+05	.244076960E+02		4
523	C4H7CHO	C 6H 100 1 G	300.00 4000.00 1000.00	1
524	8.86179270E+00 2.44574708E-02-9.08860959E-06	1.53336524E-09 -9.74116382E-14		2
525	-1.56172875E+04-1.63712955E+01 5.76395494E-01	4.73657231E-02 -3.13609797E-05		3
526	9.39481025E-09-5.51254375E-13-1.32028536E+04	2.66135077E+01		4
527	HEXENOL	C 6H 120 1 G	300.00 4000.00 1000.00	1
528	.103979970E+02 .398469010E-01-.142748760E-04	.236355490E-08-.149482190E-12		2
529	-.292509820E+05-.215428390E+02-.118271340E+01	.737594660E-01-.453636600E-04		3
530	.102038220E-07 .738389660E-12-.264012700E+05	.372503170E+02		4
531	HEXANOLOOH	C 6H 140 3 G	300.00 4000.00 1393.00	1
532	.277094420E+02 .348487880E-01-.119777002E-04	.186556340E-08-.108475524E-12		2
533	-.486083259E+05-.114399507E+03 .629165042E+00	.970053636E-01-.668336695E-04		3
534	.241186253E-07-.361669837E-11-.390326607E+05	.315310044E+02		4
535	RNC3OHOOX	C 3H 70 3 G	300.00 4000.00 1000.00	1
536	.411965608E+02 .371937787E-02-.401906883E-06	.401609731E-10-.217032561E-14		2
537	-.505341163E+05-.188000505E+03 .203813494E+01	.784218645E-01-.441306601E-04		3
538	.956957259E-08-.134730026E-11-.362640104E+05	.268180208E+02		4
539	QNC3OHOOX	C 3H 70 3 G	300.00 4000.00 1000.00	1
540	.410726584E+02 .325163393E-02-.312770829E-06	.282397537E-10-.137453673E-14		2
541	-.449667530E+05-.183380687E+03 .255294420E+01	.839412693E-01-.653740910E-04		3
542	.319006074E-07-.896548855E-11-.312800193E+05	.261620056E+02		4
543	ZNC3OHOOX	C 3H 70 5 G	300.00 4000.00 1000.00	1
544	.164918847E+02 .468250506E-01-.164871837E-04	.270739186E-08-.170379572E-12		2
545	-.513214862E+05-.386393956E+02 .131429341E+01	.103179790E+00-.802039006E-04		3
546	.264187232E-07-.137184908E-11-.487698967E+05	.341039048E+02		4
547	KEHYNC3OH	C 3H 60 4 G	300.00 4000.00 1000.00	1
548	.603831357E+00 .666768020E-01-.271765190E-04	.493142950E-08-.332781746E-12		2
549	-.637785333E+05 .469431419E+02 .227567354E+01	.864199139E-01-.619813992E-04		3
550	.165976198E-07 .130342673E-11-.669640942E+05	.287560117E+02		4
551	KEA3B3L	C 3H 40 4 G	300.00 4000.00 1387.00	1
552	.188513241E+02 .920926912E-02-.331625639E-05	.532903065E-09-.316697392E-13		2
553	-.488407829E+05-.672981510E+02 .114193480E+01	.543367117E-01-.478232702E-04		3
554	.206439596E-07-.352353283E-11-.431220565E+05	.263898462E+02		4
555	!*****Hexanol Thermo*****! !MP			
556	ESAN1OH	C 6H 140 1 G	300.00 4000.00 1000.00	1
557	.215498620E+02 .270477890E-01-.794877720E-05	.114579960E-08-.659841990E-13		2
558	-.486288910E+05-.832675700E+02 .811415610E+00	.696693440E-01-.335770780E-04		3
559	.354337360E-08 .127138890E-11-.415253200E+05	.290476130E+02		4
560	RESAN1OHA	C 6H 130 1 G	300.00 4000.00 1000.00	1
561	.224822920E+02 .220633650E-01-.560837910E-05	.726127710E-09-.387814070E-13		2
562	-.271730000E+05-.857930980E+02 .712225620E+00	.741183910E-01-.546395530E-04		3
563	.255721450E-07-.612147960E-11-.200816860E+05	.302884250E+02		4
564	RESAN1OHB	C 6H 130 1 G	300.00 4000.00 1000.00	1
565	.226977810E+02 .216816440E-01-.545814460E-05	.701621370E-09-.372876710E-13		2
566	-.252458440E+05-.868857500E+02-.372279850E+00	.818340110E-01-.718173030E-04		3
567	.412142000E-07-.112622190E-10-.180154040E+05	.348058320E+02		4
568	RESAN1OHC	C 6H 130 1 G	300.00 4000.00 1000.00	1

569	.226977810E+02	.216816440E-01-	.545814460E-05	.701621370E-09-	.372876710E-13	2
570	-.252458440E+05-	.868857500E+02-	.372279850E+00	.818340110E-01-	.718173030E-04	3
571	.412142000E-07-	.112622190E-10-	.180154040E+05	.348058320E+02		4
572	RESAN1OHD	C	6H 130 1 G	300.00	4000.00 1000.00	1
573	.226977810E+02	.216816440E-01-	.545814460E-05	.701621370E-09-	.372876710E-13	2
574	-.252458440E+05-	.868857500E+02-	.372279850E+00	.818340110E-01-	.718173030E-04	3
575	.412142000E-07-	.112622190E-10-	.180154040E+05	.348058320E+02		4
576	RESAN1OHE	C	6H 130 1 G	300.00	4000.00 1000.00	1
577	.224920710E+02	.220734010E-01-	.562121570E-05	.729891430E-09-	.391193430E-13	2
578	-.252098520E+05-	.858406450E+02	.712452890E+00	.741594210E-01-	.545500620E-04	3
579	.253264660E-07-	.599609950E-11-	.181213770E+05	.302764260E+02		4
580	RESAN1OHF	C	6H 130 1 G	300.00	4000.00 1000.00	1
581	.230495220E+02	.216574500E-01-	.550175860E-05	.714146520E-09-	.383251170E-13	2
582	-.243130620E+05-	.891266780E+02-	.208731200E+00	.797328870E-01-	.641229850E-04	3
583	.327538710E-07-	.826671460E-11-	.169163750E+05	.341480100E+02		4
584	RESAN1O	C	6H 130 1 G	300.00	4000.00 1000.00	1
585	.223293590E+02	.231753250E-01-	.612610670E-05	.818680350E-09-	.448138400E-13	2
586	-.230509100E+05-	.883801270E+02-	.599555790E+00	.741732340E-01-	.454306210E-04	3
587	.140138330E-07-	.200701590E-11-	.154257910E+05	.347537120E+02		4
588	!					
589	QC6OHOOX	C	6H 130 3 G	300.00	4000.00 1000.00	1
590	.410726584E+02	.325163393E-02-	.312770829E-06	.282397537E-10-	.137453673E-14	2
591	-.449667530E+05-	.183380687E+03	.255294420E+01	.839412693E-01-	.653740910E-04	3
592	.319006074E-07-	.896548855E-11-	.312800193E+05	.261620056E+02		4
593	RC6OHOOX	C	6H 130 3 G	300.00	4000.00 1000.00	1
594	.411965608E+02	.371937787E-02-	.401906883E-06	.401609731E-10-	.217032561E-14	2
595	-.505341163E+05-	.188000505E+03	.203813494E+01	.784218645E-01-	.441306601E-04	3
596	.956957259E-08-	.134730026E-11-	.362640104E+05	.268180208E+02		4
597	ZC6OHOOX	C	6H 130 5 G	300.00	4000.00 1000.00	1
598	.164918847E+02	.468250506E-01-	.164871837E-04	.270739186E-08-	.170379572E-12	2
599	-.513214862E+05-	.386393956E+02	.131429341E+01	.103179790E+00-	.802039006E-04	3
600	.264187232E-07-	.137184908E-11-	.487698967E+05	.341039048E+02		4
601	ETALD6	C	6H 120 2 G	300.00	4000.00 1393.00	1
602	.134576640E+02	.361254510E-01-	.126982530E-04	.207621190E-08-	.130253340E-12	2
603	-.276938870E+05-	.443481370E+02-	.480166100E+01	.824119080E-01-	.502893530E-04	3
604	.107391800E-07	.748536430E-12-	.223889220E+05	.511845550E+02		4
605	KEHYC6OH	C	6H 120 4 G	300.00	4000.00 1000.00	1
606	.603831357E+00	.666768020E-01-	.271765190E-04	.493142950E-08-	.332781746E-12	2
607	-.637785333E+05	.469431419E+02	.227567354E+01	.864199139E-01-	.619813992E-04	3
608	.165976198E-07	.130342673E-11-	.669640942E+05	.287560117E+02		4
609	!					
610	NC4-OQOOH	C	4H 80 3 G	300.00	4000.00 1388.00	1
611	.195955254E+02	.180568312E-01-	.629994700E-05	.991157547E-09-	.580382406E-13	2
612	-.461054913E+05-	.709333761E+02	.243440296E+01	.605409309E-01-	.481250984E-04	3
613	.203656751E-07-	.357059537E-11-	.402872220E+05	.205488821E+02		4
614	IC4-OQOOH	C	4H 80 3 G	300.00	4000.00 1390.00	1
615	.195047991E+02	.181701803E-01-	.634838146E-05	.999797067E-09-	.585883751E-13	2
616	-.450007951E+05-	.705122130E+02	.549934041E+00	.642751153E-01-	.501779820E-04	3
617	.203546231E-07-	.338767418E-11-	.385647626E+05	.307013051E+02		4
618	KEHYBU1	C	4H 80 4 G	300.00	4000.00 1396.00	1
619	.219367270E+02	.180406285E-01-	.626171080E-05	.981855896E-09-	.573639516E-13	2
620	-.664546784E+05-	.813588272E+02-	.445736457E+01	.947202096E-01-	.937478682E-04	3
621	.464802131E-07-	.899314409E-11-	.587131282E+05	.551970961E+02		4
622	IC4H10	C	4H 10 G	300.00	4000.00 1000.00	1
623	.508434390E+01	.331851280E-01-	.124047670E-04	.152753620E-08	.000000000E+00	2
624	-.195243797E+05-	.392308050E+01-	.128398800E+01	.519486400E-01-	.308267920E-04	3
625	.755438110E-08	.000000000E+00-	.179038400E+05	.285063500E+02		4
626	!NC4H10	C	4H 10 G	300.00	4000.00 1000.00	1
627	NC4H10	C	4H 10 G	300.00	4000.00 1000.00	1
628	.105251152E+02	.235908740E-01-	.785389060E-05	.114561140E-08-	.599309560E-13	2
629	-.204952316E+05-	.321928008E+02	.157641510E+01	.345897230E-01	.697016090E-05	3
630	-.281636370E-07	.123751170E-10-	.171470040E+05	.178727420E+02		4
631	N1C4H9OH	C	4H 100 1 G	300.000	5000.000 1400.000	1
632	! \AUTHOR: CR/KPS ! \REF: GA ! \COMMENT: FITTED WITH THERM ON 12_08_2016_14_12_47					
633	+1.48022849E+01+2.15268606E-02-7.27127618E-06+1.11937370E-09-6.45600513E-14					2
634	-4.07592510E+04-5.13528547E+01-4.59550266E-01+5.55978022E-02-3.56641050E-05					3
635	+1.15878847E-08-1.49962538E-12-3.53225632E+04+3.11360441E+01+0.00000000E+00					4
636	N2C4H9OH	C	4H 100 1 G	300.00	4000.00 1390.00	1
637	.151582366E+02	.215048627E-01-	.741631184E-05	.115764678E-08-	.674130532E-13	2
638	-.429113728E+05-	.549620416E+02-	.304705097E+00	.567446943E-01-	.387293873E-04	3
639	.141775813E-07-	.220696859E-11-	.373601662E+05	.285520284E+02		4
640	TC4H9OH	C	4H 100 1 G	300.00	4000.00 1395.00	1
640	.151183592E+02	.214941230E-01-	.730928419E-05	.113021881E-08-	.653833962E-13	2

641	-.450124898E+05-.575375902E+02-.861795957E+00	.603867730E-01-.445191256E-04	3
642	.177406426E-07-.295852901E-11-.395611057E+05	.278278048E+02	4
643	IC4H9OH C 4H 100 1 G	300.00 4000.00 1426.00	1
644	.145203606E+02 .218826590E-01-.741886985E-05	.114493281E-08-.661481541E-13	2
645	-.415815847E+05-.516504190E+02-.808654483E+00	.568695746E-01-.379891888E-04	3
646	.133635469E-07-.195588405E-11-.361485459E+05	.310126347E+02	4
647	C4H9OOH C 4H 100 2 G	300.00 4000.00 1389.00	1
648	.182257559E+02 .215996217E-01-.748424942E-05	.117205153E-08-.684096331E-13	2
649	-.342341151E+05-.670536388E+02 .607792497E+00	.624669916E-01-.444490375E-04	3
650	.167754668E-07-.265938189E-11-.280070327E+05	.278025473E+02	4
651	CYC5H4O C 5H 40 1 G	300.00 4000.00 1000.00	1
652	.558734350E+01 .254149730E-01-.929145880E-05	.112347330E-08 .000000000E+00	2
653	.339172461E+04-.552979995E+01-.427809100E+01	.546170700E-01-.380993520E-04	3
654	.105947040E-07 .000000000E+00 .589093400E+04	.446629800E+02	4
655	FURFURAL C 5H 40 2 G	300.00 4000.00 1000.00	1
656	.159553578E+02 .122096134E-01-.419491662E-05	.654219009E-09-.381060338E-13	2
657	-.255664634E+05-.596830465E+02-.186260023E+01	.570946426E-01-.476338594E-04	3
658	.197949337E-07-.326585828E-11-.197873020E+05	.347179869E+02	4
659	CYC5H6 C 5H 6 G	300.00 4000.00 1000.00	1
660	.230537462E+00 .409571826E-01-.241588958E-04	.679763480E-08-.736374421E-12	2
661	.143779465E+05 .202551234E+02-.513691194E+01	.606953453E-01-.460552837E-04	3
662	.128457201E-07 .741214852E-12 .153675713E+05	.461567559E+02	4
663	MEFU2 C 5H 60 1 G	300.00 4000.00 1000.00	1
664	.459933100E+01 .340025700E-01-.175181400E-04	.423464670E-08-.375757330E-12	2
665	-.129526080E+05 .466753790E+00-.284971730E+01	.552316440E-01-.365110720E-04	3
666	.832948240E-08 .742313490E-12-.110344430E+05	.385458850E+02	4
667	C5H8 C 5H 8 G	300.00 4000.00 1000.00	1
668	.797205310E+01 .268614160E-01-.956546320E-05	.113079120E-08 .000000000E+00	2
669	.510466811E+04-.185090870E+02 .176636500E+01	.432678800E-01-.237613290E-04	3
670	.512588110E-08 .000000000E+00 .684030700E+04	.137180600E+02	4
671	CYC5H8 C 5H 8 G	300.00 4000.00 1000.00	1
672	.772447728E+01 .283223160E-01-.115452360E-04	.215408150E-08-.150541780E-12	2
673	-.782614232E+03-.197696844E+02 .268981400E+01	.209545500E-02 .113036870E-03	3
674	-.154080700E-06 .627636580E-10 .231396630E+04	.152940560E+02	4
675	C5H8O C 5H 80 1 G	300.00 4000.00 1000.00	1
676	.154011002E+02 .203490440E-01-.699742510E-05	.109031908E-08-.634192782E-13	2
677	-.910076428E+04-.580710041E+02-.514624016E+01	.722177875E-01-.580157542E-04	3
678	.242093068E-07-.410120178E-11-.236133441E+04	.508920452E+02	4
679	MCROT C 5H 80 2 G	300.00 4000.00 1000.00	1
680	.110840220E+02 .266681570E-01-.910298150E-05	.145819250E-08-.902072000E-13	2
681	-.461868520E+05-.238654710E+02 .115411390E+01	.550597160E-01-.356332020E-04	3
682	.867407750E-08 .746845670E-12-.435806950E+05	.269868980E+02	4
683	ETMB583 C 5H 80 3 G	300.00 4000.00 1000.00	1
684	.164044820E+02 .257082970E-01-.901921340E-05	.147114070E-08-.920586850E-13	2
685	-.622657890E+05-.550660710E+02-.249091940E+01	.790685040E-01-.564648800E-04	3
686	.115540360E-07 .278656790E-11-.573317190E+05	.417407460E+02	4
687	C5EN-OQOOH-35 C 5H 80 3 G	300.00 4000.00 1389.00	1
688	.217801959E+02 .189644170E-01-.666360530E-05	.105343196E-08-.618948648E-13	2
689	-.372541821E+05-.828559128E+02 .975948412E+00	.693438350E-01-.543693801E-04	3
690	.220678107E-07-.367435527E-11-.301615960E+05	.283235620E+02	4
691	C5H8O4 C 5H 80 4 G	300.00 4000.00 1000.00	1
692	.217298154E+02 .217807665E-01-.749545594E-05	.116860895E-08-.680038942E-13	2
693	-.866505360E+05-.835752527E+02-.684199090E+01	.100610553E+00-.924172541E-04	3
694	.429800586E-07-.789719358E-11-.779623201E+05	.655426910E+02	4
695	KEHYMB C 5H 80 5 G	300.00 4000.00 1000.00	1
696	.130410150E+02 .302430520E-01-.103682550E-04	.166520830E-08-.103159200E-12	2
697	-.605793360E+05-.352927630E+02-.187604440E+01	.779613480E-01-.656695630E-04	3
698	.280818550E-07-.405575270E-11-.569013010E+05	.398655930E+02	4
699	B1M3 C 5H 10 G	300.00 4000.00 1394.00	1
700	.144242929E+02 .226454984E-01-.773646334E-05	.119999861E-08-.695711276E-13	2
701	-.114981027E+05-.530391197E+02-.964397004E+00	.568482691E-01-.366324275E-04	3
702	.123008921E-07-.171392531E-11-.593502026E+04	.302998433E+02	4
703	B2M2 C 5H 10 G	300.00 4000.00 1389.00	1
704	.140426423E+02 .227915348E-01-.774902598E-05	.119814522E-08-.693127003E-13	2
705	-.132160483E+05-.514469569E+02 .604882839E+00	.496635256E-01-.266571142E-04	3
706	.647312078E-08-.484017883E-12-.806312207E+04	.223818263E+02	4
707	B1M2 C 5H 10 G	300.00 4000.00 1392.00	1
708	.141931279E+02 .226551019E-01-.770008627E-05	.119031326E-08-.688489604E-13	2
709	-.119491010E+05-.510688681E+02-.539429136E+00	.544489715E-01-.332707895E-04	3
710	.103047694E-07-.128363329E-11-.653967251E+04	.290349986E+02	4
711	NC5H10 C 5H 10 G	300.00 4000.00 1389.00	1
712	.141108203E+02 .228348272E-01-.778626835E-05	.120627491E-08-.698795983E-13	2
713	-.114335029E+05-.501593461E+02-.541560551E+00	.539629918E-01-.323508738E-04	3

714	.977416037E-08-.118534668E-11-.598606169E+04	.297142748E+02	4
715	C4H9CHO C 5H 100 1 G	300.00 4000.00 1507.00	1
716	.197928063E+02 .217870723E-01-.780397879E-05	.124956209E-08-.740724001E-13	2
717	-.382553694E+05-.801632581E+02 .392970436E+01	.374486092E-01 .427678157E-05	3
718	-.168019085E-07 .508443447E-11-.306588984E+05	.125431056E+02	4
719	RALD5X C 5H 90 1 G	300.00 4000.00 1517.00	1
720	.190577032E+02 .197405268E-01-.706907553E-05	.113169306E-08-.670771090E-13	2
721	-.128899482E+05-.729817022E+02 .467212037E+01	.343554368E-01 .295219352E-05	3
722	-.145463894E-07 .444316435E-11-.603466621E+04	.109564879E+02	4
723	RALD5XOO C 5H 90 3 G	300.00 3500.00 1240.00	1
724	5.00092571e+01-5.34134237e-02 6.46290118e-05	-2.28766994e-08 2.64030350e-12	2
725	-4.06673528e+04-2.20829565e+02-1.12640289e+01	1.44242337e-01-1.74470699e-04	3
726	1.05671532e-07-2.32766787e-11-2.54715779e+04	8.79592018e+01	4
727	RALD5X C 5H 90 1 G	300.00 4000.00 1378.00	1
728	1.32757019E+01 3.87287541E-02-1.48883385E-05	2.46746786E-09-1.48880472E-13	2
729	-1.81757665E+04-4.13894477E+01 3.91575795E+00	5.06035891E-02-1.65881567E-05	3
730	-1.45714100E-10 6.94235310E-13-1.35519690E+04	1.30373730E+01	4
731	QA5X C 5H 90 3 G	300.00 3500.00 1020.00	1
732	3.16179272e+01-1.36493906e-02 3.39152683e-05	-1.31900640e-08 1.56959129e-12	2
733	-3.26152699e+04-1.14322463e+02-3.56697724e+00	1.24330627e-01-1.68996522e-04	3
734	1.19432021e-07-3.09358218e-11-2.54375494e+04	5.61211162e+01	4
735	ZA5X C 5H 90 5 G	300.00 3500.00 1030.00	1
736	4.82844919e+01-4.15707488e-02 6.14657190e-05	-2.30375151e-08 2.73823914e-12	2
737	-5.69207575e+04-1.98450743e+02-1.56034002e+01	2.06537570e-01-2.99857075e-04	3
738	2.10828371e-07-5.40253255e-11-4.37598517e+04	1.11659856e+02	4
739	KEA5X C 5H 80 4 G	300.00 3500.00 890.00	1
740	2.81159858e+01-1.51101039e-02 3.53666265e-05	-1.35086152e-08 1.59169636e-12	2
741	3.74972700e+04-9.42664402e+01 2.11579046e-01	1.10302960e-01-1.76003706e-04	3
742	1.44821222e-07-4.28829769e-11 4.24642543e+04	3.71043849e+01	4
743	IC4H9CHO C 5H 100 1 G	300.00 4000.00 1383.00	1
744	.170194059E+02 .223541546E-01-.759760895E-05	.117496754E-08-.679975164E-13	2
745	-.369143302E+05-.635871575E+02 .861033163E+00	.573441683E-01-.359178644E-04	3
746	.113951893E-07-.146205706E-11-.309951354E+05	.242264151E+02	4
747	C5H9OH C 5H 100 1 G	300.00 4000.00 1000.00	1
748	.107143420E+02 .300909990E-01-.104241840E-04	.168678680E-08-.105053190E-12	2
749	-.266832230E+05-.257609100E+02-.581915140E+00	.590151210E-01-.307994630E-04	3
750	.522248800E-09 .379832970E-11-.235468110E+05	.329467200E+02	4
751	IC5H9OH C 5H 100 1 G	300.00 4000.00 1394.00	1
752	.147423131E+02 .219843767E-01-.751584192E-05	.116633393E-08-.676421638E-13	2
753	-.416616600E+05-.528466211E+02-.837465362E+00	.576520639E-01-.390215462E-04	3
754	.140131231E-07-.211159111E-11-.361265628E+05	.311701525E+02	4
755	NC5H10-O C 5H 100 1 G	300.00 4000.00 1373.00	1
756	.187152768E+02 .216122625E-01-.768638433E-05	.122492227E-08-.723734176E-13	2
757	-.274341627E+05-.786690289E+02-.351633623E+01	.686975884E-01-.446579237E-04	3
758	.140670556E-07-.174934766E-11-.191663581E+05	.425589840E+02	4
759	NEOC5H10-O C 5H 100 1 G	300.00 4000.00 1406.00	1
760	.182053093E+02 .222888126E-01-.759419141E-05	.117633164E-08-.681511068E-13	2
761	-.260973639E+05-.785614741E+02-.704702259E+01	.864172552E-01-.702610933E-04	3
762	.290540959E-07-.480586102E-11-.179483330E+05	.550571499E+02	4
763	MTBE-O C 5H 100 2 G	300.00 4000.00 1397.00	1
764	.193844587E+02 .224929046E-01-.748169734E-05	.114123661E-08-.654437288E-13	2
765	-.558416627E+05-.795832532E+02-.518049059E+01	.839546669E-01-.663790553E-04	3
766	.267623941E-07-.432034827E-11-.478415885E+05	.506953652E+02	4
767	MB C 5H 100 2 G	300.00 4000.00 1380.00	1
768	.190094725E+02 .236503722E-01-.822978452E-05	.129246265E-08-.755862836E-13	2
769	-.634989152E+05-.732469099E+02 .316208825E+01	.552915358E-01-.311610102E-04	3
770	.842394129E-08-.872222021E-12-.573385240E+05	.139723817E+02	4
771	NEOC5-OQOOH C 5H 100 3 G	300.00 4000.00 1397.00	1
772	.237028187E+02 .215843890E-01-.747470111E-05	.117038715E-08-.683143724E-13	2
773	-.509464263E+05-.948314143E+02 .101097520E+01	.753376897E-01-.559848192E-04	3
774	.210040666E-07-.316727025E-11-.432003697E+05	.266737910E+02	4
775	NC5-OQOOH C 5H 100 3 G	300.00 4000.00 1389.00	1
776	.227422860E+02 .225948063E-01-.786379640E-05	.123514506E-08-.722413862E-13	2
777	-.501979972E+05-.864068664E+02 .227305950E+01	.724929431E-01-.560597536E-04	3
778	.231254746E-07-.397203084E-11-.431866364E+05	.229745558E+02	4
779	MTBE-OQOOH C 5H 100 4 G	300.00 4000.00 1386.00	1
780	.259492704E+02 .217762181E-01-.754080079E-05	.118109778E-08-.689663912E-13	2
781	-.659884236E+05-.102260628E+03 .215705064E+01	.770950997E-01-.562944956E-04	3
782	.205751475E-07-.301215733E-11-.577585957E+05	.255153989E+02	4
783	KEHYP1OH C 5H 100 4 G	300.00 4000.00 1391.00	1
784	.241671480E+02 .230357774E-01-.791201902E-05	.123189743E-08-.716178065E-13	2
785	-.696422759E+05-.907717133E+02 .209051128E+01	.771281020E-01-.592331258E-04	3
786	.236078672E-07-.383619864E-11-.622442740E+05	.268708461E+02	4

853	-.181287441E+05-.517984911E+02-.290978575E+00	.408562397E-01	.242829425E-04	3
854	-.714477617E-07 .346002146E-10-.134129780E+05	.268745637E+02		4
855	C6H6O3 C 6H 60 3 G	300.00	4000.00 1382.00	1
856	.193892545E+02 .186134462E-01-.631148097E-05	.975462374E-09-	.564561412E-13	2
857	-.492678935E+05-.716786498E+02 .598814621E+00	.618493802E-01-	.438009436E-04	3
858	.155531333E-07-.220506530E-11-.427313109E+05	.293828012E+02		4
859	CYC6H8 C 6H 8 G	300.00	4000.00 1384.00	1
860	.167797183E+02 .200748305E-01-.710732570E-05	.112925397E-08-	.665827513E-13	2
861	.22453062E+04-.729120687E+02-.719572313E+01	.780676798E-01-	.620002183E-04	3
862	.252310854E-07-.423684696E-11 .104082650E+05	.552451233E+02		4
863	!MCPTD C 6H 8 G	300.00	4000.00 1399.00	1
	!polimi			
864	! .154352848E+02 .199801707E-01-.680270423E-05	.105349633E-08-	.610336727E-13	2
865	! .447456576E+04-.636393642E+02-.665320026E+01	.744640477E-01-	.582864186E-04	3
866	! .231603543E-07-.369017129E-11 .117669311E+05	.538162769E+02		4
867	MCPTD C 6H 8 G	300.00	4000.00 1399.00	1 !
	Burcat kik 5-Methyl-1,3-CYCLOPENTADIENE			
868	1.12002638E+01 2.50104924E-02-8.94914815E-06	1.44109704E-09-8.61256818E-14		2
869	7.66096956E+03-3.68265351E+01 2.93206487E+00	1.12663266E-02 9.41193663E-05		3
870	-1.36178031E-07 5.64768524E-11 1.15372662E+04	1.42303662E+01 1.35013031E+04		4
871	!MCPTD C 6H 8 G	300.00	4000.00 1399.00	1 !
	Burcat kik 3-METHYL-1,3-CYCLOPENTADIENE			
872	! 1.11438571E+01 2.51265706E-02-9.00536078E-06	1.45167109E-09-8.68188102E-14		2
873	! 6.15685018E+03-3.61900531E+01 3.15023799E+00	1.30929547E-02 8.49819174E-05		3
874	!-1.23780433E-07 5.11852420E-11 9.89179835E+03	1.29939079E+01 1.19433443E+04		4
875	DMF C 6H 80 1 G	300.00	4000.00 1000.00	1
876	.117792073E+02 .285086757E-01-.111333319E-04	.199173491E-08-	.133982691E-12	2
877	-.211130695E+05-.374257400E+02 .803526924E+00	.443305994E-01 .419434116E-05		3
878	-.349560898E-07 .165826978E-10-.172836857E+05	.230189579E+02		4
879	C6H8O4 C 6H 80 4 G	300.00	4000.00 1398.00	1
880	.245389912E+02 .222706283E-01-.773806446E-05	.121423501E-08-	.709771757E-13	2
881	-.816610603E+05-.100550137E+03-.460104207E+01	.100736116E+00-	.905484350E-04	3
882	.413812870E-07-.752102026E-11-.725801173E+05	.522649333E+02		4
883	CYC6H10 C 6H 10 G	300.00	4000.00 1388.00	1
884	.164687940E+02 .250464584E-01-.873323457E-05	.137353265E-08-	.804138942E-13	2
885	-.977694533E+04-.696690108E+02-.607599781E+01	.751138370E-01-	.506516889E-04	3
886	.171683701E-07-.235089637E-11-.166592755E+04	.523699408E+02		4
887	C6H10 C 6H 10 G	300.00	4000.00 1413.00	1
888	.160456030E+02 .234774145E-01-.785797929E-05	.120200542E-08-	.690100029E-13	2
889	.211899382E+04-.588452460E+02-.101375402E+01	.638242808E-01-	.440653860E-04	3
890	.158295163E-07-.230830701E-11 .794033696E+04	.325056094E+02		4
891	CYC6H10-O-14 C 6H 100 1 G	300.00	4000.00 1381.00	1
892	.208569012E+02 .251723586E-01-.898344923E-05	.143508332E-08-	.849382249E-13	2
893	-.384586302E+05-.102070819E+03-.138345764E+02	.100994913E+00-	.688346635E-04	3
894	.212451763E-07-.229797219E-11-.260978348E+05	.857505804E+02		4
895	C5H9CHO C 6H 100 1 G	300.00	4000.00 1000.00	1
896	.555649280E+01 .338399710E-01-.129908190E-04	.225842790E-08-	.147803790E-12	2
897	-.155583360E+05 .376697540E+01 .117554640E+01	.506138280E-01-	.305173360E-04	3
898	.629100420E-08 .920183740E-12-.149438880E+05	.244076960E+02		4
899	CYC6H10-ONE C 6H 100 1 G	300.00	4000.00 1382.00	1
900	.189587175E+02 .263606964E-01-.929344737E-05	.147257311E-08-	.866645349E-13	2
901	-.391424596E+05-.835594309E+02-.541298687E+01	.749581025E-01-	.429010347E-04	3
902	.103686234E-07-.655858987E-12-.298390440E+05	.503037294E+02		4
903	CYC6H10-O-12 C 6H 100 1 G	300.00	4000.00 1388.00	1
904	.211309516E+02 .245922161E-01-.870218393E-05	.138238722E-08-	.815033630E-13	2
905	-.270082298E+05-.100017882E+03-.102441734E+02	.947119743E-01-	.662992744E-04	3
906	.218368996E-07-.269065692E-11-.159562249E+05	.693449458E+02		4
907	CYC6H10-O-13 C 6H 100 1 G	300.00	4000.00 1384.00	1
908	.209040427E+02 .249694592E-01-.887525958E-05	.141404459E-08-	.835397954E-13	2
909	-.281106427E+05-.100684615E+03-.120242065E+02	.974927920E-01-	.669797836E-04	3
910	.211938876E-07-.242310206E-11-.164176421E+05	.774198780E+02		4
911	HEXENAL C 6H 100 1 G	300.00	4000.00 1000.00	1
912	.163810350E+02 .253163710E-01-.817955520E-05	.126084900E-08-	.759870140E-13	2
913	-.236222230E+05-.549602890E+02 .549190040E+00	.602940540E-01-	.317306290E-04	3
914	.455543960E-08 .102256280E-11-.184722190E+05	.298272340E+02		4
915	CYC6-OQOOH-3 C 6H 100 3 G	300.00	4000.00 1421.00	1
916	.152391000E+02 .293351956E-01-.936919554E-05	.138764303E-08-	.778701917E-13	2
917	-.379802009E+05-.696293762E+02-.808436864E+01	.898617293E-01-	.693837670E-04	3
918	.282474384E-07-.463250100E-11-.306468981E+05	.532148412E+02		4
919	ALDEST C 6H 100 3 G	300.00	4000.00 1384.00	1
920	.212949599E+02 .266487791E-01-.898035403E-05	.137511216E-08-	.789865729E-13	2
921	-.762788357E+05-.785214726E+02 .521237801E+01	.613142880E-01-	.373337900E-04	3
922	.119679719E-07-.162337383E-11-.703135588E+05	.903341827E+01		4

993	-.587524861E+05-.124642473E+03-.502703972E+01	.104102110E+00-.722526077E-04	3
994	.243793077E-07-.320129183E-11-.470307327E+05	.542550536E+02	4
995	NC7H14 C 7H 14 G	300.00 4000.00 1390.00	1
996	.206190401E+02 .314852991E-01-.107162057E-04	.165827662E-08-.959911785E-13	2
997	-.196710875E+05-.822507478E+02-.116533279E+01	.790439806E-01-.496101666E-04	3
998	.158569009E-07-.205346433E-11-.117362359E+05	.359871070E+02	4
999	MCYC6 C 7H 14 G	300.00 4000.00 1381.00	1
1000	.220211359E+02 .332076617E-01-.115857900E-04	.182324838E-08-.106797390E-12	2
1001	-.311719553E+05-.103211614E+03-.890848850E+01	.969226774E-01-.576085500E-04	3
1002	.148743771E-07-.111357720E-11-.196669630E+05	.657804644E+02	4
1003	C7KETONE C 7H 14O 1 G	300.00 4000.00 1385.00	1
1004	.232764710E+02 .323525773E-01-.112350736E-04	.176201535E-08-.102947816E-12	2
1005	-.448556012E+05-.937710798E+02-.318897678E+00	.833005520E-01-.531219909E-04	3
1006	.175654519E-07-.244145064E-11-.361006378E+05	.346722541E+02	4
1007	NC7H14O C 7H 14O 1 G	300.00 4000.00 1397.00	1
1008	.231122557E+02 .333659362E-01-.114966228E-04	.179372703E-08-.104427245E-12	2
1009	-.438636425E+05-.993466782E+02-.767475343E+01	.108451023E+00-.827531084E-04	3
1010	.330380469E-07-.541492429E-11-.334640974E+05	.649157213E+02	4
1011	NC7H13OOH C 7H 14O 2 G	300.00 4000.00 1393.00	1
1012	.277094420E+02 .348487880E-01-.119777002E-04	.186556340E-08-.108475524E-12	2
1013	-.486083259E+05-.114399507E+03 .629165042E+00	.970053636E-01-.668336695E-04	3
1014	.241186253E-07-.361669837E-11-.390326607E+05	.315310044E+02	4
1015	NC7-OQOOH C 7H 14O 3 G	300.00 4000.00 1387.00	1
1016	.288332529E+02 .320168096E-01-.111508456E-04	.175226159E-08-.102520451E-12	2
1017	-.622309509E+05-.116187714E+03 .152936692E+01	.958173466E-01-.696688520E-04	3
1018	.269540382E-07-.438728126E-11-.526003608E+05	.306986714E+02	4
1019	NC7H16 C 7H 16 G	300.00 4000.00 1000.00	1
1020	.205103125E+02 .346389640E-01-.107743740E-04	.160399760E-08-.937017530E-13	2
1021	-.326499224E+05-.807081180E+02-.679531340E+00	.810756760E-01-.423279310E-04	3
1022	.697965770E-08 .837326950E-12-.256907030E+05	.329815600E+02	4
1023	NC7H15OOH C 7H 16O 2 G	300.00 4000.00 1393.00	1
1024	.277094420E+02 .348487880E-01-.119777002E-04	.186556340E-08-.108475524E-12	2
1025	-.486083259E+05-.114399507E+03 .629165042E+00	.970053636E-01-.668336695E-04	3
1026	.241186253E-07-.361669837E-11-.390326607E+05	.315310044E+02	4
1027	C8H2 C 8H 2 G	300.00 4000.00 1000.00	1
1028	.156802100E+02 .111546100E-01-.372437300E-05	.519789100E-09-.237555000E-13	2
1029	.108112300E+06-.557143700E+02 .463042700E+01	.393708000E-01-.114803500E-04	3
1030	-.256221400E-07 .167079100E-10 .110828500E+06	.807742500E+00	4
1031	!C6H5C2H C 8H 6 G	300.00 4000.00 1399.00	1
	!Polimi		
1032	! .190886756E+02 .170819066E-01-.559393248E-05	.845345947E-09-.482537486E-13	2
1033	! .280711996E+05-.790035627E+02-.377007730E+01	.792380003E-01-.711832819E-04	3
1034	! .324077613E-07-.583009863E-11 .350595597E+05	.405332699E+02	4
1035	C6H5C2H C6H5CCH T12/06C 8.H 6. 0. 0.G	200.000 6000.000 1000.	1
	!Burcat kik		
1036	1.63582907E+01 2.11974105E-02-7.65817215E-06	1.24134505E-09-7.45327960E-14	2
1037	3.10375340E+04-6.22520227E+01-2.74707918E+00	7.78284438E-02-6.69709932E-05	3
1038	2.37972496E-08-8.43279765E-13 3.61131008E+04	3.54221257E+01 3.82082350E+04	4
1039	BZFUR C 8H 6O 1 G	300.00 4000.00 1000.00	1
1040	.161267559E+02 .242942790E-01-.882919089E-05	.143722155E-08-.865592465E-13	2
1041	-.574867958E+04-.640564836E+02-.785221476E+00	.396432449E-01 .569751746E-04	3
1042	-.114831806E-06 .519411145E-10 .215748538E+03	.302655928E+02	4
1043	!C6H5C2H3 C 8H 8 G	300.00 4000.00 1000.00	1
	!Polimi		
1044	! .132118086E+02 .297097690E-01-.100379980E-04	.113030440E-08 .000000000E+00	2
1045	! .112255113E+05-.452965784E+02-.314842000E+01	.733550410E-01-.482478610E-04	3
1046	! .120551240E-07 .000000000E+00 .157685200E+05	.395339300E+02	4
1047	C6H5C2H3 Styrene T12/10C 8.H 8. 0. 0.G	200.000 6000.000 1000.	1
	!Burcat kik		
1048	1.55820120E+01 2.66093018E-02-9.56144870E-06	1.54378205E-09-9.24814823E-14	2
1049	1.03197319E+04-5.98622481E+01 1.12656107E+00	3.17044880E-02 7.38511452E-05	3
1050	-1.29131757E-07 5.65307288E-11 1.57676346E+04	2.25936971E+01 1.79366548E+04	4
1051	!C6H5C2H5 C 8H 10 G	300.00 4000.00 1000.00	1
	!Polimi		
1052	! .123967254E+02 .365194120E-01-.128125900E-04	.149467160E-08 .000000000E+00	2
1053	! -.304290347E+04-.409211516E+02-.458801200E+01	.813929890E-01-.516055260E-04	3
1054	! .123987680E-07 .000000000E+00 .171000000E+04	.472934500E+02	4
1055	C6H5C2H5 A11/04C 8.H 10. 0. 0.G	200.000 6000.000 1000.	1
	!Burcat kik		
1056	1.56901336E+01 3.23663075E-02-1.16864578E-05	1.88989562E-09-1.13201791E-13	2
1057	-4.38669907E+03-6.04442403E+01 1.24076722E+00	3.59132829E-02 7.54222474E-05	3
1058	-1.31904301E-07 5.74746803E-11 1.18391719E+03	2.24682133E+01 3.58290266E+03	4
1059	!XYLENE C 8H 10 G	300.00 4000.00 1000.00	1 !

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polimi
1060 ! .104572604E+02 .403200160E-01-.145441770E-04 .173870560E-08 .000000000E+00 2
1061 !-.392485555E+04-.316838798E+02-.365621300E+01 .742185790E-01-.400008720E-04 3
1062 ! .741031100E-08 .000000000E+00 .307000000E+03 .427477900E+02 4
1063 XYLENE o-Di-Met T 9/13C 8.H 10. 0. 0.G 200.000 6000.000 1000. 1
!Burcat kik
1064 1.38533968E+01 3.30836404E-02-1.18974456E-05 1.92231652E-09-1.15153932E-13 2
1065 -5.17475507E+03-5.00163449E+01 2.96890501E+00 2.10981093E-02 9.87221885E-05 3
1066 -1.46214604E-07 6.02721557E-11-2.13940788E+02 1.61289213E+01 2.22069515E+03 4
1067 C8H1003 C 8H 100 3 G 300.00 4000.00 1280.00 1
1068 .386588321E+02 .317536134E-02 .740594019E-05-.343506103E-08 .445199316E-12 2
1069 -.597114304E+05-.165594980E+03 .580160876E+00 .872417598E-01-.555691469E-04 3
1070 .111625328E-07 .157789482E-11-.515704990E+05 .289562016E+02 4
1071 UME7 C 8H 140 2 G 300.00 4000.00 1386.00 1
1072 .274195251E+02 .331653074E-01-.112369879E-04 .173174767E-08-.999867016E-13 2
1073 -.597230517E+05-.112624254E+03 .202528941E+01 .898844344E-01-.593620598E-04 3
1074 .203016355E-07-.286718129E-11-.505953610E+05 .247655861E+02 4
1075 IC8H16 C 8H 16 G 300.00 4000.00 1000.00 1
1076 .159403331E+02 .467083530E-01-.162445520E-04 .262105430E-08-.162114790E-12 2
1077 -.212288474E+05-.575000710E+02-.188446240E+01 .875446570E-01-.337527930E-04 3
1078 -.140196880E-07 .109753600E-10-.160534330E+05 .363096160E+02 4
1079 IC8H16O C 8H 160 1 G 300.00 4000.00 1400.00 1
1080 .286870453E+02 .350973257E-01-.120318626E-04 .187165307E-08-.108763411E-12 2
1081 -.489758985E+05-.130519447E+03-.811336944E+01 .120858100E+00-.869108786E-04 3
1082 .308943900E-07-.431018679E-11-.363657206E+05 .668763983E+02 4
1083 IC8-OQOOH C 8H 160 3 G 300.00 4000.00 1395.00 1
1084 .329665839E+02 .352889373E-01-.121856584E-04 .190423031E-08-.110989507E-12 2
1085 -.686224367E+05-.138776314E+03 .233137835E+00 .110643301E+00-.779138892E-04 3
1086 .277663606E-07-.398875833E-11-.571903320E+05 .373387625E+02 4
1087 IC8H18 C 8H 18 G 300.00 4000.00 1000.00 1
1088 .175409498E+02 .499242880E-01-.172020170E-04 .275518900E-08-.169419330E-12 2
1089 -.363533756E+05-.670046390E+02-.203218650E+01 .946845260E-01-.357433050E-04 3
1090 -.165946760E-07 .125346320E-10-.306832730E+05 .359861450E+02 4
1091 !INDENE C 9H 8 G 300.00 4000.00 1000.00 1
!polimi
1092 ! .129942100E+02 .345035980E-01-.119473340E-04 .137705200E-08 .000000000E+00 2
1093 ! .128398488E+05-.468095535E+02-.565650900E+01 .835992990E-01-.541865810E-04 3
1094 ! .131713170E-07 .000000000E+00 .180739000E+05 .501175500E+02 4
1095 INDENE T 9/96C 9.H 8. 0. 0.G 200.000 6000.000 1000. 1
!Burcat kik
1096 1.73186757E+01 2.89827586E-02-1.06050551E-05 1.73345448E-09-1.04679146E-13 2
1097 1.11514275E+04-7.15553836E+01-6.81899560E-01 4.16587045E-02 7.07413209E-05 3
1098 -1.34308856E-07 5.99158843E-11 1.77050360E+04 2.97813474E+01 1.97411898E+04 4
1099 C9H1002 C 9H 100 2 G 300.00 4000.00 1400.00 1
1100 .279893805E+02 .257305292E-01-.858901356E-05 .131357222E-08-.754726372E-13 2
1101 -.378460988E+05-.119703580E+03-.219761532E+01 .995964750E-01-.769418656E-04 3
1102 .296736479E-07-.451992280E-11-.279092089E+05 .408797910E+02 4
1103 TMBENZ C 9H 12 G 300.00 4000.00 1383.00 1
1104 .215885246E+02 .321229102E-01-.110727239E-04 .172825742E-08-.100649304E-12 2
1105 -.136169019E+05-.914142733E+02-.173308850E+01 .786049041E-01-.431048197E-04 3
1106 .100745302E-07-.585489308E-12-.471446607E+04 .366811038E+02 4
1107 NPBENZ C 9H 12 G 300.00 4000.00 1395.00 1
1108 .234758956E+02 .300348225E-01-.102493106E-04 .158931255E-08-.921475616E-13 2
1109 -.109980792E+05-.102092892E+03-.597461242E+01 .101439137E+00-.768408376E-04 3
1110 .299742828E-07-.474668103E-11-.108882285E+04 .550543799E+02 4
1111 C7H15COCHO C 9H 160 2 G 300.00 4000.00 1387.00 1
1112 .303225194E+02 .381334789E-01-.128450948E-04 .197085647E-08-.113456990E-12 2
1113 -.668175594E+05-.126355483E+03-.229351926E+00 .108754598E+00-.755330139E-04 3
1114 .275093508E-07-.415197146E-11-.560981532E+05 .380532571E+02 4
1115 ALD9 C 9H 180 1 G 300.00 4000.00 1000.00 1
1116 .106561750E+02 .676363860E-01-.253129890E-04 .432392120E-08-.279580530E-12 2
1117 -.437018400E+05-.154058910E+02-.276341620E+00 .105894390E+00-.646322300E-04 3
1118 .149734250E-07 .101003800E-11-.417122110E+05 .376426280E+02 4
1119 C10H8 C 10H 8 G 300.00 4000.00 1401.00 1
1120 .234023214E+02 .242434427E-01-.836282016E-05 .130620111E-08-.761153748E-13 2
1121 .651941329E+04-.107433208E+03-.883645988E+01 .109300567E+00-.955200914E-04 3
1122 .421647669E-07-.739851710E-11 .166533366E+05 .621064766E+02 4
1123 C10H7OH C 10H 80 1 G 300.00 4000.00 1394.00 1
1124 .262017858E+02 .245473904E-01-.859268465E-05 .135522543E-08-.795056830E-13 2
1125 -.158010339E+05-.119344614E+03-.322687986E+01 .931430619E-01-.687932451E-04 3
1126 .249753868E-07-.357353464E-11-.568766282E+04 .385570421E+02 4
1127 C10H10 C 10H 10 G 300.00 4000.00 2043.00 1
1128 .196465049E+02 .362867673E-01-.135117921E-04 .222712581E-08-.134868100E-12 2

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1129	.466515480E+04-.883925826E+02-.975555457E+01	.989343734E-01-.593843991E-04	3
1130	.154882804E-07-.129445409E-11 .148791325E+05	.708155586E+02	4
1131	TETRALIN C 10H 12 G	300.00 4000.00 1393.00	1
1132	.259510150E+02 .311178636E-01-.105072610E-04	.161945272E-08-.935513420E-13	2
1133	-.106963510E+05-.121999608E+03-.103201470E+02	.118533935E+00-.903074920E-04	3
1134	.343768814E-07-.519161790E-11 .142964373E+04	.715127353E+02	4
1135	DCYC5 C 10H 16 G	300.00 4000.00 1396.00	1
1136	.273482865E+02 .461538793E-01-.158755646E-04	.247442795E-08-.143965250E-12	2
1137	-.380245063E+05-.136978542E+03-.149885463E+02	.144180968E+00-.101905712E-03	3
1138	.365256640E-07-.527588038E-11-.233132452E+05	.905738933E+02	4
1139	KHDECA C 10H 16O 3 G	300.00 4000.00 1421.00	1
1140	.152391000E+02 .293351956E-01-.936919554E-05	.138764303E-08-.778701917E-13	2
1141	-.379802009E+05-.703238906E+02-.808436864E+01	.898617293E-01-.693837670E-04	3
1142	.282474384E-07-.463250100E-11-.306468981E+05	.525203269E+02	4
1143	DECALIN C 10H 18 G	300.00 4000.00 1396.00	1
1144	.273482865E+02 .461538793E-01-.158755646E-04	.247442795E-08-.143965250E-12	2
1145	-.380245063E+05-.136978542E+03-.149885463E+02	.144180968E+00-.101905712E-03	3
1146	.365256640E-07-.527588038E-11-.233132452E+05	.905738933E+02	4
1147	ODECAL C 10H 18 G	300.00 4000.00 1383.00	1
1148	.304308606E+02 .423969327E-01-.145305017E-04	.226051483E-08-.131385276E-12	2
1149	-.274622725E+05-.143201137E+03-.921337866E+01	.127293330E+00-.797537373E-04	3
1150	.229874961E-07-.227548927E-11-.131010829E+05	.72155536E+02	4
1151	MEALD9 C 10H 18O 3 G	300.00 4000.00 1000.00	1
1152	-.690383480E+01 .109133900E+00-.458269710E-04	.848431460E-08-.580474200E-12	2
1153	-.758799840E+05 .927347110E+02-.868940000E+00	.130857110E+00-.927276920E-04	3
1154	.252031600E-07 .168027310E-11-.817747730E+05	.466361500E+02	4
1155	NC10H20 C 10H 20 G	300.00 4000.00 1390.00	1
1156	.306417045E+02 .444757412E-01-.152579717E-04	.237363570E-08-.137907421E-12	2
1157	-.321647483E+05-.129750528E+03-.253770965E+01	.118319727E+00-.776112696E-04	3
1158	.262647573E-07-.366153318E-11-.202029921E+05	.498650630E+02	4
1159	NC10MOOH C 10H 20O 2 G	300.00 4000.00 1393.00	1
1160	.277094420E+02 .348487880E-01-.119777002E-04	.186556340E-08-.108475524E-12	2
1161	-.486083259E+05-.114399507E+03 .629165042E+00	.970053636E-01-.668336695E-04	3
1162	.241186253E-07-.361669837E-11-.390326607E+05	.315310044E+02	4
1163	NC10-OQOOH C 10H 20O 3 G	300.00 4000.00 1390.00	1
1164	.373427699E+02 .457774433E-01-.156578702E-04	.243101177E-08-.141046271E-12	2
1165	-.740262240E+05-.156527917E+03 .209018845E+01	.128739739E+00-.918467610E-04	3
1166	.350282382E-07-.560696315E-11-.617151278E+05	.328016208E+02	4
1167	NC10H22 C 10H 22 G	300.00 4000.00 1391.00	1
1168	.319882239E+02 .477244922E-01-.162276391E-04	.250963259E-08-.145215772E-12	2
1169	-.466392840E+05-.137615344E+03-.208416969E+01	.122535012E+00-.776815739E-04	3
1170	.249834877E-07-.323548038E-11-.343021863E+05	.471147911E+02	4
1171	!C10H7CHO C 11H 8O 1 G	300.00 4000.00 1391.00	1
	!Polimi		
1172	! .276532029E+02 .258287942E-01-.902879433E-05	.142281038E-08-.834251834E-13	2
1173	!-.106453206E+05-.124981465E+03-.108527081E+01	.881681978E-01-.575973932E-04	3
1174	! .170999043E-07-.173813923E-11-.356369995E+03	.307785222E+02	4
1175	C10H7CHO T 7/98C 11H 8O 1 OG	200.000 6000.000 1000.	1
	!Burcat kik		
1176	2.42593357E+01 3.16036997E-02-1.18467358E-05	1.96728679E-09-1.20096869E-13	2
1177	-7.83388781E+03-1.07718994E+02-3.75140208E-01	6.11007395E-02 4.92528177E-05	3
1178	-1.17296000E-07 5.31810720E-11 8.41138142E+02	2.88322573E+01 3.67348166E+03	4
1179	!C10H7CH3 C 11H 10 G	300.00 4000.00 1394.00	1
	!Polimi		
1180	! .269623579E+02 .288172394E-01-.100254209E-04	.157466721E-08-.921126923E-13	2
1181	! .586670370E+03-.125206708E+03-.798962224E+01	.117448428E+00-.976360478E-04	3
1182	! .414932114E-07-.710609396E-11 .120022223E+05	.599922187E+02	4
1183	C10H7CH3 T 7/98C 11H 10 0 OG	200.000 6000.000 1000.	1
	!Burcat kik		
1184	2.17939213E+01 3.60214098E-02-1.33228698E-05	2.19304403E-09-1.33071380E-13	2
1185	3.16261439E+03-9.48675403E+01-1.03043715E+00	6.03358177E-02 5.45655719E-05	3
1186	-1.22769251E-07 5.54507327E-11 1.13241014E+04	3.22970611E+01 1.39642625E+04	4
1187	CH3C10H6OH C 11H 10O 1 G	300.00 4000.00 1392.00	1
1188	.281549167E+02 .299236572E-01-.104056239E-04	.163381420E-08-.955470229E-13	2
1189	-.208064399E+05-.126965793E+03-.171335238E+01	.970093442E-01-.665430499E-04	3
1190	.223717851E-07-.293871610E-11-.102462828E+05	.342637221E+02	4
1191	C11H12O4 C 11H 12O 4 G	300.00 4000.00 1398.00	1
1192	.495886732E+02 .844753396E-02 .385179844E-05	-.232491508E-08 .315199759E-12	2
1193	-.164047630E+05-.193448260E+03 .542487420E+01	.999122905E-01-.513976516E-04	3
1194	-.430175388E-08 .876106788E-11-.572347637E+04	.356171545E+02	4
1195	UME10 C 11H 20O 2 G	300.00 4000.00 1384.00	1
1196	.374112533E+02 .458948435E-01-.156057696E-04	.241315080E-08-.139673864E-12	2
1197	-.736971925E+05-.162545741E+03 .937241013E+00	.126885097E+00-.836053178E-04	3

1198	.282312118E-07-.390359926E-11-.605539595E+05	.349335674E+02	4
1199	ETEROMD C 11H 200 3 G	300.00 4000.00 1386.00	1
1200	.418053606E+02 .443798286E-01-.151698489E-04	.235874245E-08-.137104681E-12	2
1201	-.896960798E+05-.186388223E+03-.869108022E+00	.143689897E+00-.103700029E-03	3
1202	.384483018E-07-.582555005E-11-.748416098E+05	.429341731E+02	4
1203	MDKETO C 11H 200 5 G	300.00 4000.00 1391.00	1
1204	.435827467E+02 .471875465E-01-.155121189E-04	.235632808E-08-.134947249E-12	2
1205	-.114156459E+06-.184940808E+03 .336575533E+01	.147442203E+00-.113482823E-03	3
1206	.468018272E-07-.796034235E-11-.100759720E+06	.289177372E+02	4
1207	MD C 11H 220 2 G	300.00 4000.00 1382.00	1
1208	.393230373E+02 .488368389E-01-.166923510E-04	.259065840E-08-.150309877E-12	2
1209	-.885441006E+05-.173932688E+03 .176901386E+01	.129360919E+00-.808243357E-04	3
1210	.251676921E-07-.312062272E-11-.747104475E+05	.304352079E+02	4
1211	!C12H8 C 12H 8 G	300.00 4000.00 1000.00	1
	!polimi		
1212	! .213682716E+02 .324830670E-01-.101214580E-04	.104613640E-08 .000000000E+00	2
1213	! .210494631E+05-.924787980E+02-.672892800E+01	.106967800E+00-.747993040E-04	3
1214	! .193364490E-07 .000000000E+00 .288910000E+05	.533672000E+02	4
1215	C12H8 Acenaphtyl T01/08C 12.H 8. 0. 0.G	200.000 6000.000 1000.	1
	!Burcat kik		
1216	2.15561639E+01 3.31444907E-02-1.20903392E-05	1.97278991E-09-1.19007513E-13	2
1217	2.07186570E+04-9.76752478E+01-2.14921587E+00	5.89101361E-02 6.42492047E-05	3
1218	-1.41293714E-07 6.47476866E-11 2.89379865E+04	3.36791245E+01 3.12345526E+04	4
1219	DIBZFUR C 12H 80 1 G	300.00 4000.00 1000.00	1
1220	.238928699E+02 .342239370E-01-.125916314E-04	.206592304E-08-.125089220E-12	2
1221	-.481449779E+04-.107327684E+03-.194754604E+01	.663215475E-01 .555418713E-04	3
1222	-.135401425E-06 .629515620E-10 .401745217E+04	.350605098E+02	4
1223	!BIPHENYL C 12H 10 G	300.00 4000.00 1000.00	1
	!polimi		
1224	! .214890352E+02 .375797860E-01-.121080230E-04	.129882780E-08 .000000000E+00	2
1225	! .115420788E+05-.916763235E+02-.783196500E+01	.114327200E+00-.776398370E-04	3
1226	! .194042280E-07 .000000000E+00 .198069600E+05	.608493300E+02	4
1227	BIPHENYL g 8/00C 12.H 10. 0. 0.G	200.000 6000.000 1000.00	1
	!Burcat kik		
1228	2.28963620E+01 3.68453189E-02-1.35016357E-05	2.20802787E-09-1.33358137E-13	2
1229	1.07395923E+04-1.00509573E+02 1.94600056E-01	5.35259888E-02 8.55000841E-05	3
1230	-1.63903525E-07 7.29975666E-11 1.90021492E+04	2.72148992E+01 2.19050792E+04	4
1231	C6H5OC6H5 C 12H 100 1 G	300.00 4000.00 1000.00	1
1232	.283319364E+02 .317670352E-01-.107447484E-04	.165690065E-08-.957158914E-13	2
1233	-.789446240E+04-.127230446E+03-.865410063E+01	.124988347E+00-.100933530E-03	3
1234	.413234204E-07-.675938299E-11 .409381103E+04	.686981333E+02	4
1235	C12H18 C 12H 18 G	300.00 4000.00 1000.00	1
1236	.938665800E+02 .198595000E-01-.295692400E-05	.245328200E-09-.917006600E-14	2
1237	-.897187500E+05-.457207000E+03 .374918500E+01	.185852000E+00-.868236800E-04	3
1238	.615957800E-08 .205893500E-11-.565341800E+05	.387544400E+02	4
1239	C12H22 C 12H 22 G	300.00 4000.00 1392.00	1
1240	.362943970E+02 .488870789E-01-.165740715E-04	.255852468E-08-.147868438E-12	2
1241	-.229987583E+05-.159907963E+03-.329755440E+01	.140713318E+00-.978288195E-04	3
1242	.352594898E-07-.520523450E-11-.920475977E+04	.529246931E+02	4
1243	NC12-OQOOH C 12H 240 3 G	300.00 4000.00 1678.00	1
1244	.447068212E+02 .522272795E-01-.195350799E-04	.322923457E-08-.195935332E-12	2
1245	-.818914807E+05-.192299360E+03 .877388676E+01	.119113497E+00-.561329021E-04	3
1246	.677643630E-08 .106366869E-11-.685051188E+05	.572134782E+01	4
1247	NC12H26 C 12H 26 G	300.00 4000.00 1391.00	1
1248	.385099212E+02 .563550048E-01-.191493200E-04	.296024862E-08-.171244150E-12	2
1249	-.548849270E+05-.169785166E+03-.262181594E+01	.147237711E+00-.943970271E-04	3
1250	.307441268E-07-.403602230E-11-.400654253E+05	.529882396E+02	4
1251	!FLUORENE C 13H 10 G	300.00 4000.00 1000.00	1
	!Polimi		
1252	! .231612871E+02 .392128530E-01-.125431510E-04	.133503890E-08 .000000000E+00	2
1253	! .123102892E+05-.103717257E+03-.112092800E+02	.129847800E+00-.907013380E-04	3
1254	! .232288460E-07 .000000000E+00 .219426600E+05	.748524200E+02	4
1255	FLUORENE T11/07C 13.H 10. 0. 0.G	200.000 6000.000 1000.00	1
	!Burcat kik		
1256	2.33961594E+01 3.76272122E-02-1.37117389E-05	2.24351896E-09-1.35502173E-13	2
1257	9.60546553E+03-1.04754427E+02-1.08010254E+00	5.81364450E-02 8.71414836E-05	3
1258	-1.72419903E-07 7.76417263E-11 1.83197800E+04	3.21625902E+01 2.10475422E+04	4
1259	!C6H5CH2C6H5 C 13H 12 G	300.00 4000.00 1000.00	1
	!polimi		
1260	! .185418955E+02 .513343070E-01-.178726910E-04	.207043850E-08 .000000000E+00	2
1261	! .668552054E+04-.690121392E+02-.940899900E+01	.125451300E+00-.822539730E-04	3
1262	! .202856220E-07 .000000000E+00 .144845500E+05	.760677200E+02	4
1263	C6H5CH2C6H5 T10/13C 13.H 12. 0. 0.G	200.000 6000.000 1000.0	1

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!Burcat kik MeBiPhenyl
1264 2.33823671E+01 4.36035134E-02-1.59318261E-05 2.59973976E-09-1.56760199E-13 2
1265 7.84267591E+03-1.00997944E+02 1.70749233E+00 3.70722686E-02 1.53928694E-04 3
1266 -2.41954650E-07 1.02743229E-10 1.67215993E+04 2.61209040E+01 1.98087440E+04 4
1267 ALDINS C 13H 200 1 G 300.00 4000.00 1000.00 1
1268 .938665800E+02 .198595000E-01-.295692400E-05 .245328200E-09-.917006600E-14 2
1269 -.897187500E+05-.457207000E+03 .374918500E+01 .185852000E+00-.868236800E-04 3
1270 .615957800E-08 .205893500E-11-.565341800E+05 .387544400E+02 4
1271 U2ME12 C 13H 220 2 G 300.00 4000.00 1391.00 1
1272 .422353117E+02 .524987045E-01-.181261023E-04 .283174793E-08-.165001495E-12 2
1273 -.676968189E+05-.186270028E+03 .679798314E-01 .152530074E+00-.111376081E-03 3
1274 .435663556E-07-.715842617E-11-.529996239E+05 .399987338E+02 4
1275 MEALDU12 C 13H 220 3 G 300.00 4000.00 1000.00 1
1276 .102076680E+02 .102462700E+00-.400200840E-04 .704170850E-08-.464730410E-12 2
1277 -.764049450E+05 .447871400E+01-.148239800E+01 .157342330E+00-.103758050E-03 3
1278 .246418600E-07 .237571010E-11-.758768280E+05 .556433530E+02 4
1279 !C14H10 C 14H 10 G 300.00 4000.00 1000.00 1
!polimi
1280 !.255171870E+02 .393727940E-01-.123155080E-04 .127852800E-08 .000000000E+00 2
1281 !.131224037E+05-.115618425E+03-.909474100E+01 .131333800E+00-.924017290E-04 3
1282 !.240156710E-07 .000000000E+00 .227649500E+05 .639753600E+02 4
1283 C14H10 Phenanth T 6/12C 14.H 10. 0. 0.G 200.000 6000.000 1000.00 1 !
Burcat kik
1284 2.66042825E+01 3.97675990E-02-1.45710303E-05 2.38414417E-09-1.44083321E-13 2
1285 1.15427370E+04-1.22473909E+02-3.36413181E+00 8.50677802E-02 3.75500017E-05 3
1286 -1.26667049E-07 6.14543114E-11 2.14305029E+04 4.07973319E+01 2.43189316E+04 4
1287 !C6H5C2H4C6H5 C 14H 14 G 300.00 4000.00 1000.00 1
!polimi
1288 !.183724857E+02 .606470630E-01-.215506390E-04 .254284330E-08 .000000000E+00 2
1289 !.518516081E+04-.659251182E+02-.814781700E+01 .130620600E+00-.819367560E-04 3
1290 !.194757260E-07 .000000000E+00 .126141800E+05 .718458700E+02 4
1291 !C6H5C2H4C6H5 T 5/04C 14.H 14. 0. 0.G 200.000 6000.000 1000.00 1
!Burcat kik
1292 ! 2.65979897E+01 4.68689340E-02-1.69056103E-05 2.73737090E-09-1.64235887E-13 2
1293 ! 3.18810786E+03-1.14827874E+02 1.30521842E+00 5.76220698E-02 1.22418244E-04 3
1294 !-2.18120750E-07 9.59096665E-11 1.26627763E+04 2.90742354E+01 1.63088384E+04 4
1295 C6H5C2H4C6H5 C 14H 14O 0 OG 300.00 3000.00 1000.00 1
1296 0.72920350E+01 0.92502000E-01-0.51686410E-04 0.13627090E-07-0.13811480E-11 2
1297 0.10316730E+05-0.11327380E+02-0.13889580E+02 0.17209840E+00-0.17006600E-03 3
1298 0.96018880E-07-0.23732530E-10 0.15032340E+05 0.92707360E+02 4
1299 !C16H10 C 16H 10 G 300.00 4000.00 1000.00 1
!polimi
1300 !.290747022E+02 .412337670E-01-.126077060E-04 .127453580E-08 .000000000E+00 2
1301 !.141687238E+05-.136431347E+03-.106811200E+02 .146535400E+00-.103943520E-03 3
1302 !.270645390E-07 .000000000E+00 .252715000E+05 .699617500E+02 4
1303 C16H10 Pyrene T 6/12C 16.H 10. 0. 0.G 200.000 6000.000 1000. 1
!Burcat kik
1304 2.99100370E+01 4.26680281E-02-1.57338134E-05 2.58516829E-09-1.56679506E-13 2
1305 1.27624176E+04-1.41870304E+02-4.04244612E+00 9.15520165E-02 5.14380972E-05 3
1306 -1.52760613E-07 7.30856860E-11 2.40702419E+04 4.36665325E+01 2.71212615E+04 4
1307 NC16-OQOOH C 16H 32O 3 G 300.00 4000.00 1854.00 1
1308 .488264318E+02 .825357366E-01-.292747409E-04 .467245514E-08-.276718037E-12 2
1309 -.942845289E+05-.205583924E+03 .138386904E+01 .198379105E+00-.134722947E-03 3
1310 .475955890E-07-.691333208E-11-.791319641E+05 .463051187E+02 4
1311 IC16-OQOOH C 16H 32O 3 G 300.00 4000.00 1397.00 1
1312 .620188250E+02 .682375774E-01-.235322180E-04 .367416933E-08-.214025539E-12 2
1313 -.107194396E+06-.296402060E+03-.700111687E+01 .236135134E+00-.181200158E-03 3
1314 .715715364E-07-.114883341E-10-.839739066E+05 .717765001E+02 4
1315 NC16H34 C 16H 34 G 300.00 4000.00 1391.00 1
1316 .515593854E+02 .736064257E-01-.249888737E-04 .386085377E-08-.223263662E-12 2
1317 -.713781425E+05-.234158439E+03-.369111950E+01 .196612966E+00-.127777824E-03 3
1318 .422323349E-07-.562967041E-11-.515927302E+05 .647080513E+02 4
1319 IC16H34 C 16H 34 G 300.00 4000.00 1400.00 1
1320 .565856523E+02 .692869560E-01-.234931111E-04 .362720220E-08-.209665225E-12 2
1321 -.820366778E+05-.276851694E+03-.107545408E+02 .233995831E+00-.178076331E-03 3
1322 .696956034E-07-.110282035E-10-.595981394E+05 .818346760E+02 4
1323 UME16 C 17H 32O 2 G 300.00 4000.00 1000.00 1
1324 .333606142E+02 .106719124E+00-.429500189E-04 .790457654E-08-.546125152E-12 2
1325 -.868236054E+05-.126816968E+03 .114310960E+02 .102101194E+00 .102480878E-03 3
1326 -.181385357E-06 .698603588E-10-.778209017E+05 .206428096E+01 4
1327 ETEROMPA C 17H 32O 3 G 300.00 4000.00 1000.00 1

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1328 .406345250E+02 .963702350E-01-.332815250E-04 .536978820E-08-.333546480E-12 2
1329 -.105022900E+06-.161181400E+03-.374618910E+01 .216936450E+00-.134184780E-03 3
1330 .217036750E-07 .800116570E-11-.930412810E+05 .677468110E+02 4
1331 MPA C 17H 340 2 G 300.00 4000.00 1000.00 1
1332 .355305296E+02 .109746228E+00-.440981772E-04 .810571172E-08-.559469785E-12 2
1333 -.102923616E+06-.145292419E+03 .117629996E+02 .108027697E+00 .103662595E-03 3
1334 -.187190120E-06 .724616510E-10-.933306777E+05-.643066315E+01 4
1335 KHMLIN1 C 19H 300 5 G 300.00 4000.00 1843.00 1
1336 .597680898E+02 .832144998E-01-.302817533E-04 .491632066E-08-.294624551E-12 2
1337 -.961002787E+05-.258440317E+03-.347354324E+01 .238348931E+00-.171810701E-03 3
1338 .624560833E-07-.914836595E-11-.760003616E+05 .770024622E+02 4
1339 MLIN1 C 19H 320 2 G 300.00 4000.00 1834.00 1
1340 .520202170E+02 .871284776E-01-.313984409E-04 .506450961E-08-.302130761E-12 2
1341 -.727531890E+05-.226713941E+03-.298592567E+01 .218746556E+00-.148096154E-03 3
1342 .511216154E-07-.719451974E-11-.549290521E+05 .662774857E+02 4
1343 MLINO C 19H 340 2 G 300.00 4000.00 1833.00 1
1344 .524257963E+02 .910351615E-01-.326514183E-04 .524998946E-08-.312507814E-12 2
1345 -.869039436E+05-.227879204E+03-.158761924E+01 .219526542E+00-.145761172E-03 3
1346 .495347572E-07-.688636525E-11-.693288124E+05 .600962817E+02 4
1347 MLIN1OOH C 19H 340 4 G 300.00 4000.00 1833.00 1
1348 .524257963E+02 .910351615E-01-.326514183E-04 .524998946E-08-.312507814E-12 2
1349 -.869039436E+05-.227879204E+03-.158761924E+01 .219526542E+00-.145761172E-03 3
1350 .495347572E-07-.688636525E-11-.693288124E+05 .600962817E+02 4
1351 MEOLE C 19H 360 2 G 300.00 4000.00 1831.00 1
1352 .528856562E+02 .948572658E-01-.338668063E-04 .542873444E-08-.322458135E-12 2
1353 -.101075125E+06-.229348639E+03-.267573662E+00 .220639742E+00-.143861659E-03 3
1354 .481699649E-07-.661786902E-11-.837166223E+05 .542791001E+02 4
1355 MLINOOH C 19H 360 4 G 300.00 4000.00 1833.00 1
1356 .524257963E+02 .910351615E-01-.326514183E-04 .524998946E-08-.312507814E-12 2
1357 -.869039436E+05-.227879204E+03-.158761924E+01 .219526542E+00-.145761172E-03 3
1358 .495347572E-07-.688636525E-11-.693288124E+05 .600962817E+02 4
1359 MSTEAKETO C 19H 360 5 G 300.00 4000.00 1857.00 1
1360 .628573476E+02 .927885184E-01-.331648431E-04 .532086973E-08-.316267196E-12 2
1361 -.142644021E+06-.277684268E+03-.711176329E+00 .251338095E+00-.180571731E-03 3
1362 .664483461E-07-.990089173E-11-.122716422E+06 .585265768E+02 4
1363 MSTEA C 19H 380 2 G 300.00 4000.00 1000.00 1
1364 .418174710E+02 .117959830E+00-.465265590E-04 .845319460E-08-.579171090E-12 2
1365 -.110862900E+06-.175601040E+03 .114771030E+02 .131225240E+00 .898738730E-04 3
1366 -.183685190E-06 .722337400E-10-.991500330E+05-.163992920E+01 4
1367 BIN1B C 20H 10 G 300.00 4000.00 1000.00 1
1368 -.570256700E+01 .143432300E+00-.880724700E-04 .276799200E-07-.352289900E-11 2
1369 .277808900E+05 .434481200E+02-.570256700E+01 .143432300E+00-.880724700E-04 3
1370 .276799200E-07-.352289900E-11 .277808900E+05 .434481200E+02 4
1371 BIN1A C 20H 16 G 300.00 4000.00 1000.00 1
1372 -.324173600E+01 .158222900E+00-.946183500E-04 .281843100E-07-.356131000E-11 2
1373 .217869900E+05 .300825300E+02-.324173600E+01 .158222900E+00-.946183500E-04 3
1374 .281843100E-07-.356131000E-11 .217869900E+05 .300825300E+02 4
1375 C24H28O4 C 24H 280 4 G 300.00 4000.00 1398.00 1
1376 .495886732E+02 .844753396E-02 .385179844E-05-.232491508E-08 .315199759E-12 2
1377 -.164047630E+05-.193448260E+03 .542487420E+01 .999122905E-01-.513976516E-04 3
1378 -.430175388E-08 .876106788E-11-.572347637E+04 .356171545E+02 4
1379 !O O 1 G 300.00 4000.00 700.00 1
1380 ! .854006043E+00-.488003453E-02 .104572169E-04-.522729913E-08 .771608734E-12 2
1381 ! .306893420E+05 .173763860E+02 .000000000E+00 .000000000E+00 .000000000E+00 3
1382 ! .473195502E-08-.278526775E-11 .308089029E+05 .211918689E+02 4
1383 O ATcT3EO 1 0 0 OG 200.00 6000.00 1000.00 1
! [Ghobad] O <g> ATcT ver. 1.122, DHf298 = 249.229 \B1 0.002 kJ/mol - fit MAR17
1384 2.55160087E+00-3.83085457E-05 8.43197478E-10 4.01267136E-12-4.17476574E-16 2
1385 2.92287628E+04 4.87617014E+00 3.15906526E+00-3.21509999E-03 6.49255543E-06 3
1386 -5.98755115E-09 2.06876117E-12 2.91298453E+04 2.09078344E+00 2.99753606E+04 4
1387 !H H 1 G 300.00 4000.00 1000.00 1
1388 ! .250000000E+01 .000000000E+00 .000000000E+00 .000000000E+00 .000000000E+00 2
1389 ! .254736600E+05-.446682850E+00 .250000000E+01 .000000000E+00 .000000000E+00 3
1390 ! .000000000E+00 .000000000E+00 .254736600E+05-.446682850E+00 4
1391 H ATcT3EH 1 0 0 OG 200.00 6000.00 1000.00 1
! [Ghobad] H <g> ATcT ver. 1.122, DHf298 = 217.998 \B1 0.000 kJ/mol - fit MAR17
1392 2.49985211E+00 2.34582548E-07-1.16171641E-10 2.25708298E-14-1.52992005E-18 2
1393 2.54738024E+04-4.45864645E-01 2.49975925E+00 6.73824499E-07 1.11807261E-09 3
1394 -3.70192126E-12 2.14233822E-15 2.54737665E+04-4.45574009E-01 2.62191345E+04 4
1395 !OH H 1O 1 G 300.00 4000.00 1000.00 1
1396 ! .283853033E+01 .110741289E-02-.294000209E-06 .420698729E-10-.242289890E-14 2
1397 ! .369780808E+04 .584494652E+01 .399198424E+01-.240106655E-02 .461664033E-05 3
1398 !-.387916306E-08 .136319502E-11 .336889836E+04-.103998477E+00 4

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1399 OH ATcT3EH 10 1 0 OG 200.00 6000.00 1000.00 1
! [Ghobad] OH <g> ATcT ver. 1.122, DHf298 = 37.490 \B1 0.027 kJ/mol - fit MAR17
1400 2.84581721E+00 1.09723818E-03-2.89121101E-07 4.09099910E-11-2.31382258E-15 2
1401 3.71706610E+03 5.80339915E+00 3.97585165E+00-2.28555291E-03 4.33442882E-06 3
1402 -3.59926640E-09 1.26706930E-12 3.39341137E+03-3.55397262E-02 4.50901087E+03 4
1403 !HO2 H 10 2 G 300.00 4000.00 1000.00 1
1404 ! .417228741E+01 .188117627E-02-.346277286E-06 .194657549E-10 .176256905E-15 2
1405 ! .310206839E+02 .295767672E+01 .430179807E+01-.474912097E-02 .211582905E-04 3
1406 !-.242763914E-07 .929225225E-11 .264018485E+03 .371666220E+01 4
1407 HO2 ATcT3EH 10 2 0 OG 200.00 6000.00 1000.00 1
! [Ghobad] HO2 <g> ATcT ver. 1.122, DHf298 = 12.26 \B1 0.16 kJ/mol - fit MAR17
1408 4.10564010E+00 2.04046836E-03-3.65877562E-07 1.85973044E-11 4.98818315E-16 2
1409 4.32898769E+01 3.30808126E+00 4.26251250E+00-4.45642032E-03 2.05164934E-05 3
1410 -2.35794011E-08 9.05614257E-12 2.62442356E+02 3.88223684E+00 1.47417835E+03 4
1411 ! C C 1 G 300.00 4000.00 1000.00 1
1412 ! .843301655E+00-.481886660E-02 .103261427E-04-.515161356E-08 .759963466E-12 2
1413 ! .868941443E+05 .170134676E+02 .000000000E+00 .000000000E+00 .000000000E+00 3
1414 ! .468280808E-08-.275232998E-11 .870122065E+05 .207811260E+02 4
1415 CSOLID C 1 G 300.00 4000.00 1000.00 1
1416 .159828070E+01 .143065097E-02-.509435105E-06 .864401302E-10-.534349530E-14 2
1417 -.745940284E+03-.930332005E+01-.303744539E+00 .436036227E-02 .198268825E-05 3
1418 -.643472598E-08 .299601320E-11-.109458288E+03 .108301475E+01 4
1419 CH C 1H 1 G 300.00 4000.00 1000.00 1
1420 .252093690E+01 .176536390E-02-.461476600E-06 .592896750E-10-.334745010E-14 2
1421 .709948780E+05 .740518290E+01 .348975830E+01 .324321600E-03-.168997510E-05 3
1422 .316284200E-08-.140618030E-11 .706607550E+05 .208428410E+01 4
1423 !HCO C 1H 10 1 G 300.00 4000.00 1000.00 1
1424 ! .392001542E+01 .252279324E-02-.671004164E-06 .105615948E-09-.743798261E-14 2
1425 ! .365342928E+04 .358077056E+01 .423754610E+01-.332075257E-02 .140030264E-04 3
1426 !-.134239995E-07 .437416208E-11 .387241185E+04 .330834869E+01 4
1427 HCO ATcT3EC 1H 10 1 OG 200.00 6000.00 1000.00 1
! [Ghobad] HCO <g> ATcT ver. 1.122, DHf298 = 41.803 \B1 0.099 kJ/mol - fit MAR17
1428 3.85781113E+00 2.64113950E-03-7.44177294E-07 1.23313230E-10-8.88958718E-15 2
1429 3.61642883E+03 3.92451197E+00 3.97074749E+00-1.49121608E-03 9.54041776E-06 3
1430 -8.82720349E-09 2.67645129E-12 3.84203291E+03 4.44660361E+00 5.02774557E+03 4
1431 HCO3 C 1H 10 3 G 300.00 4000.00 1000.00 1
1432 .726425669E+01 .532196974E-02-.196520055E-05 .323182996E-09-.195989250E-13 2
1433 -.159242239E+05-.103647520E+02 .364808935E+01 .957717212E-02 .755287366E-05 3
1434 -.181264650E-07 .827293980E-11-.146544449E+05 .967735548E+01 4
1435 CH2 C 1H 2 G 300.00 4000.00 1000.00 1
1436 .314631886E+01 .303671259E-02-.996474439E-06 .150483580E-09-.857335515E-14 2
1437 .460412605E+05 .472341711E+01 .371757846E+01 .127391260E-02 .217347251E-05 3
1438 -.348858500E-08 .165208866E-11 .458723866E+05 .175297945E+01 4
1439 CH2(S) C 1H 2 G 300.00 4000.00 1000.00 1
1440 .313501686E+01 .289593926E-02-.816668090E-06 .113572697E-09-.636262835E-14 2
1441 .505040504E+05 .406030621E+01 .419331325E+01-.233105184E-02 .815676451E-05 3
1442 -.662985981E-08 .193233199E-11 .503662246E+05-.746734310E+00 4
1443 CH3 C 1H 3 G 300.00 4000.00 1000.00 1
1444 .297812060E+01 .579785200E-02-.197558000E-05 .307297900E-09-.179174160E-13 2
1445 .165095130E+05 .472247990E+01 .365717970E+01 .212659790E-02 .545838830E-05 3
1446 -.661810030E-08 .246570740E-11 .164227160E+05 .167353540E+01 4
1447 CH3O C 1H 3O 1 G 300.00 4000.00 1000.00 1
1448 .475779238E+01 .744142474E-02-.269705176E-05 .438090504E-09-.263537098E-13 2
1449 .390139164E+03-.196680028E+01 .371180502E+01-.280463306E-02 .376550971E-04 3
1450 -.473072089E-07 .186588420E-10 .130772484E+04 .657240864E+01 4
1451 CH2OH C 1H 3O 1 G 300.00 4000.00 1000.00 1
1452 .509312037E+01 .594758550E-02-.206496524E-05 .323006703E-09-.188125052E-13 2
1453 -.405813228E+04-.184690613E+01 .447832317E+01-.135069687E-02 .278483707E-04 3
1454 -.364867397E-07 .147906775E-10-.352476728E+04 .330911984E+01 4
1455 CH3O2 C 1H 3O 2 G 300.00 4000.00 1000.00 1
1456 .480390863E+01 .995844638E-02-.385301026E-05 .684740497E-09-.458402955E-13 2
1457 -.747135460E+03 .145281400E+01 .362497097E+01 .359397933E-02 .226538097E-04 3
1458 -.295391947E-07 .111977570E-10 .793040410E+02 .996382194E+01 4
1459 C2H C 2H 1 G 300.00 4000.00 1000.00 1
1460 .366270248E+01 .382492252E-02-.136632500E-05 .213455040E-09-.123216848E-13 2
1461 .671683790E+05 .392205792E+01 .289867676E+01 .132988489E-01-.280733327E-04 3
1462 .289484755E-07-.107502351E-10 .670616050E+05 .618547632E+01 4
1463 HCCO C 2H 1O 1 G 300.00 4000.00 1000.00 1
1464 .591479333E+01 .371408730E-02-.130137010E-05 .206473345E-09-.121476759E-13 2
1465 .193596301E+05-.550567269E+01 .187607969E+01 .221205418E-01-.358869325E-04 3
1466 .305402541E-07-.101281069E-10 .201633840E+05 .136968290E+02 4
1467 C2H3 C 2H 3 G 300.00 4000.00 1000.00 1
1468 .415026763E+01 .754021341E-02-.262997847E-05 .415974048E-09-.245407509E-13 2

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1469 .338566380E+05 .172812235E+01 .336377642E+01 .265765722E-03 .279620704E-04 3
1470 -.372986942E-07 .151590176E-10 .344749589E+05 .791510092E+01 4
1471 CH3CO C 2H 3O 1 G 300.00 4000.00 1000.00 1
1472 .531371650E+01 .917377930E-02-.332203860E-05 .539474560E-09-.324523680E-13 2
1473 -.364504140E+04-.167575580E+01 .403587050E+01 .877294870E-03 .307100100E-04 3
1474 -.392475650E-07 .152968690E-10-.268207380E+04 .786176820E+01 4
1475 CH2CHO C 2H 3O 1 G 300.00 4000.00 1000.00 1
1476 .653928338E+01 .780238629E-02-.276413612E-05 .442098906E-09-.262954290E-13 2
1477 -.118858659E+04-.872091393E+01 .279502600E+01 .101099472E-01 .161750645E-04 3
1478 -.310303145E-07 .139436139E-10 .162944975E+03 .123646657E+02 4
1479 CH3CO2 C 2H 3O 2 G 300.00 4000.00 1000.00 1
1480 .700171955E+01 .101977290E-01-.365621800E-05 .589475086E-09-.352561321E-13 2
1481 -.226135780E+05-.905267669E+01 .475563598E+01 .780915313E-02 .162272935E-04 3
1482 -.241210787E-07 .942644561E-11-.215157456E+05 .478096491E+01 4
1483 CH3CO3 C 2H 3O 3 G 300.00 4000.00 1000.00 1
1484 .102188027E+02 .888408630E-02-.222887620E-05 .166265570E-09 .000000000E+00 2
1485 -.256023886E+05-.219354293E+02 .384065500E+01 .218595100E-01-.904528040E-05 3
1486 .385393800E-09 .000000000E+00-.234946000E+05 .124829900E+02 4
1487 C2H5 C 2H 5 G 300.00 4000.00 1000.00 1
1488 .432195633E+01 .123930542E-01-.439680960E-05 .703519917E-09-.418435239E-13 2
1489 .121759475E+05 .171103809E+00 .424185905E+01-.356905235E-02 .482667202E-04 3
1490 -.585401009E-07 .225804514E-10 .129690344E+05 .444703782E+01 4
1491 PC2H4OH C 2H 5O 1 G 300.00 4000.00 1000.00 1
1492 .701348674E+01 .120204391E-01-.421992012E-05 .670675981E-09-.397135273E-13 2
1493 -.616161779E+04-.862052409E+01 .420954137E+01 .912964578E-02 .247462263E-04 3
1494 -.392945764E-07 .166541312E-10-.491511371E+04 .830445413E+01 4
1495 CH3OCH2 C 2H 5O 1 G 300.00 4000.00 1000.00 1
1496 .594067593E+01 .129906358E-01-.456921036E-05 .726888932E-09-.430599587E-13 2
1497 -.258503562E+04-.452841964E+01 .453195381E+01 .781884271E-02 .194968539E-04 3
1498 -.274538336E-07 .106521135E-10-.170629244E+04 .506122980E+01 4
1499 SC2H4OH C 2H 5O 1 G 300.00 4000.00 1000.00 1
1500 .635842302E+01 .124356276E-01-.433096839E-05 .684530381E-09-.403713238E-13 2
1501 -.953018581E+04-.605106112E+01 .422283250E+01 .512174798E-02 .348386522E-04 3
1502 -.491943637E-07 .201183723E-10-.835622088E+04 .801675700E+01 4
1503 C2H5O2 C 2H 5O 2 G 300.00 4000.00 1000.00 1
1504 .888872432E+01 .135833179E-01-.491116949E-05 .792343362E-09-.473525704E-13 2
1505 -.744107388E+04-.190789836E+02 .450099327E+01 .687965342E-02 .474143971E-04 3
1506 -.692287127E-07 .287395324E-10-.539547911E+04 .791490068E+01 4
1507 C2H4O2H C 2H 5O 2 G 300.00 4000.00 1000.00 1
1508 .941379980E+01 .133542122E-01-.468067639E-05 .743230845E-09-.439824231E-13 2
1509 .198459602E+04-.224516643E+02 .507456388E+01 .132389561E-01 .253758646E-04 3
1510 -.438089546E-07 .189061540E-10 .371063204E+04 .272289544E+01 4
1511 DME-OO C 2H 5O 3 G 300.00 4000.00 1359.00 1
1512 .120501213E+02 .123072703E-01-.435221905E-05 .690896352E-09-.407091104E-13 2
1513 -.227977573E+05-.323415629E+02 .515628105E+01 .216783339E-01-.561847228E-05 3
1514 -.192807296E-08 .859447044E-12-.196244836E+05 .725163812E+01 4
1515 DME-QOOH C 2H 5O 3 G 300.00 4000.00 1367.00 1
1516 .140894827E+02 .105710448E-01-.375281006E-05 .597314407E-09-.352604582E-13 2
1517 -.191406716E+05-.429268872E+02 .543520255E+01 .272005914E-01-.150210893E-04 3
1518 .370396290E-08-.309396378E-12-.157034464E+05 .495012674E+01 4
1519 C2-OOQOOH C 2H 5O 4 G 300.00 4000.00 1387.00 1
1520 .145471032E+02 .123393823E-01-.427259469E-05 .668763337E-09-.390196721E-13 2
1521 -.196338761E+05-.408784236E+02 .590031872E+01 .305658528E-01-.185905950E-04 3
1522 .567871605E-08-.702799577E-12-.163916571E+05 .633051038E+01 4
1523 DME-OOQOOH C 2H 5O 5 G 300.00 4000.00 1382.00 1
1524 .146274659E+02 .163794767E-01-.563311171E-05 .877481381E-09-.510186598E-13 2
1525 -.370029335E+05-.399555488E+02 .771229157E+01 .301140957E-01-.165996092E-04 3
1526 .533577253E-08-.842885930E-12-.341808026E+05-.165902348E+01 4
1527 C3H2 C 3H 2 G 300.00 4000.00 1000.00
1 ! Modified 1712
1528 .667324762E+01 .557728845E-02-.199180164E-05 .320289156E-09-.191216272E-13 2
1529 .607571184E+05-.972894405E+01 .243417332E+01 .173013063E-01-.118294047E-04 3
1530 .102756396E-08 .162626314E-11 .619074892E+05 .121012230E+02 4
1531 C3H3 C 3H 3 G 300.00 4000.00 1000.00 1
1532 .714221719E+01 .761902211E-02-.267460030E-05 .424914904E-09-.251475443E-13 2
1533 .395709594E+05-.125848690E+02 .135110873E+01 .327411291E-01-.473827407E-04 3
1534 .376310220E-07-.118541128E-10 .407679941E+05 .152058598E+02 4
1535 C3H5-A C 3H 5 G 300.00 4000.00 1000.00 1
1536 .674633155E+01 .131071760E-01-.460059113E-05 .731029510E-09-.432759674E-13 2
1537 .171151431E+05-.125248814E+02 .165533607E+01 .163688750E-01 .210544223E-04 3
1538 -.424018394E-07 .192638759E-10 .189454047E+05 .161040987E+02 4
1539 C3H5-T C 3H 5 G 300.00 4000.00 1000.00 1
1540 .611018050E+01 .146733950E-01-.536768220E-05 .869049320E-09-.519320060E-13 2

1541 .255324420E+05-.835557120E+01 .255440330E+01 .109867980E-01 .301743050E-04 3
1542 -.472535680E-07 .197710730E-10 .271502420E+05 .132075920E+02 4
1543 C3H5-S C 3H 5 G 300.00 4000.00 1000.00 1
1544 .605091412E+01 .134052084E-01-.473450586E-05 .755380897E-09-.448421084E-13 2
1545 .290860210E+05-.673692060E+01 .333277282E+01 .106102499E-01 .217559727E-04 3
1546 -.347145235E-07 .144476835E-10 .303404530E+05 .978922358E+01 4
1547 C3H5O C 3H 5O 1 G 300.00 4000.00 1402.00 1
1548 .102638186E+02 .117609932E-01-.389837957E-05 .592650815E-09-.338867417E-13 2
1549 .725938472E+04-.275108651E+02 .824068673E+00 .346749909E-01-.251786795E-04 3
1550 .956781953E-08-.148085302E-11 .104203725E+05 .228283070E+02 4
1551 RALD3BG C 3H 5O 1 G 300.00 4000.00 1366.00 1
1552 .979372730E+01 .168079281E-01-.684815970E-05 .118460585E-08-.738195109E-13 2
1553 -.875662870E+04-.294639062E+02 .667614768E+01 .261082031E-02 .280410577E-04 3
1554 -.226802600E-07 .516442572E-11-.510504908E+04-.439698728E+01 4
1555 CH3COCH2 C 3H 5O 1 G 300.00 4000.00 1000.00 1
1556 .754410697E+01 .143443222E-01-.508381081E-05 .813200521E-09-.483673315E-13 2
1557 -.748672286E+04-.114792587E+02 .470187196E+01 .551653762E-02 .427505858E-04 3
1558 -.594680816E-07 .240685378E-10-.592845491E+04 .712932590E+01 4
1559 C3H5OO C 3H 5O 2 G 300.00 4000.00 1375.00 1
1560 .120289627E+02 .126220050E-01-.443107280E-05 .699998849E-09-.411059161E-13 2
1561 .440592543E+04-.346276747E+02 .316765415E+01 .300862111E-01-.169786280E-04 3
1562 .462955698E-08-.501220245E-12 .789477349E+04 .142601307E+02 4
1563 CH3CHOOCHOL C 3H 5O 3 G 300.00 4000.00 1375.00 1
1564 .168446948E+02 .108808472E-01-.388442566E-05 .620614245E-09-.367342997E-13 2
1565 -.242215993E+05-.597283331E+02 .351827789E+01 .399638014E-01-.273701195E-04 3
1566 .894188675E-08-.112554087E-11-.194047940E+05 .125456874E+02 4
1567 CH2CHOOHCHOL C 3H 5O 3 G 300.00 4000.00 1387.00 1
1568 .165672086E+02 .109861375E-01-.388980958E-05 .618066089E-09-.364435558E-13 2
1569 -.159737374E+05-.559457656E+02 .175858492E+01 .494637636E-01-.434833502E-04 3
1570 .195880861E-07-.355128051E-11-.111728737E+05 .222887088E+02 4
1571 CH2OOCCHOOHCHOL C 3H 5O 5 G 300.00 4000.00 1387.00 1
1572 .207806034E+02 .116953349E-01-.414531832E-05 .659225856E-09-.388964379E-13 2
1573 -.355954399E+05-.753605279E+02 .563102793E+01 .452923139E-01-.313606807E-04 3
1574 .100926022E-07-.119108613E-11-.302385330E+05 .649991022E+01 4
1575 NC3H7 C 3H 7 G 300.00 4000.00 1000.00 1
1576 .649636579E+01 .177337992E-01-.624898046E-05 .995389495E-09-.590199770E-13 2
1577 .885973885E+04-.856389710E+01 .408211458E+01 .523240341E-02 .513554466E-04 3
1578 -.699343598E-07 .281819493E-10 .104074558E+05 .839534919E+01 4
1579 IC3H7 C 3H 7 G 300.00 4000.00 1000.00 1
1580 .530597255E+01 .189854588E-01-.674315384E-05 .107993730E-08-.642785036E-13 2
1581 .778748910E+04-.223233935E+01 .547421257E+01-.842536682E-02 .804607759E-04 3
1582 -.949287824E-07 .359830971E-10 .904939013E+04 .340542323E+01 4
1583 CH3CH2CHOH C 3H 7O 1 G 300.000 5000.000 1388.000 31
!\AUTHOR: CR/KPS !\REF: GA !\COMMENT: FITTED WITH THERM ON 11_08_2016_20_43_11
1584 1.14795375E+01 1.45881429E-02-4.88359380E-06 7.47606975E-10-4.29608360E-14 2
1585 -1.46832088E+04-3.36825807E+01 1.13614529E+00 3.68850655E-02-2.24073579E-05 3
1586 6.62398992E-09-7.32206246E-13-1.09273174E+04 2.24919343E+01 4
1587 CH3CH2CH2O C 3H 7O 1 OG 300.000 5000.000 1386.000 21
!\AUTHOR: CR/KPS !\REF: GA !\COMMENT: FITTED WITH THERM ON 11_08_2016_20_43_11
1588 1.15279177E+01 1.53775991E-02-5.23946272E-06 8.11382512E-10-4.69927603E-14 2
1589 -9.85099866E+03-3.54233008E+01 2.57486880E+00 3.07100600E-02-1.20048836E-05 3
1590 3.40807021E-12 7.25275283E-13-6.20913350E+03 1.45966401E+01 4
1591 CH2CHOHCH3 C 3H 7O 1 G 300.00 4000.00 1388.00 1
1592 .110944203E+02 .153549108E-01-.523574640E-05 .810964124E-09-.469665855E-13 2
1593 -.134769536E+05-.307070215E+02 .584672920E+00 .407370189E-01-.294865043E-04 3
1594 .116950656E-07-.196228356E-11-.984929391E+04 .255429190E+02 4
1595 CH2CH2CH2OH C 3H 7O 1 OG 300.000 5000.000 1402.000 31
!\AUTHOR: CR/KPS !\REF: GA !\COMMENT: FITTED WITH THERM ON 11_08_2016_20_43_11
1596 1.08178935E+01 1.53027604E-02-5.15746733E-06 7.92717531E-10-4.56680640E-14 2
1597 -1.14319965E+04-2.79700973E+01 2.58072848E-01 3.90347698E-02-2.51378459E-05 3
1598 8.26896578E-09-1.09178202E-12-7.68516846E+03 2.90500173E+01 4
1599 CH3COHCH3 C 3H 7O 1 G 300.00 4000.00 1388.00 1
1600 .115026438E+02 .149881248E-01-.510421075E-05 .789864272E-09-.457135659E-13 2
1601 -.164821894E+05-.347655748E+02 .118802517E+01 .410410262E-01-.314650841E-04 3
1602 .133514692E-07-.237788249E-11-.130177234E+05 .200655998E+02 4
1603 CH3CHCH2OH C 3H 7O 1 G 300.000 5000.000 1393.000 31
!\AUTHOR: CR/KPS !\REF: GA !\COMMENT: FITTED WITH THERM ON 11_08_2016_20_43_11
1604 1.04922579E+01 1.55907665E-02-5.25786983E-06 8.08382729E-10-4.65762492E-14 2
1605 -1.20531154E+04-2.64451618E+01 2.48398386E+00 3.14461742E-02-1.62613388E-05 3
1606 3.80532805E-09-2.66318786E-13-8.95721842E+03 1.76242658E+01 4
1607 NC3-QOOH C 3H 7O 2 G 300.00 4000.00 1374.00 1
1608 .146139980E+02 .143723015E-01-.488635144E-05 .756519620E-09-.438364992E-13 2
1609 -.646101457E+04-.457478245E+02 .191005011E+01 .411666833E-01-.251630217E-04 3

1610	.711856873E-08-.698838732E-12-.179305093E+04	.234514457E+02	4
1611	IC3-QOOH C 3H 70 2 G	300.00 4000.00 1399.00	1
1612	.155030898E+02 .139802008E-01-.481811216E-05	.751835399E-09-.437743118E-13	2
1613	-.741643030E+04-.523911482E+02-.184042862E+00	.564670638E-01-.501611253E-04	3
1614	.230526863E-07-.423866481E-11-.252333896E+04	.298354826E+02	4
1615	NC3H7O2 C 3H 70 2 G	300.00 4000.00 1388.00	1
1616	.127230991E+02 .167336808E-01-.575943184E-05	.897769493E-09-.522275065E-13	2
1617	-.108816595E+05-.381965321E+02 .156301709E+01	.426192697E-01-.296615075E-04	3
1618	.114187326E-07-.189894471E-11-.688086375E+04	.219842933E+02	4
1619	IC3H7O2 C 3H 70 2 G	300.00 4000.00 1392.00	1
1620	.132610651E+02 .162501084E-01-.558631798E-05	.870057473E-09-.505849469E-13	2
1621	-.131937089E+05-.421023499E+02 .103495454E+01	.469942369E-01-.366525520E-04	3
1622	.157084173E-07-.281956117E-11-.906344820E+04	.229566921E+02	4
1623	NC3-OOQOOH C 3H 70 4 G	300.00 4000.00 1388.00	1
1624	.185146106E+02 .164157074E-01-.573085844E-05	.901975314E-09-.528299084E-13	2
1625	-.231819444E+05-.618247164E+02 .254387733E+01	.570847379E-01-.472164204E-04	3
1626	.208289492E-07-.378162942E-11-.178600410E+05	.229447574E+02	4
1627	IC3-OOQOOH C 3H 70 4 G	300.00 4000.00 1391.00	1
1628	.191234208E+02 .158457151E-01-.552231946E-05	.868162288E-09-.508094203E-13	2
1629	-.255253957E+05-.661419362E+02 .175906535E+01	.624712381E-01-.554930416E-04	3
1630	.257973727E-07-.483190839E-11-.200009572E+05	.251348546E+02	4
1631	C4H3 C 4H 3 G	300.00 4000.00 1000.00	1
1632	.107527376E+02 .538115300E-02-.554963720E-06-	.305226590E-09 .576173970E-13	2
1633	.612141980E+05-.297302533E+02 .415388100E+01	.172628700E-01-.238937390E-06	3
1634	-.101870000E-07 .434050410E-11 .633807200E+05	.603650600E+01	4
1635	C4H3O C 4H 30 1 G	300.00 4000.00 1000.00	1
1636	.129455763E+02 .795235476E-02-.280679691E-05	.445205248E-09-.262240810E-13	2
1637	.175946397E+05-.478819894E+02-.584674088E+01	.620875882E-01-.630010605E-04	3
1638	.306882361E-07-.575456234E-11 .230253176E+05	.492940922E+02	4
1639	C4H5 C 4H 5 G	300.00 4000.00 1000.00	1
1640	.128659744E+02 .794336940E-02-.862646570E-06-	.465563500E-09 .895113110E-13	2
1641	.378355213E+05-.418250446E+02 .299524000E+01	.228845610E-01 .197547090E-05	3
1642	-.114824500E-07 .319782310E-11 .414221800E+05	.128945400E+02	4
1643	C4H71-4 C 4H 7 G	300.00 4000.00 1000.00	1
1644	.664945270E+01 .226232110E-01-.806420670E-05	.954149200E-09 .000000000E+00	2
1645	.206794519E+05-.786429084E+01 .283048200E+00	.386777000E-01-.210739710E-04	3
1646	.427582900E-08 .000000000E+00 .225247800E+05	.254564400E+02	4
1647	IC4H7 C 4H 7 G	300.00 4000.00 1000.00	1
1648	.616543300E+01 .257842760E-01-.936521250E-05	.112618500E-08 .000000000E+00	2
1649	.114713700E+05-.676561500E+01 .476952000E+01	.167724920E-01 .213011010E-04	3
1650	-.275874430E-07 .845501100E-11 .126384700E+05	.401309300E+01	4
1651	C4H71-3 C 4H 7 G	300.00 4000.00 1000.00	1
1652	.714879043E+01 .219663880E-01-.774471300E-05	.907477370E-09 .000000000E+00	2
1653	.124589843E+05-.117547735E+02-.442598200E+00	.422160100E-01-.254697900E-04	3
1654	.597432100E-08 .000000000E+00 .145672100E+05	.276086500E+02	4
1655	RALD4X C 4H 70 1 G	300.00 4000.00 1378.00	1
1656	.109543855E+02 .241148701E-01-.952821930E-05	.161222652E-08-.988398314E-13	2
1657	-.118963413E+05-.334390867E+02 .575601777E+01	.186084099E-01 .131646529E-04	3
1658	-.151687447E-07 .367436225E-11-.792068905E+04	.141446613E+01	4
1659	RIBALDB C 4H 70 1 G	300.00 4000.00 1000.00	1
1660	.355152000E+01 .294219200E-01-.104255000E-04	.171367900E-08-.107873000E-12	2
1661	.000000000E+00 .104367300E+02-.823550500E+00	.485680000E-01-.340648100E-04	3
1662	.109786600E-07-.495457100E-12 .000000000E+00	.303407900E+02	4
1663	RIBALDG C 4H 70 1 G	300.00 4000.00 1000.00	1
1664	.499900800E+01 .269364000E-01-.923615800E-05	.148292200E-08-.918125000E-13	2
1665	-.348819900E+04 .571944000E+01-.277712900E+01	.617368400E-01-.610123800E-04	3
1666	.338144900E-07-.767826900E-11-.241914600E+04	.416421800E+02	4
1667	RMP3 C 4H 70 2 G	300.00 4000.00 1376.00	1
1668	.154260382E+02 .169789201E-01-.593961909E-05	.936106835E-09-.548809672E-13	2
1669	-.343012110E+05-.525677530E+02 .406577480E+01	.388324925E-01-.208048750E-04	3
1670	.506251249E-08-.421741752E-12-.297848227E+05	.102796868E+02	4
1671	QA4X C 4H 70 3 G	300.00 4000.00 1000.00	1
1672	.778775690E+01 .301204420E-01-.104582260E-04	.169501670E-08-.105681860E-12	2
1673	-.162963980E+05 .404129030E+00 .111242760E+01	.661709530E-01-.649819340E-04	3
1674	.331132210E-07-.636964220E-11-.160735140E+05	.288202740E+02	4
1675	RIBALDGOO C 4H 70 3 G	300.00 4000.00 1000.00	1
1676	.688742900E+01 .315358900E-01-.111087400E-04	.181743800E-08-.113981500E-12	2
1677	-.209771000E+05 .101528900E+01-.131763500E+01	.654173000E-01-.523002100E-04	3
1678	.187106700E-07-.151244600E-11-.199258600E+05	.391267300E+02	4
1679	QIBALDB3 C 4H 70 3 G	300.00 4000.00 1000.00	1
1680	0.77877569E+01 0.30120442E-01-0.10458226E-04	0.16950167E-08-0.10568186E-12	2
1681	-0.16296398E+05 0.40412903E+00 0.11124276E+01	0.66170953E-01-0.64981934E-04	3
1682	0.33113221E-07-0.63696422E-11-0.16073514E+05	0.28820274E+02	4

1683	RIBALD	BOO	C	4H	70	3	G	300.00	4000.00	1000.00	1
1684	0.72319469E+01	0.32013219E-01	-0.11485144E-04	0.19037878E-08	-0.12050984E-12						2
1685	-0.22166488E+05	-0.72145844E+00	-0.23625577E-01	0.64917222E-01	-0.53189186E-04						3
1686	0.19445174E-07	-0.16272577E-11	-0.21545568E+05	0.31875837E+02							4
1687	QIBALD	G3	C	4H	70	3	G	300.00	4000.00	1000.00	1
1688	.815273500E+01	.289866500E-01	-.985444500E-05	.157305600E-08	-.970256900E-13						2
1689	-.143742500E+05	-.200325000E+01	-.862350600E+00	.706020100E-01	-.697863100E-04						3
1690	.360017200E-07	-.720299500E-11	-.133755300E+05	.389215900E+02							4
1691	QIBALD	G2	C	4H	70	3	G	300.00	4000.00	1000.00	1
1692	0.45559053E+01	0.35916157E-01	-0.13290762E-04	0.22510276E-08	-0.14461383E-12						2
1693	-0.18124246E+05	0.16529331E+02	0.15762151E+01	0.67029655E-01	-0.68767891E-04						3
1694	0.36980971E-07	-0.75502798E-11	-0.19410281E+05	0.24012136E+02							4
1695	RALD4	OOX	C	4H	70	3	G	300.00	4000.00	1000.00	1
1696	.723194690E+01	.320132190E-01	-.114851440E-04	.190378780E-08	-.120509840E-12						2
1697	-.221664880E+05	-.721458440E+00	-.236255770E-01	.649172220E-01	-.531891860E-04						3
1698	.194451740E-07	-.162725770E-11	-.215455680E+05	.318758370E+02							4
1699	ZIBALD	B3	C	4H	70	5	G	300.00	4000.00	1000.00	1
1700	.101088800E+02	.334733300E-01	-.116762600E-04	.189872800E-08	-.118662800E-12						2
1701	-.318892400E+05	-.778537800E+01	.612429000E+00	.741854800E-01	-.608675100E-04						3
1702	.207212300E-07	-.985714500E-12	-.308839900E+05	.356398800E+02							4
1703	ZIBALD	G2	C	4H	70	5	G	300.00	4000.00	1000.00	1
1704	0.67585382E+01	0.40589843E-01	-0.15337158E-04	0.26372311E-08	-0.17129352E-12						2
1705	-0.34054738E+05	0.10674515E+02	0.13726847E+01	0.78338057E-01	-0.69229740E-04						3
1706	0.25735014E-07	-0.17713571E-11	-0.35033230E+05	0.29777508E+02							4
1707	ZA4X		C	4H	70	5	G	300.00	4000.00	1000.00	1
1708	.675853820E+01	.405898430E-01	-.153371580E-04	.263723110E-08	-.171293520E-12						2
1709	-.340547380E+05	.106745150E+02	.137268470E+01	.783380570E-01	-.692297400E-04						3
1710	.257350140E-07	-.177135710E-11	-.350332300E+05	.297775080E+02							4
1711	ZIBALD	G3	C	4H	70	5	G	300.00	4000.00	1000.00	1
1712	.101088800E+02	.334733300E-01	-.116762600E-04	.189872800E-08	-.118662800E-12						2
1713	-.318892400E+05	-.778537800E+01	.612429000E+00	.741854800E-01	-.608675100E-04						3
1714	.207212300E-07	-.985714500E-12	-.308839900E+05	.356398800E+02							4
1715	PC4H9		C	4H	9		G	300.00	4000.00	1000.00	1
1716	.285927140E+01	.339093470E-01	-.129634890E-04	.162487360E-08	.000000000E+00						2
1717	.644131902E+04	.136765387E+02	.361027200E+00	.446560900E-01	-.269622400E-04						3
1718	.737512580E-08	.000000000E+00	.679487900E+04	.252696800E+02							4
1719	TC4H9		C	4H	9		G	300.00	4000.00	1000.00	1
1720	.678309830E+01	.275756420E-01	-.999251920E-05	.119923980E-08	.000000000E+00						2
1721	.130943964E+04	-.110379681E+02	-.668177200E+00	.478197410E-01	-.281268890E-04						3
1722	.654078610E-08	.000000000E+00	.334806900E+04	.274761900E+02							4
1723	SC4H9		C	4H	9		G	300.00	4000.00	1000.00	1
1724	.182440000E+01	.354350280E-01	-.136901980E-04	.172985780E-08	.000000000E+00						2
1725	.521137543E+04	.190721830E+02	.882678800E+00	.419813690E-01	-.239577090E-04						3
1726	.639274900E-08	.000000000E+00	.513670700E+04	.226104800E+02							4
1727	IC4H9		C	4H	9		G	300.00	4000.00	1000.00	1
1728	.672898190E+01	.277240280E-01	-.100574610E-04	.120817530E-08	.000000000E+00						2
1729	.390175463E+04	-.921990655E+01	-.514098700E+00	.469939600E-01	-.268680800E-04						3
1730	.599194290E-08	.000000000E+00	.591746700E+04	.283543100E+02							4
1731	CH3CH2	CHOHCH2	C	4H	90	1	G	300.00	4000.00	1390.00	1
1732	.147487308E+02	.193476286E-01	-.668165997E-05	.104395798E-08	-.608330722E-13						2
1733	-.178485397E+05	-.492109234E+02	.467890397E+00	.521732276E-01	-.362067190E-04						3
1734	.135025449E-07	-.213961182E-11	-.127480216E+05	.278224820E+02							4
1735	CH3CHCH2	CH3	C	4H	90	1	G	300.00	4000.00	1422.00	1
1736	.148239632E+02	.195938055E-01	-.674334212E-05	.105133556E-08	-.611769464E-13						2
1737	-.154937986E+05	-.535942326E+02	-.581327100E+00	.539666459E-01	-.358338761E-04						3
1738	.122179671E-07	-.171024843E-11	-.995421675E+04	.297619860E+02							4
1739	CH3CH2	COHCH3	C	4H	90	1	G	300.00	4000.00	1390.00	1
1740	.151619233E+02	.189741815E-01	-.654734215E-05	.102237774E-08	-.595503510E-13						2
1741	-.208549516E+05	-.532957109E+02	.108860217E+01	.524153990E-01	-.380997951E-04						3
1742	.151074363E-07	-.254404184E-11	-.159195374E+05	.222613243E+02							4
1743	CH2CHCH2	OHCH3	C	4H	90	1	G	300.00	4000.00	1422.00	1
1744	.140854789E+02	.197806925E-01	-.671026390E-05	.103599950E-08	-.598718336E-13						2
1745	-.165129917E+05	-.457671006E+02	-.566170728E-01	.523981203E-01	-.356379876E-04						3
1746	.128198684E-07	-.192264202E-11	-.115334457E+05	.303769293E+02							4
1747	CH3CH2	CHCH2OH	C	4H	90	1	OG	300.000	5000.000	1394.000	41
	!\AUTHOR: CR/KPS !\REF: GA !\COMMENT: FITTED WITH THERM ON 12_08_2016_14_12_47										
1748	+1.38348463E+01	+1.99255957E-02	-6.74388288E-06	+1.03943751E-09	-5.99954849E-14						2
1749	-1.62408295E+04	-4.28940661E+01	+2.16591909E+00	+4.43770980E-02	-2.54941588E-05						3
1750	+7.22842042E-09	-7.87011274E-13	-1.18784302E+04	+2.08188392E+01	+0.00000000E+00						4
1751	CH3CH	CHOHCH3	C	4H	90	1	G	300.00	4000.00	1387.00	1
1752	.142049192E+02	.195897318E-01	-.671801693E-05	.104483881E-08	-.606940644E-13						2
1753	-.190416934E+05	-.463876157E+02	.933300006E+00	.472805232E-01	-.278316313E-04						3
1754	.797039080E-08	-.870532264E-12	-.140666468E+05	.261224696E+02							4

1755 CH2CH2CHOHCH3 C 4H 90 1 G 300.00 4000.00 1390.00 1
1756 .147487308E+02 .193476286E-01-.668165997E-05 .104395798E-08-.608330722E-13 2
1757 -.178485397E+05-.492109234E+02 .467890397E+00 .521732276E-01-.362067190E-04 3
1758 .135025449E-07-.213961182E-11-.127480216E+05 .278224820E+02 4
1759 CH3CCH2OHCH3 C 4H 90 1 G 300.00 4000.00 1682.00 1
1760 .125605997E+02 .210637488E-01-.715019648E-05 .110439262E-08-.638428695E-13 2
1761 -.183183621E+05-.368996627E+02 .329612707E+01 .347649647E-01-.102505618E-04 3
1762 -.204641931E-08 .118879408E-11-.142607619E+05 .157499123E+02 4
1763 RTC4H8OH C 4H 90 2 G 300.00 4000.00 1395.00 1
1764 .146782533E+02 .193935063E-01-.660052048E-05 .102120044E-08-.590998119E-13 2
1765 -.199408575E+05-.505292168E+02-.836665970E-01 .558040633E-01-.420184309E-04 3
1766 .171111519E-07-.290735214E-11-.149499995E+05 .281627857E+02 4
1767 CH3CHCH3CHOH C 4H 90 1 G 300.00 4000.00 1673.00 1
1768 .145354872E+02 .193544788E-01-.655352544E-05 .101052180E-08-.583473661E-13 2
1769 -.195307842E+05-.500528678E+02 .524328525E+00 .528985884E-01-.379651080E-04 3
1770 .147054933E-07-.239054621E-11-.147012758E+05 .249822692E+02 4
1771 RTC4H9O C 4H 90 1 G 300.00 4000.00 1391.00 1
1772 .154820006E+02 .191120896E-01-.659337031E-05 .102954283E-08-.599712426E-13 2
1773 -.189474281E+05-.587209701E+02-.652960434E+00 .575360662E-01-.423660204E-04 3
1774 .165461682E-07-.269335532E-11-.133634774E+05 .277645681E+02 4
1775 CH3CH2CH2CHOH C 4H 90 1 OG 300.000 5000.000 1392.000 41
! \AUTHOR: CR/KPS ! \REF: GA ! \COMMENT: FITTED WITH THERM ON 12_08_2016_14_12_47
1776 +1.47813217E+01+1.89692972E-02-6.38671427E-06+9.81341181E-10-5.65332084E-14 2
1777 -1.88487062E+04-4.98892364E+01+7.72566993E-01+5.00429367E-02-3.20163534E-05 3
1778 +1.02913291E-08-1.30709217E-12-1.38421800E+04+2.58928300E+01+0.00000000E+00 4
1779 CH3CH2CH2CH2O C 4H 90 1 OG 300.000 5000.000 1382.000 41
! \AUTHOR: CR/KPS ! \REF: GA ! \COMMENT: FITTED WITH THERM ON 12_08_2016_14_12_47
1780 +1.52662649E+01+1.94024981E-02-6.71808947E-06+1.05163276E-09-6.13656485E-14 2
1781 -1.43012793E+04-5.43382882E+01+1.93228064E+00+4.47128724E-02-2.24881300E-05 3
1782 +4.12226630E-09+3.99342930E-14-9.07148053E+03+1.93703892E+01+0.00000000E+00 4
1783 CH3CHCH2CH2OH C 4H 90 1 OG 300.000 5000.000 1521.000 41
! \AUTHOR: CR/KPS ! \REF: GA ! \COMMENT: FITTED WITH THERM ON 12_08_2016_14_12_47
1784 +1.36682761E+01+1.97440068E-02-6.61586418E-06+1.01311840E-09-5.82212400E-14 2
1785 -1.70603748E+04-4.19313460E+01+9.12869135E-01+4.43138287E-02-2.14369517E-05 3
1786 +3.12967216E-09+3.57475931E-13-1.22046904E+04+2.82635095E+01+0.00000000E+00 4
1787 CH3CH2CHOCH3 C 4H 90 1 G 300.00 4000.00 1382.00 1
1788 .157118766E+02 .189436692E-01-.663728010E-05 .104718616E-08-.614402720E-13 2
1789 -.169625442E+05-.584079611E+02-.123566480E+00 .537328693E-01-.359804830E-04 3
1790 .125064763E-07-.182873667E-11-.111514942E+05 .275750096E+02 4
1791 CH2CH2CH2CH2OH C 4H 90 1 OG 300.000 5000.000 1401.000 41
! \AUTHOR: CR/KPS ! \REF: GA ! \COMMENT: FITTED WITH THERM ON 12_08_2016_14_12_47
1792 +1.41519859E+01+1.96439700E-02-6.64537615E-06+1.02402720E-09-5.91001981E-14 2
1793 -1.56141213E+04-4.43658958E+01-6.95634721E-02+5.20263179E-02-3.44849029E-05 3
1794 +1.17704221E-08-1.63047436E-12-1.06053581E+04+3.22854711E+01+0.00000000E+00 4
1795 IC4H9P-OO C 4H 90 2 G 300.00 4000.00 1391.00 1
1796 .160321835E+02 .211162441E-01-.726598082E-05 .113244436E-08-.658740064E-13 2
1797 -.161760498E+05-.559920048E+02 .591660961E+00 .579744782E-01-.422019324E-04 3
1798 .167841571E-07-.283252682E-11-.107815683E+05 .268393730E+02 4
1799 IC4H9T-OO C 4H 90 2 G 300.00 4000.00 1392.00 1
1800 .167547908E+02 .205266172E-01-.706765238E-05 .110199004E-08-.641203511E-13 2
1801 -.197490954E+05-.625129056E+02 .429458545E+00 .619305024E-01-.492178248E-04 3
1802 .213391061E-07-.385156685E-11-.142778206E+05 .242205126E+02 4
1803 NC4H9-OO C 4H 90 2 G 300.00 4000.00 1392.00 1
1804 .164199470E+02 .207668293E-01-.714061871E-05 .111233445E-08-.646799300E-13 2
1805 -.172909027E+05-.576444825E+02 .859225542E+00 .589774363E-01-.445935184E-04 3
1806 .184502497E-07-.321329944E-11-.119598721E+05 .254554544E+02 4
1807 NC4-QOOH C 4H 90 2 G 300.00 4000.00 1391.00 1
1808 .182943014E+02 .184250091E-01-.627217889E-05 .971379578E-09-.562825607E-13 2
1809 -.128564704E+05-.650917535E+02 .986162058E+00 .585630676E-01-.416710545E-04 3
1810 .151223447E-07-.222454695E-11-.684048054E+04 .279289603E+02 4
1811 IC4P-QOOH C 4H 90 2 G 300.00 4000.00 1396.00 1
1812 .181457399E+02 .188972595E-01-.650258715E-05 .101363925E-08-.589752496E-13 2
1813 -.103249571E+05-.654833345E+02-.253900783E+00 .658110437E-01-.535280232E-04 3
1814 .228723790E-07-.398637599E-11-.429699727E+04 .319918975E+02 4
1815 IC4T-QOOH C 4H 90 2 G 300.00 4000.00 1397.00 1
1816 .188631296E+02 .183239932E-01-.631233086E-05 .984688082E-09-.573186521E-13 2
1817 -.138981290E+05-.708829284E+02-.425033602E+00 .698121411E-01-.606175877E-04 3
1818 .274812344E-07-.501908797E-11-.779203954E+04 .305104370E+02 4
1819 QBU1OOX C 4H 90 3 G 300.00 4000.00 1386.00 1
1820 .129455763E+02 .795235476E-02-.280679691E-05 .445205248E-09-.262240810E-13 2
1821 .175946397E+05-.478819894E+02-.584674088E+01 .620875882E-01-.630010605E-04 3
1822 .306882361E-07-.575456234E-11 .230253176E+05 .492940922E+02 4
1823 RBU1OOX C 4H 90 3 G 300.00 4000.00 1392.00 1

1824	.179101133E+02	.211247449E-01-	.724787505E-05	.112742547E-08-	.654930094E-13	2				
1825	-.371878276E+05-	.612769774E+02	.289779336E+01	.560720331E-01-	.390996379E-04	3				
1826	.147174953E-07-	.234862827E-11-	.318812119E+05	.195265598E+02		4				
1827	IC4T-OOQOOH	C	4H	90	4	G	300.00	4000.00	1391.00	1
1828	.225796674E+02	.201772761E-01-	.702773819E-05	.110438266E-08-	.646157968E-13	2				
1829	-.320684788E+05-	.852469773E+02	.152317721E+01	.757827720E-01-	.656981278E-04	3				
1830	.300159936E-07-	.556277284E-11-	.252715176E+05	.257762885E+02		4				
1831	IC4P-OOQOOH	C	4H	90	4	G	300.00	4000.00	1390.00	1
1832	.218612263E+02	.207812365E-01-	.723484570E-05	.113659545E-08-	.664871920E-13	2				
1833	-.284979533E+05-	.798472350E+02	.156900216E+01	.724191880E-01-	.596183448E-04	3				
1834	.260680737E-07-	.468228506E-11-	.217597632E+05	.278260039E+02		4				
1835	NC4-OOQOOH	C	4H	90	4	G	300.00	4000.00	1393.00	1
1836	.231119306E+02	.196469811E-01-	.682730172E-05	.107124796E-08-	.626109519E-13	2				
1837	-.320261199E+05-	.872192509E+02	.109604492E+01	.794472856E-01-	.714221316E-04	3				
1838	.334124791E-07-	.626730135E-11-	.251118713E+05	.282288973E+02		4				
1839	ZBU10OX	C	4H	90	5	G	300.00	4000.00	1397.00	1
1840	.236719411E+02	.205751255E-01-	.708127339E-05	.110392970E-08-	.642301320E-13	2				
1841	-.515463449E+05-	.860806755E+02	.475209184E+01	.678608013E-01-	.534336966E-04	3				
1842	.221852722E-07-	.378003417E-11-	.452511232E+05	.144907043E+02		4				
1843	C5H5	C	5H	50	1	G	300.00	4000.00	1000.00	1
1844	.421464919E+01	.271834728E-01-	.133173209E-04	.308980119E-08-	.277879873E-12	2				
1845	.288952416E+05-	.305999781E-01-	.737844042E+01	.972391818E-01-	.169579138E-03	3				
1846	.151818667E-06-	.512075479E-10	.305514662E+05	.512829539E+02		4				
1847	C5H5O	C	5H	50	1	G	300.00	4000.00	1395.00	1
1848	.149072105E+02	.136369619E-01-	.470762207E-05	.736028654E-09-	.429314124E-13	2				
1849	.143724130E+05-	.569296345E+02-	.414628450E+01	.623584874E-01-	.528374678E-04	3				
1850	.224628793E-07-	.380136191E-11	.204992627E+05	.437921058E+02		4				
1851	C5H7	C	5H	7		G	300.00	4000.00	1000.00	1
1852	.671323690E+01	.274278890E-01-	.994311090E-05	.119373240E-08	.000000000E+00	2				
1853	.235116384E+05-	.112735252E+02	.759315300E+00	.432678800E-01-	.237613290E-04	3				
1854	.512588110E-08	.000000000E+00	.251686000E+05	.196131100E+02		4				
1855	RMCROTA	C	5H	70	2	G	300.00	4000.00	1000.00	1
1856	.151681730E+02	.178142000E-01-	.496258460E-05	.688767770E-09-	.386765100E-13	2				
1857	-.320532540E+05-	.462913590E+02-	.242828070E+00	.630479530E-01-	.556979940E-04	3				
1858	.265678430E-07-	.501508770E-11-	.278218120E+05	.329157640E+02		4				
1859	NC5H9-3	C	5H	9		G	300.00	4000.00	1383.00	1
1860	.140838604E+02	.208584950E-01-	.722620456E-05	.113154433E-08-	.660424465E-13	2				
1861	.542225436E+04-	.515371079E+02-	.697079542E+00	.514354766E-01-	.304500502E-04	3				
1862	.880925852E-08-	.994458078E-12	.110172568E+05	.293601364E+02		4				
1863	ERC4H8CHO	C	5H	90	1	G	300.00	4000.00	1517.00	1
1864	.190577032E+02	.197405268E-01-	.706907553E-05	.113169306E-08-	.670771090E-13	2				
1865	-.128899482E+05-	.729817022E+02	.467212037E+01	.343554368E-01	.295219352E-05	3				
1866	-.145463894E-07	.444316435E-11-	.603466621E+04	.109564879E+02		4				
1867	C5EN-QOOH	C	5H	90	2	G	300.00	4000.00	1392.00	1
1868	.203810644E+02	.199415880E-01-	.695158032E-05	.109308002E-08-	.639829228E-13	2				
1869	-.198146484E+02-	.759778447E+02	.111814871E+01	.671698903E-01-	.526574214E-04	3				
1870	.218036776E-07-	.373297383E-11	.652627032E+04	.268196384E+02		4				
1871	C5EN-OO	C	5H	90	2	G	300.00	4000.00	1392.00	1
1872	.186695690E+02	.216228347E-01-	.748565666E-05	.117148772E-08-	.683420517E-13	2				
1873	-.458976288E+04-	.678082548E+02	.338814185E+00	.676913346E-01-	.538434525E-04	3				
1874	.231725654E-07-	.414643363E-11	.158489053E+04	.297116190E+02		4				
1875	RMBX	C	5H	90	2	G	300.00	4000.00	1382.00	1
1876	.193382201E+02	.209401493E-01-	.732209753E-05	.115371679E-08-	.676297088E-13	2				
1877	-.412852468E+05-	.755834444E+02	.231680806E+01	.569247905E-01-	.356059275E-04	3				
1878	.110212330E-07-	.136558032E-11-	.349304634E+05	.172843303E+02		4				
1879	RMBOOX	C	5H	90	4	G	300.00	4000.00	1000.00	1
1880	.211938570E+02	.222144000E-01-	.631327380E-05	.888168590E-09-	.502931100E-13	2				
1881	-.572489530E+05-	.734085620E+02	.256566330E+01	.606897660E-01-	.678613150E-05	3				
1882	-.390168040E-07	.205529000E-10-	.518452190E+05	.251823650E+02		4				
1883	C5EN-OOQOOH-35	C	5H	90	4	G	300.00	4000.00	1000.00	1
1884	.251889054E+02	.206642290E-01-	.723193822E-05	.114017997E-08-	.668636462E-13	2				
1885	-.189404232E+05-	.976775550E+02	.705279661E+00	.861579519E-01-	.769448689E-04	3				
1886	.356373390E-07-	.663192053E-11-	.111524362E+05	.310665731E+02		4				
1887	QMBOOX	C	5H	90	4	G	300.00	4000.00	1000.00	1
1888	.211938570E+02	.222144000E-01-	.631327380E-05	.888168590E-09-	.502931100E-13	2				
1889	-.572489530E+05-	.734085620E+02	.256566330E+01	.606897660E-01-	.678613150E-05	3				
1890	-.390168040E-07	.205529000E-10-	.518452190E+05	.251823650E+02		4				
1891	ZMBOOX	C	5H	90	6	G	300.00	4000.00	1000.00	1
1892	.261471200E+02	.215283560E-01-	.581135510E-05	.785452200E-09-	.431572980E-13	2				
1893	-.689643590E+05-	.913329620E+02	.443715430E+01	.699071290E-01-	.165602940E-04	3				
1894	-.356586160E-07	.205531550E-10-	.628690510E+05	.226288070E+02		4				
1895	NC5H11	C	5H	11		G	300.00	4000.00	1384.00	1
1896	.131340658E+02	.260923466E-01-	.897731137E-05	.139920325E-08-	.813970860E-13	2				

1897	-.427735231E+04-.434455998E+02-.304386354E+01	.581995422E-01-.316090839E-04	3
1898	.790004927E-08-.665198232E-12 .199185425E+04	.455946950E+02	4
1899	IC5H11 C 5H 11 G	300.00 4000.00 1389.00	1
1900	.153818750E+02 .241141042E-01-.827847584E-05	.128831856E-08-.748649188E-13	2
1901	-.184296128E+04-.564907641E+02-.592409395E+00	.586734947E-01-.365981110E-04	3
1902	.118412541E-07-.159845819E-11 .405970723E+04	.304115490E+02	4
1903	NEOC5H11 C 5H 11 G	300.00 4000.00 1396.00	1
1904	.166235914E+02 .227037884E-01-.771624835E-05	.119289853E-08-.690060600E-13	2
1905	-.396429146E+04-.644693953E+02-.158140132E+01	.657175067E-01-.468120314E-04	3
1906	.174732793E-07-.268709925E-11 .230933742E+04	.331296742E+02	4
1907	RIPENTOHB C 5H 110 1 G	300.00 4000.00 1374.00	1
1908	.178146436E+02 .231777549E-01-.776038398E-05	.118900766E-08-.683934164E-13	2
1909	-.225247765E+05-.648614694E+02 .204135308E+00	.588299650E-01-.324898705E-04	3
1910	.750026128E-08-.365893927E-12-.159312048E+05	.315479677E+02	4
1911	RIPENTOHA C 5H 110 1 G	300.00 4000.00 1394.00	1
1912	.176264597E+02 .239817014E-01-.815640882E-05	.126137771E-08-.729792490E-13	2
1913	-.238094100E+05-.651182426E+02 .287733983E+00	.650700888E-01-.461663158E-04	3
1914	.176228098E-07-.282635934E-11-.177872581E+05	.278924962E+02	4
1915	RPENT1O C 5H 110 1 G	300.00 5000.00 1396.00	1
1916	1!\AUTHOR: CR/KPS !\REF: GA !\COMMENT: FITTED WITH THERM ON 11_08_2016_20_43_11		
1917	+1.87118024E+01+2.36054696E-02-8.05610528E-06+1.24900841E-09-7.23989034E-14		2
1918	-1.84133036E+04-7.11769229E+01+1.61443159E+00+5.84449099E-02-3.26027513E-05		3
1919	+7.76525028E-09-4.48739932E-13-1.20210227E+04+2.23620686E+01		4
1919	RPENT1OHB C 5H 110 1 G	300.00 5000.00 1394.00	1
1920	1!\AUTHOR: CR/KPS !\REF: GA !\COMMENT: FITTED WITH THERM ON 11_08_2016_20_43_11		
1921	+1.71780951E+01+2.42601001E-02-8.22986526E-06+1.27049816E-09-7.34155598E-14		2
1922	-2.04290445E+04-5.93472290E+01+1.84753679E+00+5.73086840E-02-3.47271444E-05		3
1923	+1.06516139E-08-1.30777652E-12-1.47995754E+04+2.40150308E+01		4
1923	RPENT1OHE C 5H 110 1 G	300.00 5000.00 1400.00	1
1924	1!\AUTHOR: CR/KPS !\REF: GA !\COMMENT: FITTED WITH THERM ON 11_08_2016_20_43_11		
1925	+1.74868543E+01+2.39842944E-02-8.13298324E-06+1.25529418E-09-7.25301446E-14		2
1926	-1.97969015E+04-6.07667197E+01-3.94307020E-01+6.50012333E-02-4.38043364E-05		3
1927	+1.52539819E-08-2.16516288E-12-1.35258816E+04+3.55083245E+01		4
1927	RPENT1OHD C 5H 110 1 G	300.00 5000.00 2022.00	1
1928	1!\AUTHOR: CR/KPS !\REF: GA !\COMMENT: FITTED WITH THERM ON 11_08_2016_20_43_11		
1929	1.65897836E+01 2.53826913E-02-9.43220215E-06 1.55249347E-09-9.39190299E-14		2
1930	-2.10435752E+04-5.62532844E+01 3.69891615E-01 5.63524034E-02-2.76588983E-05		3
1931	4.35237097E-09 2.03539591E-13-1.50416080E+04 3.28904903E+01		4
1931	RIPENTO C 5H 110 1 G	300.00 4000.00 1390.00	1
1932	.179852494E+02 .240897408E-01-.828641852E-05	.129144549E-08-.751291843E-13	2
1933	-.197891737E+05-.690290731E+02-.769895465E+00	.660085470E-01-.438697957E-04	3
1934	.150115512E-07-.211319317E-11-.130499892E+05	.324309009E+02	4
1935	RPENT1OHA C 5H 110 1 G	300.00 5000.00 1394.00	1
1936	1!\AUTHOR: CR/KPS !\REF: GA !\COMMENT: FITTED WITH THERM ON 11_08_2016_20_43_11		
1937	+1.80953018E+01+2.33361161E-02-7.88463541E-06+1.21428332E-09-7.00616136E-14		2
1938	-2.30206675E+04-6.61675776E+01+4.26049539E-01+6.31258286E-02-4.15122762E-05		3
1939	+1.38895665E-08-1.86732010E-12-1.67596661E+04+2.92144308E+01		4
1939	RIPENTOHD C 5H 110 1 G	300.00 4000.00 1394.00	1
1940	.172306012E+02 .242975217E-01-.826186089E-05	.127755536E-08-.739123165E-13	2
1941	-.208013525E+05-.618034685E+02-.237764707E+00	.644135904E-01-.436552710E-04	3
1942	.156133960E-07-.232736806E-11-.146304196E+05	.323161057E+02	4
1943	RPENT1OHC C 5H 110 1 G	300.00 5000.00 1042.00	1
1944	1!\AUTHOR: CR/KPS !\REF: GA !\COMMENT: FITTED WITH THERM ON 11_08_2016_20_43_11		
1945	+1.68143234E+01+2.44876194E-02-8.29372543E-06+1.27921101E-09-7.38804613E-14		2
1946	-2.12567818E+04-5.74573295E+01+5.41167712E-01+5.66862244E-02-2.94678472E-05		3
1947	+5.84904634E-09-3.31866470E-14-1.50943752E+04+3.18827465E+01		4
1947	RIPENTOHC C 5H 110 1 G	300.00 4000.00 1381.00	1
1948	.157053942E+02 .255921700E-01-.870811298E-05	.134716260E-08-.779628294E-13	2
1949	-.226082350E+05-.522449991E+02 .309642922E+01	.468661615E-01-.183869508E-04	3
1950	.820832987E-09 .767460794E-12-.173551008E+05	.184684107E+02	4
1951	RMTBE C 5H 110 1 G	300.00 4000.00 1386.00	1
1952	.191923401E+02 .226496418E-01-.770522799E-05	.119249279E-08-.690514122E-13	2
1953	-.223486482E+05-.717004889E+02-.284403552E+00	.706092470E-01-.543641242E-04	3
1954	.224557925E-07-.385680161E-11-.157511970E+05	.321647207E+02	4
1955	NEOC5H11-OO C 5H 110 2 G	300.00 4000.00 1396.00	1
1956	.202154849E+02 .245786365E-01-.841704919E-05	.130775217E-08-.759095109E-13	2
1957	-.224777899E+05-.796085899E+02 .730403748E+00	.705036948E-01-.502866599E-04	3
1958	.189083885E-07-.294948183E-11-.157211898E+05	.249439750E+02	4
1959	NEOC5-QOOH C 5H 110 2 G	300.00 4000.00 1396.00	1
1960	.218550366E+02 .228989820E-01-.786956915E-05	.122572909E-08-.712760383E-13	2
1961	-.164801773E+05-.857429310E+02 .115441893E+01	.724266160E-01-.535668095E-04	3
1962	.205704339E-07-.323425526E-11-.941504872E+04	.250054329E+02	4
1963	NC5-QOOH C 5H 110 2 G	300.00 4000.00 1396.00	1

1964	.220245928E+02	.228314385E-01-	.786198359E-05	.122609365E-08-	.713571493E-13	2
1965	-.179960313E+05-	.864387261E+02-	.607426660E+00	.818016374E-01-	.685494236E-04	3
1966	.302071532E-07-	.540750321E-11-	.106868081E+05	.330450153E+02		4
1967	NC5H1200	C	5H 110 2	G	300.00 4000.00 1392.00	1
1968	.199150940E+02	.250390538E-01-	.861981469E-05	.134386616E-08-	.781893344E-13	2
1969	-.238472344E+05-	.769667628E+02	.235935841E+00	.739755736E-01-	.572379508E-04	3
1970	.241234657E-07-	.425357119E-11-	.171710700E+05	.279024996E+02		4
1971	RPENT100X	C	5H 110 3	G	300.00 4000.00 1394.00	1
1972	.235310388E+02	.257989924E-01-	.888660144E-05	.138620388E-08-	.806892959E-13	2
1973	-.591984578E+05-	.904223960E+02	.177546391E+01	.768095280E-01-	.550828141E-04	3
1974	.206638345E-07-	.320646569E-11-	.516288295E+05	.264068764E+02		4
1975	QIPENTOXX	C	5H 110 3	G	300.00 4000.00 1393.00	1
1976	.229723533E+02	.230366475E-01-	.771154566E-05	.118147984E-08-	.679624947E-13	2
1977	-.349052726E+05-	.847531774E+02	.275419521E+01	.666225847E-01-	.414002404E-04	3
1978	.119392262E-07-	.118354877E-11-	.276318447E+05	.249380687E+02		4
1979	RIPENTOXX	C	5H 110 3	G	300.00 4000.00 1394.00	1
1980	.229563234E+02	.264776592E-01-	.906923239E-05	.140937564E-08-	.818234063E-13	2
1981	-.583968852E+05-	.878789834E+02	.176378684E+01	.755411075E-01-	.526303110E-04	3
1982	.191090062E-07-	.286212429E-11-	.509737373E+05	.261265484E+02		4
1983	MTBE-OO	C	5H 110 3	G	300.00 4000.00 1386.00	1
1984	.219476262E+02	.253064866E-01-	.877948807E-05	.137597948E-08-	.803553517E-13	2
1985	-.383949561E+05-	.811182382E+02	.226233362E+01	.712292692E-01-	.511734982E-04	3
1986	.199100134E-07-	.329751069E-11-	.314029562E+05	.248780910E+02		4
1987	QPENT100X	C	5H 110 3	G	300.00 4000.00 1393.00	1
1988	.246066807E+02	.226714906E-01-	.788343040E-05	.123763348E-08-	.723672450E-13	2
1989	-.382649798E+05-	.958452159E+02	.148247361E+01	.786233062E-01-	.604614335E-04	3
1990	.240553703E-07-	.391498689E-11-	.304133501E+05	.276855455E+02		4
1991	MTBE-QOOH	C	5H 110 3	G	300.00 4000.00 1401.00	1
1992	.214971173E+02	.259064341E-01-	.848605930E-05	.127921441E-08-	.726936886E-13	2
1993	-.312441531E+05-	.765479844E+02	.134883146E+01	.795292274E-01-	.643595941E-04	3
1994	.280404405E-07-	.497823206E-11-	.249060790E+05	.293286141E+02		4
1995	NEOC5-OOQOOH	C	5H 110 4	G	300.00 4000.00 1392.00	1
1996	.248490803E+02	.252599638E-01-	.873651764E-05	.136662251E-08-	.797082603E-13	2
1997	-.350133010E+05-	.961825156E+02	.265748524E+01	.758789336E-01-	.526594216E-04	3
1998	.186692316E-07-	.269820831E-11-	.271776626E+05	.234450387E+02		4
1999	NC5-OOQOOH	C	5H 110 4	G	300.00 4000.00 1391.00	1
2000	.257270270E+02	.247172056E-01-	.859292907E-05	.134865114E-08-	.788382618E-13	2
2001	-.361631686E+05-	.100728579E+03	.135798731E+01	.877212925E-01-	.735867140E-04	3
2002	.327395450E-07-	.595540146E-11-	.281695250E+05	.282261555E+02		4
2003	ZIPENTOXX	C	5H 110 5	G	300.00 4000.00 1400.00	1
2004	.258845592E+02	.261151092E-01-	.903875069E-05	.141449719E-08-	.825222954E-13	2
2005	-.550208255E+05-	.962071206E+02	.391413178E+01	.765170930E-01-	.535251760E-04	3
2006	.194861484E-07-	.294077918E-11-	.472474207E+05	.222011325E+02		4
2007	MTBE-OOQOOH	C	5H 110 5	G	300.00 4000.00 1391.00	1
2008	.264681284E+02	.261757287E-01-	.899393547E-05	.140058534E-08-	.814301239E-13	2
2009	-.504985383E+05-	.992053288E+02	.454595241E+01	.801871705E-01-	.616423289E-04	3
2010	.254521416E-07-	.437448229E-11-	.430642384E+05	.177072264E+02		4
2011	ZPENT100X	C	5H 110 5	G	300.00 4000.00 1400.00	1
2012	.286303066E+02	.232317088E-01-	.801616025E-05	.125197153E-08-	.729415409E-13	2
2013	-.577713687E+05-	.109745016E+03	.345682525E+01	.876757175E-01-	.724014952E-04	3
2014	.308846552E-07-	.532198779E-11-	.496056070E+05	.234305819E+02		4
2015	C6H3	C	6H 3	G	300.00 4000.00 1000.00	1
2016	.120132339E+02	.114461128E-01-	.408884040E-05	.657753914E-09-	.392832116E-13	2
2017	.825892145E+05-	.335118700E+02	.150089155E+01	.545901804E-01-	.788221454E-04	3
2018	.627969099E-07-	.200768594E-10	.849133510E+05	.176237455E+02		4
2019	!C6H5	C	6H 5	G	300.00 4000.00 1000.00	1
	!polimi					
2020	!.157758892E+02	.965110900E-02-	.942941600E-06-	.546911100E-09	.102652200E-12	2
2021	!.330269797E+05-	.617628096E+02	.114355700E+00	.362732400E-01	.115828600E-05	3
2022	!-.219696400E-07	.846355600E-11	.383605400E+05	.238011700E+02		4
2023	!C6H5 phenyl radi	T07/10C	6.H 5. 0. 0.G	200.000 6000.000	B 77.10390	1
2024	C6H5	C	6H 5	G	300.00 4000.00 1000.00	1
	!Burcat kik					
2025	1.09540673E+01	1.82072569E-02-	6.63331157E-06	1.08125690E-09-	6.51736617E-14	2
2026	3.51098413E+04-	3.64320659E+01	4.91024498E-01	1.72669813E-02	7.02556406E-05	3
2027	-1.13389805E-07	4.89202543E-11	3.92340510E+04	2.42505364E+01	4.05676342E+04	4
2028	LC6H5	C	6H 5	G	300.00 4000.00 1000.00	1
2029	.134117680E+02	.147202210E-01-	.508177050E-05	.798863540E-09-	.469508440E-13	2
2030	.585037160E+05-	.416520320E+02	.779297070E+00	.543721260E-01-	.478738140E-04	3
2031	.161871640E-07	.337357440E-12	.616503120E+05	.221285920E+02		4
2032	C6H5O	C	6H 5O 1	G	300.00 4000.00 1000.00	1
2033	.137221720E+02	.174688771E-01-	.635504520E-05	.103492308E-08-	.623410504E-13	2
2034	.287274751E+03-	.488181680E+02-	.466204455E+00	.413443975E-01	.132412991E-04	3

2035	-.572872769E-07	.289763707E-10	.477858391E+04	.276990274E+02						4
2036	DMF-3YL	C	6H	70	1	G	300.00	4000.00	1000.00	1
2037	.118002735E+02	.257930235E-01-	.101089409E-04	.181299326E-08-	.122176870E-12					2
2038	.130508362E+05-	.352008048E+02	.197118616E+01	.384836786E-01	.786460722E-05					3
2039	-.354301012E-07	.162325679E-10	.165648455E+05	.193223377E+02						4
2040	CYC6H9	C	6H	9		G	300.00	4000.00	1381.00	1
2041	.166730638E+02	.227088190E-01-	.801509353E-05	.127088484E-08-	.748275111E-13					2
2042	.698387216E+04-	.723601536E+02-	.631908086E+01	.726795534E-01-	.484456826E-04					3
2043	.157628084E-07-	.202092558E-11	.153574632E+05	.524769640E+02						4
2044	RC6H9A	C	6H	9		G	300.00	4000.00	1400.00	1
2045	.170842767E+02	.208842788E-01-	.714529004E-05	.110943563E-08-	.643676989E-13					2
2046	.201040204E+05-	.639326012E+02-	.266715213E+01	.726196475E-01-	.605323920E-04					3
2047	.266000571E-07-	.474613408E-11	.264415017E+05	.402220332E+02						4
2048	RALDEST	C	6H	90	3	G	300.00	4000.00	1373.00	1
2049	.215153215E+02	.236419666E-01-	.830694270E-05	.131026314E-08-	.767602984E-13					2
2050	-.530993462E+05-	.770487448E+02	.687062608E+01	.492844450E-01-	.217786396E-04					3
2051	.243527207E-08	.464021620E-12-	.470662293E+05	.479532953E+01						4
2052	CYC6H11	C	6H	11		G	300.00	4000.00	1674.00	1
2053	.146799252E+02	.309324453E-01-	.112934485E-04	.183887582E-08-	.110464203E-12					2
2054	-.197594614E+03-	.590168221E+02-	.757310296E+01	.766896480E-01-	.424441426E-04					3
2055	.941423236E-08-	.439999709E-12	.764576045E+04	.620172120E+02						4
2056	CYC6-QOOH-4	C	6H	110	2	G	300.00	4000.00	1374.00	1
2057	.241250295E+02	.262273012E-01-	.925328534E-05	.146724451E-08-	.864028312E-13					2
2058	-.163808524E+05-	.106267870E+03-	.596804450E+01	.893075551E-01-	.558813589E-04					3
2059	.152003723E-07-	.125762311E-11-	.534935832E+04	.576800888E+02						4
2060	CYC6-OO	C	6H	110	2	G	300.00	4000.00	1380.00	1
2061	.225527144E+02	.280656231E-01-	.990087442E-05	.156942170E-08-	.923867180E-13					2
2062	-.209455781E+05-	.994788807E+02-	.594021024E+01	.887171975E-01-	.569424328E-04					3
2063	.171601250E-07-	.191055830E-11-	.104841379E+05	.556048484E+02						4
2064	CYC6-QOOH-2	C	6H	110	2	G	300.00	4000.00	1375.00	1
2065	.243899542E+02	.262326944E-01-	.930434909E-05	.148019558E-08-	.873538395E-13					2
2066	-.163135893E+05-	.107549099E+03-	.378907832E+01	.841562901E-01-	.510965662E-04					3
2067	.133666762E-07-	.102528616E-11-	.580881865E+04	.464783226E+02						4
2068	CYC6-QOOH-3	C	6H	110	2	G	300.00	4000.00	1374.00	1
2069	.241250295E+02	.262273012E-01-	.925328534E-05	.146724451E-08-	.864028312E-13					2
2070	-.163808524E+05-	.106267870E+03-	.596804450E+01	.893075551E-01-	.558813589E-04					3
2071	.152003723E-07-	.125762311E-11-	.534935832E+04	.576800888E+02						4
2072	CYC6-OOQOOH-4	C	6H	110	4	G	300.00	4000.00	1383.00	1
2073	.291238921E+02	.270060308E-01-	.959994599E-05	.152947435E-08-	.903544360E-13					2
2074	-.353659440E+05-	.128893429E+03-	.534585270E+01	.106448443E+00-	.790742157E-04					3
2075	.290275771E-07-	.426034434E-11-	.233396667E+05	.565320100E+02						4
2076	CYC6-OOQOOH-3	C	6H	110	4	G	300.00	4000.00	1383.00	1
2077	.291238921E+02	.270060308E-01-	.959994599E-05	.152947435E-08-	.903544360E-13					2
2078	-.353659440E+05-	.128198915E+03-	.534585270E+01	.106448443E+00-	.790742157E-04					3
2079	.290275771E-07-	.426034434E-11-	.233396667E+05	.572265244E+02						4
2080	CYC6-OOQOOH-2	C	6H	110	4	G	300.00	4000.00	1383.00	1
2081	.291238921E+02	.270060308E-01-	.959994599E-05	.152947435E-08-	.903544360E-13					2
2082	-.353659440E+05-	.128198915E+03-	.534585270E+01	.106448443E+00-	.790742157E-04					3
2083	.290275771E-07-	.426034434E-11-	.233396667E+05	.572265244E+02						4
2084	RDIPe	C	6H	130	1	G	300.00	4000.00	1389.00	1
2085	.195346832E+02	.300586517E-01-	.103564671E-04	.161544621E-08-	.940217507E-13					2
2086	-.289625035E+05-	.700231442E+02-	.545711430E-01	.748436725E-01-	.509801332E-04					3
2087	.191769721E-07-	.313046382E-11-	.218696353E+05	.358513387E+02						4
2088	!C7H7	C	7H	7		G	300.00	4000.00	1000.00	1 !
	Polimi									
2089	!.126890424E+02	.248754040E-01-	.820402330E-05	.901804910E-09	.000000000E+00					2
2090	!.179417186E+05-	.454264236E+02-	.296228400E+01	.659171040E-01-	.433334430E-04					3
2091	!.106408510E-07	.000000000E+00	.223472400E+05	.359657700E+02						4
2092	C7H7 Benzyl rad	T08/90C	7H	7	0	OG	200.000	6000.000	1000.	1 !
	Burcat kik									
2093	0.14043980E+02	0.23493873E-01-	0.85375367E-05	0.13890841E-08-	0.83614420E-13					2
2094	0.18564203E+05-	0.51665589E+02	0.48111540E+00	0.38512832E-01	0.32861492E-04					3
2095	-0.76972721E-07	0.35423068E-10	0.23307027E+05	0.23548820E+02	0.25317186E+05					4
2096	!CH3C6H4	C	7H	7		G	300.00	4000.00	1000.00	1
	POLIMI									
2097	!.989521100E+01	.281997140E-01-	.985390310E-05	.114532240E-08	.000000000E+00					2
2098	!.307512908E+05-	.257557742E+02-	.298827000E+01	.621039310E-01-	.390118950E-04					3
2099	!.928257830E-08	.000000000E+00	.343676800E+05	.412025200E+02						4
2100	CH3C6H4 o-Tolu RadT10/13C	7.H	7.	0.	0.G	200.000	6000.000	1000.		1 !
	Burcat kik 1706									
2101	1.28543060E+01	2.42712778E-02-	8.75277064E-06	1.41703290E-09-	8.50082345E-14					2
2102	3.10872386E+04-	4.29177096E+01	2.43474215E+00	2.10368651E-02	7.20305506E-05					3
2103	-1.14038924E-07	4.82416036E-11	3.53949018E+04	1.83045052E+01	3.74896416E+04					4

2104 !
 2105 !CH3C6H4 C 7H 7 0 OG 300.000 5000.000 1393.000
 11 !Zhang
 2106 ! 1.50088040E+01 2.08076711E-02-7.18274868E-06 1.12201995E-09-6.53756838E-14 2
 2107 ! 2.89360689E+04-5.63866198E+01-2.51731357E+00 6.18263711E-02-4.43238513E-05 3
 2108 ! 1.66517959E-08-2.59379321E-12 3.50509401E+04 3.77723973E+01 4
 2109 !
 2110 RCRESOLO C 7H 7O 1 G 300.00 4000.00 1000.00 1
 2111 .632623400E+01 .370920700E-01-.137369600E-04 .232847100E-08-.149701800E-12 2
 2112 -.156635900E+04-.468621100E+01-.403964400E+01 .739909500E-01-.515945300E-04 3
 2113 .120372800E-07 .143210200E-11 .225707600E+03 .453169300E+02 4
 2114 RCRESOLC C 7H 7O 1 G 300.00 4000.00 1000.00 1
 2115 .689970000E+01 .376640500E-01-.142499000E-04 .245139600E-08-.159215300E-12 2
 2116 -.104378100E+04-.796692700E+01-.415304900E+01 .776998800E-01-.583028700E-04 3
 2117 .178677900E-07-.536299700E-12 .896696700E+03 .453288900E+02 4
 2118 RMCYC6 C 7H 13 G 300.00 4000.00 2030.00 1
 2119 .173202469E+02 .361144629E-01-.130438584E-04 .210911191E-08-.126098895E-12 2
 2120 -.514813032E+04-.717714814E+02-.853970231E+01 .919151844E-01-.546389770E-04 3
 2121 .144889205E-07-.127842414E-11 .374687760E+04 .679730355E+02 4
 2122 NC7H13 C 7H 13 G 300.00 4000.00 1383.00 1
 2123 .140838604E+02 .208584950E-01-.722620456E-05 .113154433E-08-.660424465E-13 2
 2124 .542225436E+04-.515371079E+02-.697079542E+00 .514354766E-01-.304500502E-04 3
 2125 .880925852E-08-.994458078E-12 .110172568E+05 .293601364E+02 4
 2126 MCYC6-QOOH C 7H 13O 2 G 300.00 4000.00 2055.00 1
 2127 .234331685E+02 .347621964E-01-.124048044E-04 .199225952E-08-.118633947E-12 2
 2128 -.195868561E+05-.990888361E+02-.694095755E+01 .104651350E+00-.698281467E-04 3
 2129 .219897276E-07-.260222584E-11-.958151058E+04 .634587763E+02 4
 2130 RMCYC6-OO C 7H 13O 2 G 300.00 4000.00 1386.00 1
 2131 .252650839E+02 .325458915E-01-.113494502E-04 .178540172E-08-.104551384E-12 2
 2132 -.262255150E+05-.112686720E+03-.606776148E+01 .998265984E-01-.637962761E-04 3
 2133 .191011484E-07-.207496071E-11-.148337709E+05 .575547331E+02 4
 2134 MCYC6T-QOOH C 7H 13O 2 G 300.00 4000.00 2055.00 1
 2135 .234331685E+02 .347621964E-01-.124048044E-04 .199225952E-08-.118633947E-12 2
 2136 -.195868561E+05-.990888361E+02-.694095755E+01 .104651350E+00-.698281467E-04 3
 2137 .219897276E-07-.260222584E-11-.958151058E+04 .634587763E+02 4
 2138 MCYC6-OOQOOH C 7H 13O 4 G 300.00 4000.00 1394.00 1
 2139 .305321225E+02 .326136355E-01-.113442944E-04 .178165385E-08-.104214977E-12 2
 2140 -.403458401E+05-.135302325E+03-.434829022E+01 .112403701E+00-.796910207E-04 3
 2141 .277878216E-07-.380650779E-11-.281870009E+05 .524217373E+02 4
 2142 MCYC6T-OOQOOH C 7H 13O 4 G 300.00 4000.00 1394.00 1
 2143 .305321225E+02 .326136355E-01-.113442944E-04 .178165385E-08-.104214977E-12 2
 2144 -.403458401E+05-.135302325E+03-.434829022E+01 .112403701E+00-.796910207E-04 3
 2145 .277878216E-07-.380650779E-11-.281870009E+05 .524217373E+02 4
 2146 NC7H15 C 7H 15 G 300.00 4000.00 1382.00 1
 2147 .216371448E+02 .323324804E-01-.109273807E-04 .168357060E-08-.971774091E-13 2
 2148 -.105877217E+05-.852228493E+02-.379155767E-01 .756726570E-01-.407473634E-04 3
 2149 .932678943E-08-.492360745E-12-.235605303E+04 .337321506E+02 4
 2150 NC7H15-OO C 7H 15O 2 G 300.00 4000.00 1393.00 1
 2151 .272928290E+02 .327034748E-01-.112483701E-04 .175282538E-08-.101955579E-12 2
 2152 -.235449480E+05-.109307876E+03 .137396160E+01 .925294066E-01-.644403647E-04 3
 2153 .235223293E-07-.356678305E-11-.144154775E+05 .302419431E+02 4
 2154 NC7-QOOH C 7H 15O 2 G 300.00 4000.00 1000.00 1
 2155 .449365222E+02 .384325070E-02-.181753210E-06-.116055420E-10 .168632530E-14 2
 2156 -.301866739E+05-.207157897E+03 .169959950E+01 .943723540E-01-.755904260E-04 3
 2157 .401131540E-07-.120065810E-10-.147076150E+05 .283145640E+02 4
 2158 NC7-OOQOOH C 7H 15O 4 G 300.00 4000.00 1395.00 1
 2159 .269436049E+02 .351661203E-01-.120111248E-04 .186268617E-08-.107974911E-12 2
 2160 -.478858130E+05-.104588181E+03 .234060326E+01 .923428863E-01-.637138459E-04 3
 2161 .236026902E-07-.368902757E-11-.392112217E+05 .278171493E+02 4
 2162 !C6H4C2H C 8H 5 G 300.00 4000.00 1000.00 1
 !polimi
 2163 ! .286860656E+02-.138698600E-01 .227211900E-04-.998822700E-08 .140859000E-11 2
 2164 ! .560473490E+05-.127502636E+03-.293242200E+01 .660436800E-01-.395005000E-04 3
 2165 !-.318303810E-08 .853003870E-11 .653240430E+05 .380586850E+02 4
 2166 C6H4C2H C6H4-CCH T10/13C 8.H 5. 0. 0.G 200.000 6000.000 1000. 1
 !Burcat kik
 2167 1.51356812E+01 1.95393656E-02-7.04783919E-06 1.14147499E-09-6.85061656E-14 2
 2168 6.04891517E+04-5.42442195E+01-6.76311844E-01 5.42227756E-02-1.44506489E-05 3
 2169 -2.83755064E-08 1.79798680E-11 6.51966135E+04 2.93260540E+01 6.72297466E+04 4
 2170 !C6H5C2H2 C 8H 7 G 300.00 4000.00 1394.00 1
 !Polimi
 2171 ! .187667289E+02 .200619262E-01-.690883699E-05 .107799789E-08-.627759176E-13 2
 2172 ! .376789029E+05-.760287256E+02-.272251268E+01 .709701368E-01-.527526320E-04 3

2173 ! .197369835E-07-.295890798E-11 .450007235E+05 .390143531E+02 4
 2174 C6H5C2H2 n-styryl T12/07C 8.H 7. 0. 0.G 200.000 6000.000 1000. 1
 !Burcat kik
 2175 1.60668682E+01 2.35522834E-02-8.47352807E-06 1.36928204E-09-8.20829942E-14 2
 2176 3.98109546E+04-6.01469382E+01 2.78678850E-01 4.12517677E-02 4.27417783E-05 3
 2177 -9.66212597E-08 4.47818574E-11 4.52024803E+04 2.70544015E+01 4.73269020E+04 4
 2178 !RXYLENE C 8H 9 G 300.00 4000.00 1000.00 1
 2179 ! .808697123E+01 .442230490E-01-.196920930E-04 .391313300E-08-.286780230E-12 2
 2180 ! .152828351E+05-.180507988E+02-.244083000E+01 .750206000E-01-.520941000E-04 3
 2181 ! .184357000E-07-.267709000E-11 .180599500E+05 .358328500E+02 4
 2182 RXYLENE T 9/13C 8.H 9. 0. 0.G 200.000 6000.000 1000. 1
 !Burcat kik 2-3C6H4CH2*
 2183 1.56947853E+01 2.95619506E-02-1.06097584E-05 1.71214533E-09-1.02481459E-13 2
 2184 1.41477221E+04-5.99627856E+01 5.72547012E-01 4.45565169E-02 4.13301302E-05 3
 2185 -9.20754733E-08 4.18729206E-11 1.95112053E+04 2.43021144E+01 2.18652673E+04 4
 2186 !C6H5CHCH3 C 8H 9 G 300.00 4000.00 1000.00 1
 !EBenz old polimi
 2187 ! .179749910E+02 .239625180E-01-.715492520E-05 .103757720E-08-.596944840E-13 2
 2188 ! .194242850E+05-.693345570E+02-.526520200E+01 .889877600E-01-.754492360E-04 3
 2189 ! .341497320E-07-.666954430E-11 .259605610E+05 .509400020E+02 4
 2190 C6H5CHCH3 AlCHCH3 T 1/14C 8.H 9. 0. 0.G 200.000 6000.000 1000. 1
 !Burcat kik
 2191 1.52771567E+01 2.96305787E-02-1.06968599E-05 1.72910274E-09-1.03530176E-13 2
 2192 1.47917666E+04-5.54929193E+01 2.27328453E+00 3.30022851E-02 6.58045139E-05 3
 2193 -1.15196192E-07 4.99525562E-11 1.98294339E+04 1.91733305E+01 2.23513746E+04 4
 2194 RUME7 C 8H 130 2 G 300.00 4000.00 1376.00 1
 2195 .270534591E+02 .305004468E-01-.106520501E-04 .167796515E-08-.983020287E-13 2
 2196 -.363346010E+05-.107800076E+03 .366021323E+01 .765652941E-01-.421034444E-04 3
 2197 .990005395E-08-.618141131E-12-.272971814E+05 .209764369E+02 4
 2198 RME7 C 8H 150 2 G 300.00 4000.00 1382.00 1
 2199 .283088733E+02 .346001847E-01-.117889297E-04 .182346779E-08-.105527368E-12 2
 2200 -.507031223E+05-.115791454E+03 .312712425E+01 .886538094E-01-.550709022E-04 3
 2201 .172495936E-07-.218153163E-11-.414147165E+05 .212562509E+02 4
 2202 IC8H17 C 8H 17 G 300.00 4000.00 1000.00 1
 2203 .210071027E+02 .400670210E-01-.122220840E-04 .179139180E-08-.103364050E-12 2
 2204 -.156827594E+05-.841376688E+02-.142527150E+01 .952433870E-01-.515412500E-04 3
 2205 .269038680E-08 .557281520E-11-.909216410E+04 .335841900E+02 4
 2206 IC8-QOOH C 8H 170 2 G 300.00 4000.00 1400.00 1
 2207 .323288504E+02 .354286616E-01-.121434812E-04 .188811322E-08-.109661472E-12 2
 2208 -.319868602E+05-.136609837E+03-.150530420E+01 .118500203E+00-.910186246E-04 3
 2209 .362481173E-07-.587667874E-11-.206807572E+05 .436006519E+02 4
 2210 IC8H17-OO C 8H 170 2 G 300.00 4000.00 1397.00 1
 2211 .307492955E+02 .368544999E-01-.126522533E-04 .196915974E-08-.114442369E-12 2
 2212 -.380116818E+05-.129042218E+03-.126574300E+01 .113828908E+00-.844050615E-04 3
 2213 .328104935E-07-.525271208E-11-.270886887E+05 .421608430E+02 4
 2214 IC8T-QOOH C 8H 170 2 G 300.00 4000.00 1400.00 1
 2215 .323288504E+02 .354286616E-01-.121434812E-04 .188811322E-08-.109661472E-12 2
 2216 -.319868602E+05-.136609837E+03-.150530420E+01 .118500203E+00-.910186246E-04 3
 2217 .362481173E-07-.587667874E-11-.206807572E+05 .436006519E+02 4
 2218 IC8-OOQOOH C 8H 170 4 G 300.00 4000.00 1398.00 1
 2219 .362956073E+02 .372755603E-01-.128091685E-04 .199516372E-08-.116026947E-12 2
 2220 -.507708950E+05-.153592254E+03 .134208862E+01 .119507370E+00-.864939904E-04 3
 2221 .319097725E-07-.475802942E-11-.387629197E+05 .338018650E+02 4
 2222 !INDENYL C 9H 7 G 300.00 4000.00 1389.00 1
 !polimi
 2223 ! .210619876E+02 .219045968E-01-.772700080E-05 .122481766E-08-.721012249E-13 2
 2224 ! .270100509E+05-.947705468E+02-.627808779E+01 .881610767E-01-.698280991E-04 3
 2225 ! .280009421E-07-.454051640E-11 .362473103E+05 .511874555E+02 4
 2226 INDENYL T 9/96C 9.H 7. 0. 0.G 200.000 6000.000 1000. 1
 !Burcat kik 1-indenyl
 2227 1.85549761E+01 2.50350502E-02-9.14573755E-06 1.49348099E-09-9.01328268E-14 2
 2228 2.57211482E+04-7.63004782E+01-2.66986010E+00 6.21770959E-02 1.50674040E-05 3
 2229 -7.96461960E-08 4.09191931E-11 3.23869684E+04 3.78611069E+01 3.43495696E+04 4
 2230 RC9H11 C 9H 11 G 300.00 4000.00 1385.00 1
 2231 .227307929E+02 .291439937E-01-.101635526E-04 .159859987E-08-.935933623E-13 2
 2232 .481056390E+04-.975266902E+02-.180604559E+01 .826070356E-01-.539943357E-04 3
 2233 .177716542E-07-.237645289E-11 .137819561E+05 .357292291E+02 4
 2234 !C10H7 C 10H 7 G 300.00 4000.00 1000.00 1
 !polimi
 2235 ! .146529084E+02 .356159360E-01-.121796480E-04 .138747960E-08 .000000000E+00 2
 2236 ! .405898415E+05-.575649187E+02-.631700500E+01 .913910790E-01-.608201990E-04 3
 2237 ! .152228010E-07 .000000000E+00 .464268700E+05 .512234700E+02 4
 2238 C10H7 Naphtyl rad T 7/98C 10H 7 0 OG 200.000 6000.000 1000. 1


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!Burcat kik
2239 1.83535073E+01 2.77474314E-02-1.00885968E-05 1.64229575E-09-9.89002001E-14 2
2240 3.89261241E+04-7.48978150E+01-1.89559772E+00 5.83077290E-02 2.79388931E-05 3
2241 -9.14375172E-08 4.46422302E-11 4.55409775E+04 3.52453263E+01 4.76546183E+04 4
2242 !C10H7O C 10H 7O 1 G 300.00 4000.00 1387.00 1
!polimi
2243 !.252263199E+02 .234793777E-01-.827533154E-05 .131107385E-08-.771548491E-13 2
2244 !.188945294E+04-.112699321E+03-.234081413E+01 .850055448E-01-.590412510E-04 3
2245 !.195981954E-07-.248272174E-11 .116463286E+05 .362009562E+02 4
2246 C10H7O Radical T 7/98C 10.H 7.O 1. 0.G 200.000 6000.000 1000.00 1
!Burcat kik
2247 2.10591364E+01 2.82563070E-02-1.03328686E-05 1.68867034E-09-1.01974767E-13 2
2248 4.09143507E+03-8.84963398E+01-1.15176448E+00 6.11354512E-02 3.20151083E-05 3
2249 -9.94285290E-08 4.79990043E-11 1.14058756E+04 3.25584836E+01 1.38887800E+04 4
2250 RTETRALIN C 10H 11 G 300.00 4000.00 1393.00 1
2251 .274897602E+02 .290231662E-01-.101643070E-04 .160474752E-08-.942455736E-13 2
2252 .498834588E+04-.134140516E+03-.103201226E+02 .112759920E+00-.777366610E-04 3
2253 .248527119E-07-.289510552E-11 .183518811E+05 .701782401E+02 4
2254 RTETRAOO C 10H 11O 2 G 300.00 4000.00 1393.00 1
2255 .325696052E+02 .270322587E-01-.103226960E-04 .172977036E-08-.105947326E-12 2
2256 -.797598133E+04-.153101057E+03-.133437809E+02 .139730780E+00-.110918062E-03 3
2257 .406822937E-07-.565600132E-11 .639529388E+04 .899902305E+02 4
2258 RODECA C 10H 17 G 300.00 4000.00 1393.00 1
2259 .266885367E+02 .438181872E-01-.149997894E-04 .233096426E-08-.135354849E-12 2
2260 -.142864228E+05-.128706101E+03-.137726588E+02 .134621624E+00-.905467076E-04 3
2261 .298633466E-07-.381482514E-11-.121358784E+02 .896659972E+02 4
2262 RDECALIN C 10H 17 G 300.00 4000.00 1393.00 1
2263 .266885367E+02 .438181872E-01-.149997894E-04 .233096426E-08-.135354849E-12 2
2264 -.142864228E+05-.128706101E+03-.137726588E+02 .134621624E+00-.905467076E-04 3
2265 .298633466E-07-.381482514E-11-.121358784E+02 .896659972E+02 4
2266 RDECOO C 10H 17O 2 G 300.00 4000.00 1379.00 1
2267 .223721095E+02 .276799389E-01-.974217376E-05 .154194767E-08-.906767646E-13 2
2268 -.211451384E+05-.984373555E+02-.491663898E+01 .836156703E-01-.498338842E-04 3
2269 .127483629E-07-.918573704E-12-.109593466E+05 .507734668E+02 4
2270 QDECOOH C 10H 17O 2 G 300.00 4000.00 1379.00 1
2271 .223721095E+02 .276799389E-01-.974217376E-05 .154194767E-08-.906767646E-13 2
2272 -.211451384E+05-.984373555E+02-.491663898E+01 .836156703E-01-.498338842E-04 3
2273 .127483629E-07-.918573704E-12-.109593466E+05 .507734668E+02 4
2274 ZDECA C 10H 17O 4 G 300.00 4000.00 1379.00 1
2275 .223721095E+02 .276799389E-01-.974217376E-05 .154194767E-08-.906767646E-13 2
2276 -.211451384E+05-.984373555E+02-.491663898E+01 .836156703E-01-.498338842E-04 3
2277 .127483629E-07-.918573704E-12-.109593466E+05 .507734668E+02 4
2278 NC10H19 C 10H 19 G 300.00 4000.00 1383.00 1
2279 .140838604E+02 .208584950E-01-.722620456E-05 .113154433E-08-.660424465E-13 2
2280 .542225436E+04-.515371079E+02-.697079542E+00 .514354766E-01-.304500502E-04 3
2281 .880925852E-08-.994458078E-12 .110172568E+05 .293601364E+02 4
2282 NC10H21 C 10H 21 G 300.00 4000.00 1385.00 1
2283 .314447580E+02 .452778532E-01-.153145696E-04 .236072411E-08-.136311835E-12 2
2284 -.229702700E+05-.131435127E+03-.930536886E+00 .113137924E+00-.664034118E-04 3
2285 .183220872E-07-.177128003E-11-.109890165E+05 .451328034E+02 4
2286 NC10-QOOH C 10H 21O 2 G 300.00 4000.00 1392.00 1
2287 .364873664E+02 .456938220E-01-.154604572E-04 .238346695E-08-.137626430E-12 2
2288 -.370093465E+05-.152798812E+03 .883511244E+00 .125360621E+00-.820308363E-04 3
2289 .270294818E-07-.354081617E-11-.243570772E+05 .395546233E+02 4
2290 NC10H21-OO C 10H 21O 2 G 300.00 4000.00 1392.00 1
2291 .347424373E+02 .481682266E-01-.165183738E-04 .256870455E-08-.149189141E-12 2
2292 -.416206773E+05-.145293449E+03 .109633829E+01 .123998092E+00-.822926235E-04 3
2293 .288935474E-07-.426829326E-11-.295195291E+05 .366210584E+02 4
2294 NC10-OOQOOH C 10H 21O 4 G 300.00 4000.00 1393.00 1
2295 .419701067E+02 .470326141E-01-.162065055E-04 .252885796E-08-.147242779E-12 2
2296 -.568721943E+05-.179987435E+03 .270340236E+01 .134161981E+00-.884509572E-04 3
2297 .291143638E-07-.380678318E-11-.428023111E+05 .324857210E+02 4
2298 !C10H7CH2 C 11H 9 G 300.00 4000.00 1389.00 1
!polimi
2299 !.266596927E+02 .269903845E-01-.949827903E-05 .150313533E-08-.883831941E-13 2
2300 !.210179470E+05-.122975754E+03-.551514480E+01 .106245066E+00-.857510752E-04 3
2301 !.355122444E-07-.598055713E-11 .318146452E+05 .484291679E+02 4
2302 C10H7CH2 T 7/98C 11H 9 0 OG 200.000 6000.000 1000. 1
!Burcat kik 1-C10H7-CH2*
2303 2.18977539E+01 3.26102636E-02-1.18401218E-05 1.92574628E-09-1.15903442E-13 2
2304 2.24571098E+04-9.41050741E+01-2.53234304E+00 7.32920338E-02 2.02974707E-05 3
2305 -9.36547823E-08 4.70753594E-11 3.02906705E+04 3.79638513E+01 3.28097266E+04 4
2306 !C10H6CH3 C 11H 9 G 300.00 4000.00 1387.00 1

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!polimi
2307 ! .241866524E+02 .287085863E-01-.100040198E-04 .157283341E-08-.920615442E-13 2
2308 ! .317595121E+05-.107209439E+03-.148986180E+01 .837301572E-01-.531437515E-04 3
2309 ! .161159556E-07-.183550466E-11 .411521411E+05 .324161445E+02 4
2310 C10H6CH3 T11/13C 11.H 9. 0. 0.G 200.000 6000.000 1000. 1
!burcat kik 1-Naphthyl-3-Methyl Radical 1-C10H6*-3-CH3
2311 2.06757697E+01 3.29978114E-02-1.19213860E-05 1.93272353E-09-1.16069177E-13 2
2312 3.42587805E+04-8.79526119E+01-2.07498418E+00 6.80090538E-02 2.63761043E-05 3
2313 -9.53060559E-08 4.65647314E-11 4.17116175E+04 3.57867673E+01 4.41824233E+04 4
2314 CH3C10H6O C 11H 90 1 G 300.00 4000.00 1386.00 1
2315 .281108749E+02 .281427040E-01-.986090177E-05 .155620703E-08-.913337710E-13 2
2316 -.350666986E+04-.125748079E+03-.108570461E+01 .905308669E-01-.577474885E-04 3
2317 .167977934E-07-.168045736E-11 .709977655E+04 .329292729E+02 4
2318 RUME10 C 11H 190 2 G 300.00 4000.00 1400.00 1
2319 .333201898E+02 .479399831E-01-.157699228E-04 .238393079E-08-.135735725E-12 2
2320 -.400970534E+05-.137405141E+03 .142231026E+01 .127120401E+00-.922642215E-04 3
2321 .364453822E-07-.599028369E-11-.294852312E+05 .322500169E+02 4
2322 RMDX C 11H 210 2 G 300.00 4000.00 1376.00 1
2323 .385051195E+02 .464902832E-01-.162008540E-04 .254969816E-08-.149299808E-12 2
2324 -.649901621E+05-.166525707E+03 .345128941E+01 .114960511E+00-.621890037E-04 3
2325 .140937438E-07-.752795690E-12-.513892174E+05 .266431624E+02 4
2326 QMDOOH C 11H 210 4 G 300.00 4000.00 1378.00 1
2327 .463512360E+02 .442905004E-01-.156791241E-04 .249437540E-08-.147109263E-12 2
2328 -.802179278E+05-.202701285E+03 .505901193E+01 .130586874E+00-.811966955E-04 3
2329 .236808295E-07-.254638441E-11-.648189073E+05 .227472201E+02 4
2330 RMDOOX C 11H 210 4 G 300.00 4000.00 1384.00 1
2331 .426675367E+02 .481355870E-01-.164385340E-04 .254942818E-08-.147838407E-12 2
2332 -.850035553E+05-.184014175E+03 .443641793E+01 .133210481E+00-.883606205E-04 3
2333 .302231077E-07-.426647212E-11-.712160785E+05 .229630078E+02 4
2334 ZMDOOH C 11H 210 6 G 300.00 4000.00 1384.00 1
2335 .493171232E+02 .461887725E-01-.155948619E-04 .242596048E-08-.141314237E-12 2
2336 -.997314376E+05-.213131636E+03 .613115269E+01 .145831804E+00-.103807590E-03 3
2337 .382530920E-07-.579145154E-11-.845666547E+05 .193222210E+02 4
2338 !C12H7 C 12H 7 G 300.00 4000.00 1000.00 1
!polimi
2339 ! .119534365E+02 .523860720E-01-.276952580E-04 .698583900E-08-.684938540E-12 2
2340 ! .531995141E+05-.403925438E+02-.733802700E+01 .111965800E+00-.932829430E-04 3
2341 ! .358663430E-07-.426602200E-11 .580597660E+05 .573507160E+02 4
2342 C12H7 AcenaphtynylT01/08C 12.H 7. 0. 0.G 200.000 6000.000 1000.00 1
!Burcat kik
2343 2.16586138E+01 3.04696316E-02-1.11497201E-05 1.82316781E-09-1.10144488E-13 2
2344 5.28451416E+04-9.73300058E+01-2.23704309E+00 6.20074173E-02 4.69635631E-05 3
2345 -1.20874263E-07 5.68318739E-11 6.08867652E+04 3.38045560E+01 6.31787081E+04 4
2346 !C12H9 C 12H 9 G 300.00 4000.00 1000.00 1
!polimi
2347 ! .214890352E+02 .375797860E-01-.121080230E-04 .129882780E-08 .000000000E+00 2
2348 ! .415521488E+05-.916763235E+02-.783196500E+01 .114327200E+00-.776398370E-04 3
2349 ! .194042280E-07 .000000000E+00 .498170300E+05 .608493300E+02 4
2350 C12H9 C 12H 9 G 300.00 6000.00 1000.00 1
!Burcat kik P2-
2351 2.25692222E+01 3.45619984E-02-1.27020877E-05 2.08111819E-09-1.25849407E-13 2
2352 4.05907457E+04-9.57787051E+01 4.07668089E-01 5.42794698E-02 7.12515775E-05 3
2353 -1.44404112E-07 6.48497982E-11 4.85351870E+04 2.81980814E+01 5.14438013E+04 4
2354 NC12H25 C 12H 25 G 300.00 4000.00 1387.00 1
2355 .379559371E+02 .541231481E-01-.184408520E-04 .285618139E-08-.165452331E-12 2
2356 -.312698454E+05-.166157365E+03-.117025753E+01 .136564242E+00-.813840519E-04 3
2357 .231564976E-07-.240764498E-11-.167979250E+05 .471339366E+02 4
2358 NC12-QOOH C 12H 250 2 G 300.00 4000.00 1392.00 1
2359 .427882927E+02 .547351985E-01-.185693137E-04 .286771608E-08-.165782124E-12 2
2360 -.451897912E+05-.183774591E+03 .457142729E+00 .149660990E+00-.984019129E-04 3
2361 .327982507E-07-.438634589E-11-.301386488E+05 .448987214E+02 4
2362 NC12H25-OO C 12H 250 2 G 300.00 4000.00 1392.00 1
2363 .410672882E+02 .571682582E-01-.196096581E-04 .304996352E-08-.177163659E-12 2
2364 -.498119415E+05-.176403781E+03 .761653139E+00 .147870053E+00-.980093227E-04 3
2365 .342486611E-07-.502171364E-11-.353144020E+05 .415448990E+02 4
2366 NC12-QOOOH C 12H 250 4 G 300.00 4000.00 1393.00 1
2367 .478223133E+02 .563342752E-01-.193784199E-04 .302016363E-08-.175696376E-12 2
2368 -.648031378E+05-.208209874E+03 .250560092E+01 .157994999E+00-.105503812E-03 3
2369 .358709948E-07-.494871123E-11-.486270464E+05 .366890378E+02 4
2370 !C14H9 C 14H 9 G 300.00 4000.00 1000.00 1
!polimi
2371 ! .255171870E+02 .393727940E-01-.123155080E-04 .127852800E-08 .000000000E+00 2
2372 ! .431324738E+05-.115618425E+03-.909474100E+01 .131333800E+00-.924017290E-04 3

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2373	!	.240156710E-07	.000000000E+00	.527750200E+05	.639753600E+02	4	
2374	C14H9 4-Phenantr	T11/07C 14.H 9.	0.	0.G	298.150 5000.000 1000.00	1	
	!Burcat kik assume 4-Phenanthryl rad as it is active site to from pyrene						
2375		2.68173412E+01	3.76935761E-02	-1.45586251E-05	2.58486800E-09	-1.73198001E-13	2
2376		4.14405846E+04	-1.21547559E+02	-1.08929968E+01	1.41537035E-01	-1.14205532E-04	3
2377		3.57710437E-08	0.00000000E+00	5.21136455E+04	7.37137024E+01	5.42184687E+04	4
2378	C16H9	C 16H	9	G	300.00 4000.00 1000.00	1	
2379		.161628784E+02	.696969850E-01	-.371786410E-04	.946306230E-08	-.935417110E-12	2
2380		.461067047E+05	-.652717249E+02	-.114972670E+02	.151166960E+00	-.116351410E-03	3
2381		.317097570E-07	.218082760E-11	.532378630E+05	.757195740E+02		4
2382	IC16H33	C 16H	33	G	300.00 4000.00 1398.00	1	
2383		.560389730E+02	.668182464E-01	-.225681513E-04	.347608102E-08	-.200620637E-12	2
2384		-.583645424E+05	-.270643351E+03	-.953227198E+01	.224283987E+00	-.166371012E-03	3
2385		.627848165E-07	-.951119300E-11	-.362947496E+05	.795385858E+02		4
2386	NC16H33	C 16H	33	G	300.00 4000.00 1387.00	1	
2387		.510324990E+02	.711045684E-01	-.240491592E-04	.370710805E-08	-.214054039E-12	2
2388		-.477151440E+05	-.228063103E+03	-.243005348E+01	.186692969E+00	-.115724867E-03	3
2389		.350879669E-07	-.405848895E-11	-.282942913E+05	.622394761E+02		4
2390	IC16H33-OO	C 16H	330 2	G	300.00 4000.00 1397.00	1	
2391		.600009189E+02	.697612153E-01	-.240119992E-04	.374399505E-08	-.217877031E-12	2
2392		-.771125672E+05	-.288496873E+03	-.807177622E+01	.238256241E+00	-.186291159E-03	3
2393		.758296536E-07	-.125956694E-10	-.544214916E+05	.737310481E+02		4
2394	NC16-QOOH	C 16H	330 2	G	300.00 4000.00 1394.00	1	
2395		.557196631E+02	.758805933E-01	-.260092776E-04	.404350192E-08	-.234807139E-12	2
2396		-.852319237E+05	-.250905152E+03	-.858601178E+00	.204663464E+00	-.138309577E-03	3
2397		.488963438E-07	-.717831502E-11	-.651200924E+05	.543621098E+02		4
2398	IC16-QOOH	C 16H	330 2	G	300.00 4000.00 1399.00	1	
2399		.615798034E+02	.683372119E-01	-.235040286E-04	.366308625E-08	-.213104512E-12	2
2400		-.710887760E+05	-.294961987E+03	-.836284759E+01	.243137667E+00	-.193204766E-03	3
2401		.794478202E-07	-.132585716E-10	-.480052296E+05	.765156723E+02		4
2402	NC16H33-OO	C 16H	330 2	G	300.00 4000.00 1392.00	1	
2403		.537254976E+02	.751675700E-01	-.257930312E-04	.401271756E-08	-.233130903E-12	2
2404		-.661992854E+05	-.238675214E+03	.121036107E+00	.195526928E+00	-.129332034E-03	3
2405		.448994551E-07	-.651714304E-11	-.469097176E+05	.512502917E+02		4
2406	IC16T-QOOH	C 16H	330 2	G	300.00 4000.00 1397.00	1	
2407		.619590914E+02	.670805941E-01	-.228781110E-04	.354645272E-08	-.205581639E-12	2
2408		-.737750910E+05	-.297686975E+03	-.828638110E+01	.240615134E+00	-.188046280E-03	3
2409		.753924180E-07	-.122092604E-10	-.505105835E+05	.759168895E+02		4
2410	IC16T-OOQOOH	C 16H	330 4	G	300.00 4000.00 1396.00	1	
2411		.664600695E+02	.692200495E-01	-.239811044E-04	.375550159E-08	-.219211037E-12	2
2412		-.927495777E+05	-.318609160E+03	-.734744585E+01	.256652224E+00	-.210530384E-03	3
2413		.896944245E-07	-.155165690E-10	-.685533247E+05	.725686554E+02		4
2414	NC16-OOQOOH	C 16H	330 4	G	300.00 4000.00 1393.00	1	
2415		.605564321E+02	.743085731E-01	-.255622121E-04	.398394439E-08	-.231762903E-12	2
2416		-.812450313E+05	-.270973587E+03	.185761468E+01	.205470409E+00	-.136236709E-03	3
2417		.460471713E-07	-.632675050E-11	-.602164277E+05	.464682670E+02		4
2418	IC16-OOQOOH	C 16H	330 4	G	300.00 4000.00 1395.00	1	
2419		.657312368E+02	.698159219E-01	-.241818212E-04	.378635278E-08	-.220988765E-12	2
2420		-.891725518E+05	-.313140345E+03	-.709314164E+01	.252307521E+00	-.202956898E-03	3
2421		.848048060E-07	-.144255682E-10	-.650715559E+05	.736645741E+02		4
2422	RUME16	C 17H	310 2	G	300.00 4000.00 1836.00	1	
2423		.492312959E+02	.809629787E-01	-.290414743E-04	.466984560E-08	-.277987170E-12	2
2424		-.712766099E+05	-.212350222E+03	.581847898E+00	.197335153E+00	-.132222747E-03	3
2425		.454132116E-07	-.638160297E-11	-.555076491E+05	.468001664E+02		4
2426	RMPAX	C 17H	330 2	G	300.00 4000.00 1000.00	1	
2427		.347969412E+02	.108174887E+00	-.436560662E-04	.805036686E-08	-.557001848E-12	2
2428		-.833532968E+05	-.136711346E+03	.118429649E+02	.108281798E+00	.937470576E-04	3
2429		-.175260710E-06	.681980157E-10	-.741770519E+05	.304443036E+01		4
2430	RMPA00X	C 17H	330 4	G	300.00 4000.00 1384.00	1	
2431		.426675367E+02	.481355870E-01	-.164385340E-04	.254942818E-08	-.147838407E-12	2
2432		-.850035553E+05	-.184014175E+03	.443641793E+01	.133210481E+00	-.883606205E-04	3
2433		.302231077E-07	-.426647212E-11	-.712160785E+05	.229630078E+02		4
2434	QMPA00H	C 17H	330 4	G	300.00 4000.00 1378.00	1	
2435		.463512360E+02	.442905004E-01	-.156791241E-04	.249437540E-08	-.147109263E-12	2
2436		-.802179278E+05	-.202701285E+03	.505901193E+01	.130586874E+00	-.811966955E-04	3
2437		.236808295E-07	-.254638441E-11	-.648189073E+05	.227472201E+02		4
2438	ZMPA00H	C 17H	330 6	G	300.00 4000.00 1384.00	1	
2439		.493171232E+02	.461887725E-01	-.155948619E-04	.242596048E-08	-.141314237E-12	2
2440		-.997314376E+05	-.213131636E+03	.613115269E+01	.145831804E+00	-.103807590E-03	3
2441		.382530920E-07	-.579145154E-11	-.845666547E+05	.193222210E+02		4
2442	RMLIN1X	C 19H	310 2	G	300.00 4000.00 1830.00	1	
2443		.515951901E+02	.848982968E-01	-.306132424E-04	.493978264E-08	-.294767670E-12	2
2444		-.437090861E+05	-.222319284E+03	-.124182769E+01	.210470141E+00	-.141012967E-03	3

2445	.480938977E-07-.668889816E-11-.265018940E+05	.594297783E+02	4
2446	RMLIN1A C 19H 310 2 G	300.00 4000.00 1830.00	1
2447	.515951901E+02 .848982968E-01-.306132424E-04	.493978264E-08-.294767670E-12	2
2448	-.437090861E+05-.222319284E+03-.124182769E+01	.210470141E+00-.141012967E-03	3
2449	.480938977E-07-.668889816E-11-.265018940E+05	.594297783E+02	4
2450	RMLIN1OOX C 19H 310 4 G	300.00 4000.00 1854.00	1
2451	.566771062E+02 .848718923E-01-.306165992E-04	.494186779E-08-.294961213E-12	2
2452	-.712260452E+05-.243221478E+03-.182318626E+01	.229267759E+00-.163619600E-03	3
2453	.597071790E-07-.884702825E-11-.526983896E+05	.668009912E+02	4
2454	QMLIN1OOX C 19H 310 4 G	300.00 4000.00 1859.00	1
2455	.597198037E+02 .825172318E-01-.298594827E-04	.482987333E-08-.288709215E-12	2
2456	-.679692648E+05-.260058551E+03-.300959205E+01	.239625356E+00-.176824958E-03	3
2457	.662378545E-07-.999748235E-11-.483423909E+05	.715224170E+02	4
2458	ZMLIN1OOX C 19H 310 6 G	300.00 4000.00 1844.00	1
2459	.633953698E+02 .840133680E-01-.304696355E-04	.493592631E-08-.295352525E-12	2
2460	-.861431583E+05-.275575442E+03 .377427203E+00	.239045319E+00-.172299424E-03	3
2461	.627369839E-07-.920510825E-11-.661691485E+05	.585014961E+02	4
2462	RMLINX C 19H 330 2 G	300.00 4000.00 1386.00	1
2463	.611078575E+02 .762751735E-01-.262266430E-04	.408707626E-08-.237771674E-12	2
2464	-.683962704E+05-.275956500E+03-.144781566E+01	.215019809E+00-.142192171E-03	3
2465	.476963895E-07-.649336150E-11-.458716461E+05	.627347784E+02	4
2466	RMLINA C 19H 330 2 G	300.00 4000.00 1386.00	1
2467	.611078575E+02 .762751735E-01-.262266430E-04	.408707626E-08-.237771674E-12	2
2468	-.683962704E+05-.275956500E+03-.144781566E+01	.215019809E+00-.142192171E-03	3
2469	.476963895E-07-.649336150E-11-.458716461E+05	.627347784E+02	4
2470	RMLIN1OH C 19H 330 3 G	300.00 4000.00 1000.00	1
2471	.109866520E+03 .423976550E-02-.805195410E-07-	.170406780E-10 .168247750E-14	2
2472	-.106680810E+06-.543129330E+03 .690969590E+00	.209334020E+00-.125946550E-03	3
2473	.409375960E-07-.109953440E-10-.661363050E+05	.579650690E+02	4
2474	RMLINOOX C 19H 330 4 G	300.00 4000.00 1840.00	1
2475	.561396497E+02 .898573320E-01-.323076347E-04	.520295879E-08-.310043109E-12	2
2476	-.835647272E+05-.240835194E+03 .146002415E+01	.221120424E+00-.149309126E-03	3
2477	.517229930E-07-.733489301E-11-.658774535E+05	.502873652E+02	4
2478	QMLINOOX C 19H 330 4 G	300.00 4000.00 1830.00	1
2479	.592334771E+02 .871071695E-01-.313329462E-04	.504827960E-08-.300945381E-12	2
2480	-.780101129E+05-.256778117E+03-.383425349E+00	.231626065E+00-.160960610E-03	3
2481	.566395921E-07-.805109149E-11-.589322117E+05	.599912602E+02	4
2482	RMLIN1OHOO C 19H 330 5 G	300.00 4000.00 1000.00	1
2483	.251712040E+02 .137856480E+00-.512202200E-04	.870306320E-08-.560550030E-12	2
2484	-.886761250E+05-.568400270E+02-.493498520E+01	.253526120E+00-.181310740E-03	3
2485	.532790980E-07-.715418010E-12-.841542810E+05	.856818080E+02	4
2486	ZMLINOOX C 19H 330 6 G	300.00 4000.00 1183.00	1
2487	.601829822E+02 .877246704E-01-.308673874E-04	.490011538E-08-.289106438E-12	2
2488	-.959756017E+05-.274111539E+03 .888177201E+00	.245491279E+00-.188867182E-03	3
2489	.756398491E-07-.122061299E-10-.781464330E+05	.361650421E+02	4
2490	RMEOLEA C 19H 350 2 G	300.00 4000.00 1386.00	1
2491	.617968812E+02 .797287018E-01-.272798012E-04	.423721781E-08-.245941529E-12	2
2492	-.826622063E+05-.278715034E+03-.296860913E-01	.215538273E+00-.139084893E-03	3
2493	.453526106E-07-.596335185E-11-.602711250E+05	.564905254E+02	4
2494	RMEOLLES C 19H 350 2 G	300.00 4000.00 1386.00	1
2495	.617968812E+02 .797287018E-01-.272798012E-04	.423721781E-08-.245941529E-12	2
2496	-.826622063E+05-.278715034E+03-.296860913E-01	.215538273E+00-.139084893E-03	3
2497	.453526106E-07-.596335185E-11-.602711250E+05	.564905254E+02	4
2498	RMEOLEOOX C 19H 350 4 G	300.00 4000.00 1799.00	1
2499	.565118676E+02 .949710722E-01-.342666750E-04	.553134168E-08-.330143553E-12	2
2500	-.121723087E+06-.240377715E+03 .312228984E+01	.215930145E+00-.133878272E-03	3
2501	.413627115E-07-.514696341E-11-.103763030E+06	.464356398E+02	4
2502	QMEOLEOOH C 19H 350 4 G	300.00 4000.00 1825.00	1
2503	.578903822E+02 .960618008E-01-.345783142E-04	.557312937E-08-.332293982E-12	2
2504	-.145787244E+06-.248797880E+03-.121085721E+01	.236084007E+00-.157011163E-03	3
2505	.530523572E-07-.729693062E-11-.126516243E+06	.664772594E+02	4
2506	ZMEOLEOOX C 19H 350 6 G	300.00 4000.00 1175.00	1
2507	.558298346E+02 .101939581E+00-.350749088E-04	.548251413E-08-.319925836E-12	2
2508	-.108843753E+06-.228788516E+03 .196924109E+01	.244903891E+00-.177892306E-03	3
2509	.692918136E-07-.110530115E-10-.926192007E+05	.531689573E+02	4
2510	RSTEAX C 19H 370 2 G	300.00 4000.00 1000.00	1
2511	.410838828E+02 .116388491E+00-.460844475E-04	.839784976E-08-.576703150E-12	2
2512	-.912925804E+05-.167019971E+03 .115570681E+02	.131479341E+00 .799583356E-04	3
2513	-.171755777E-06 .679701047E-10-.799964069E+05	.174630364E+01	4
2514	RMEOLEOH C 19H 370 3 G	300.00 4000.00 1000.00	1
2515	.113871410E+03 .775875800E-02-.452147480E-06	.136135370E-10-.133024960E-16	2
2516	-.136912560E+06-.564887510E+03 .250303720E+01	.215053450E+00-.121530550E-03	3
2517	.330490980E-07-.788034390E-11-.955148750E+05	.486207620E+02	4

2518	QMSTEA00H	C	19H	370	4	G	300.00	3500.00	1230.00	1
2519	-1.30612112e+02	6.00365407e-01	-4.85197507e-04	1.58690694e-07	-1.80918278e-11					2
2520	1.24045712e+04	7.12083733e+02	2.15554520e+01	1.05511541e-01	1.18282818e-04					3
2521	-1.68398913e-07	4.83897995e-11	-2.50286495e+04	-5.35376428e+01						4
2522	RMSTEA00X	C	19H	370	4	G	300.00	3500.00	1250.00	1
2523	-1.20700825e+02	5.67736647e-01	-4.52750605e-04	1.47317719e-07	-1.67528750e-11					2
2524	1.02039730e+04	6.60024010e+02	1.91170969e+01	1.20319296e-01	8.41502164e-05					3
2525	-1.39029386e-07	4.05165459e-11	-2.47505076e+04	-4.57161098e+01						4
2526	RMEOLE00O	C	19H	370	5	G	300.00	4000.00	1000.00	1
2527	.133736930E+02	.167858470E+00	-.644862230E-04	.112143850E-07	-.733979720E-12					2
2528	-.112646060E+06	.973074340E+01	-.366680260E+01	.261956100E+00	-.180087150E-03					3
2529	.445610300E-07	.429013550E-11	-.113462220E+06	.787735670E+02						4
2530	ZMSTEA00H	C	19H	370	6	G	300.00	3500.00	1250.00	1
2531	-6.22995292e+01	3.41575945e-01	-2.69706994e-04	8.71969173e-08	-9.87435445e-12					2
2532	1.57160052e+04	3.57020399e+02	1.61954271e+01	9.03920846e-02	3.17136383e-05					3
2533	-7.35607532e-08	2.22771796e-11	-3.90773390e+03	-3.91880337e+01						4
2534	!C10H8	C	10H	8		G	300.00	4000.00	1401.00	1
	!polimi									
2535	! .234023214E+02	.242434427E-01	-.836282016E-05	.130620111E-08	-.761153748E-13					2
2536	! .651941329E+04	-.107433208E+03	-.883645988E+01	.109300567E+00	-.955200914E-04					3
2537	! .421647669E-07	-.739851710E-11	.166533366E+05	.621064766E+02						4
2538	C10H8 Naphthalene T 7/98C	10H	8	0	0G	200.000	6000.000	1000.		1
	!Burcat kik									
2539	1.86129884E+01	3.04494175E-02	-1.11224825E-05	1.81615474E-09	-1.09601281E-13					2
2540	8.91578988E+03	-8.00230396E+01	-1.04919475E+00	4.62970781E-02	7.07591636E-05					3
2541	-1.38408111E-07	6.20475407E-11	1.59848987E+04	3.02121626E+01	1.81107678E+04					4
2542	NC3H7O2	C	3H	70	2	G	300.00	4000.00	1388.00	1
2543	.127230991E+02	.167336808E-01	-.575943184E-05	.897769493E-09	-.522275065E-13					2
2544	-.108816595E+05	-.381965321E+02	.156301709E+01	.426192697E-01	-.296615075E-04					3
2545	.114187326E-07	-.189894471E-11	-.688086375E+04	.219842933E+02						4
2546	IC3H7O2	C	3H	70	2	G	300.00	4000.00	1392.00	1
2547	.132610651E+02	.162501084E-01	-.558631798E-05	.870057473E-09	-.505849469E-13					2
2548	-.131937089E+05	-.421023499E+02	.103495454E+01	.469942369E-01	-.366525520E-04					3
2549	.157084173E-07	-.281956117E-11	-.906344820E+04	.229566921E+02						4
2550	NC3-QOOH	C	3H	70	2	G	300.00	4000.00	1374.00	1
2551	.146139980E+02	.143723015E-01	-.488635144E-05	.756519620E-09	-.438364992E-13					2
2552	-.646101457E+04	-.457478245E+02	.191005011E+01	.411666833E-01	-.251630217E-04					3
2553	.711856873E-08	-.698838732E-12	-.179305093E+04	.234514457E+02						4
2554	IC3-QOOH	C	3H	70	2	G	300.00	4000.00	1399.00	1
2555	.155030898E+02	.139802008E-01	-.481811216E-05	.751835399E-09	-.437743118E-13					2
2556	-.741643030E+04	-.523911482E+02	-.184042862E+00	.564670638E-01	-.501611253E-04					3
2557	.230526863E-07	-.423866481E-11	-.252333896E+04	.298354826E+02						4
2558	NC3-OOQOOH	C	3H	70	4	G	300.00	4000.00	1388.00	1
2559	.185146106E+02	.164157074E-01	-.573085844E-05	.901975314E-09	-.528299084E-13					2
2560	-.231819444E+05	-.618247164E+02	.254387733E+01	.570847379E-01	-.472164204E-04					3
2561	.208289492E-07	-.378162942E-11	-.178600410E+05	.229447574E+02						4
2562	IC3-OOQOOH	C	3H	70	4	G	300.00	4000.00	1391.00	1
2563	.191234208E+02	.158457151E-01	-.552231946E-05	.868162288E-09	-.508094203E-13					2
2564	-.255253957E+05	-.661419362E+02	.175906535E+01	.624712381E-01	-.554930416E-04					3
2565	.257973727E-07	-.483190839E-11	-.200009572E+05	.251348546E+02						4
2566	CHOCH2CHO	C	3H	40	2	G	300.00	4000.00	1000.00	1
2567	.104962923E+02	.120559957E-01	-.434149310E-05	.699425892E-09	-.418003976E-13					2
2568	-.437332461E+05	-.275425657E+02	.124227207E+01	.300698605E-01	-.148206586E-05					3
2569	-.242738150E-07	.133121686E-10	-.408667843E+05	.219242842E+02						4
2570	C3H6O	C	3H	60	1	G	300.00	4000.00	1000.00	1
2571	.801491079E+01	.173919953E-01	-.626027968E-05	.101188256E-08	-.606239111E-13					2
2572	-.151980838E+05	-.188279964E+02	.342806676E+01	.625176642E-02	.613196311E-04					3
2573	-.860387185E-07	.351371393E-10	-.128446646E+05	.104244994E+02						4
2574	NC3H7OH	C	3H	80	1	G	300.00	4000.00	1000.00	1
2575	.852377408E+01	.210371210E-01	-.748398370E-05	.119958663E-08	-.714873013E-13					2
2576	-.350702414E+05	-.177857176E+02	.541877541E+01	-.575566129E-03	.851215375E-04					3
2577	-.111060442E-06	.443007063E-10	-.328368377E+05	.529974117E+01						4
2578	IC3H7OH	C	3H	80	1	G	300.00	4000.00	1000.00	1
2579	.964183701E+01	.200230715E-01	-.711967189E-05	.114138950E-08	-.679935249E-13					2
2580	-.374835623E+05	-.256288343E+02	.430755345E+01	.102582798E-01	.619565411E-04					3
2581	-.902973802E-07	.373936384E-10	-.349249212E+05	.755995822E+01						4
2582	C3H7OOH	C	3H	80	2	G	300.00	4000.00	1000.00	1
2583	.104115631E+02	.213763889E-01	-.755819870E-05	.120207180E-08	-.711798090E-13					2
2584	-.268935445E+05	-.235428789E+02	.708977756E+01	-.486163264E-02	.103253531E-03					3
2585	-.133200956E-06	.530799252E-10	-.244194556E+05	.174859215E+01						4
2586	C3-QOOH	C	3H	60	3	G	300.00	4000.00	1391.00	1
2587	.170285271E+02	.130716784E-01	-.459310856E-05	.726135156E-09	-.426658337E-13					2
2588	-.416334217E+05	-.592513577E+02	.768933034E+00	.546905880E-01	-.465072405E-04					3

2589	.203159585E-07-.358398999E-11-.363238861E+05	.268291637E+02	4
2590	CH3CH2CH2O C 3H 70 1 G	300.00 4000.00 1000.00	1
2591	.838041157E+01 .195206120E-01-.697374143E-05	.112144919E-08-.669467831E-13	2
2592	-.848625211E+04-.189916219E+02 .421934640E+01	.738556641E-02 .602825529E-04	3
2593	-.838680247E-07 .339623435E-10-.623491852E+04	.808139850E+01	4
2594	CH2OHCH2CHO C 3H 60 2 G	300.00 4000.00 1382.00	1
2595	.118936666E+02 .144153203E-01-.477525443E-05	.726036430E-09-.415285995E-13	2
2596	-.459271652E+05-.327285750E+02 .266613285E+01	.346302298E-01-.214380719E-04	3
2597	.690469334E-08-.916939105E-12-.425706303E+05	.173358364E+02	4
2598	CH3CH2CHOH C 3H 70 1 G	300.00 4000.00 1386.00	1
2599	.110500439E+02 .152562747E-01-.517257413E-05	.798146428E-09-.461030406E-13	2
2600	-.142779432E+05-.312276095E+02 .149130595E+01	.376502110E-01-.258507542E-04	3
2601	.978662277E-08-.158835656E-11-.109017244E+05	.201908977E+02	4
2602	CH2CHOHCH3 C 3H 70 1 G	300.00 4000.00 1388.00	1
2603	.110944203E+02 .153549108E-01-.523574640E-05	.810964124E-09-.469665855E-13	2
2604	-.134769536E+05-.307070215E+02 .584672920E+00	.407370189E-01-.294865043E-04	3
2605	.116950656E-07-.196228356E-11-.984929391E+04	.255429190E+02	4
2606	CH2CH2CH2OH C 3H 70 1 G	300.00 4000.00 1392.00	1
2607	.106573810E+02 .155684549E-01-.527663821E-05	.814099260E-09-.470228616E-13	2
2608	-.112728087E+05-.272448749E+02 .975268381E+00	.369225253E-01-.232066980E-04	3
2609	.768472523E-08-.106762046E-11-.774554528E+04	.252661698E+02	4
2610	CH3COHCH3 C 3H 70 1 G	300.00 4000.00 1388.00	1
2611	.115026438E+02 .149881248E-01-.510421075E-05	.789864272E-09-.457135659E-13	2
2612	-.164821894E+05-.347655748E+02 .118802517E+01	.410410262E-01-.314650841E-04	3
2613	.133514692E-07-.237788249E-11-.130177234E+05	.200655998E+02	4
2614	CH3CHCH2OH C 3H 70 1 G	300.00 4000.00 1674.00	1
2615	.931287816E+01 .167579212E-01-.575555480E-05	.900584362E-09-.526566836E-13	2
2616	-.119163093E+05-.195564662E+02 .120494302E+01	.330857885E-01-.163893637E-04	3
2617	.318103918E-08-.684229288E-13-.902896295E+04	.246601603E+02	4
2618	CH3CO2H C 2H 40 2 G	300.00 4000.00 1000.00	1
2619	.767084601E+01 .135152602E-01-.525874333E-05	.893184479E-09-.553180543E-13	2
2620	-.557560970E+05-.154677315E+02 .278950201E+01	.999941719E-02 .342572245E-04	3
2621	-.509031329E-07 .206222185E-10-.534752488E+05	.141053123E+02	4
2622	HCOOH C 1H 20 2 G	300.00 4000.00 1000.00	1
2623	1 POLIMI .461383160E+01 .644963640E-02-.229082510E-05	.367160470E-09-.218736750E-13	2
2624	-.453303180E+05 .847883830E+00 .389836160E+01-	.355877950E-02 .355205380E-04	3
2625	-.438499590E-07 .171077690E-10-.467785744E+05	.734953970E+01	4
2626	HCO3 C 1H 10 3 G	300.00 4000.00 1000.00	1
2627	.726425669E+01 .532196974E-02-.196520055E-05	.323182996E-09-.195989250E-13	2
2628	-.159242239E+05-.103647520E+02 .364808935E+01	.957717212E-02 .755287366E-05	3
2629	-.181264650E-07 .827293980E-11-.146544449E+05	.967735548E+01	4
2630	HCO3H C 1H 20 3 G	300.00 4000.00 1378.00	1
2631	.987503581E+01 .464663708E-02-.167230522E-05	.268624413E-09-.159595232E-13	2
2632	-.380502456E+05-.224938942E+02 .242464726E+01	.219706380E-01-.168705546E-04	3
2633	.625612194E-08-.911645843E-12-.354828006E+05	.175027796E+02	4
2634	H2 TPIS78H 2 0 0 OG	200.000 6000.00 1000.00	1
2635	2.93286575E+00 8.26608026E-04-1.46402364E-07	1.54100414E-11-6.88804800E-16	2
2636	-8.13065581E+02-1.02432865E+00 2.34433112E+00	7.98052075E-03-1.94781510E-05	3
2637	2.01572094E-08-7.37611761E-12-9.17935173E+02	6.83010238E-01 0.00000000E+00	4
2638	H L 6/94H 1 0 0 OG	200.000 6000.00 1000.00	1
2639	0.25000000E+01 0.00000000E+00 0.00000000E+00	0.00000000E+00 0.00000000E+00	2
2640	0.25473660E+05-0.44668285E+00 0.25000000E+01	0.00000000E+00 0.00000000E+00	3
2641	0.00000000E+00 0.00000000E+00 0.25473660E+05-	0.44668285E+00 0.26219035E+05	4
2642	O2 RUS 890 2 0 0 OG	200.000 6000.00 1000.00	1
2643	3.66096065E+00 6.56365811E-04-1.41149627E-07	2.05797935E-11-1.29913436E-15	2
2644	-1.21597718E+03 3.41536279E+00 3.78245636E+00-	2.99673416E-03 9.84730201E-06	3
2645	-9.68129509E-09 3.24372837E-12-1.06394356E+03	3.65767573E+00 0.00000000E+00	4
2646	O L 1/900 1 0 0 OG	200.000 6000.00 1000.00	1
2647	2.54363697E+00-2.73162486E-05-4.19029520E-09	4.95481845E-12-4.79553694E-16	2
2648	2.92260120E+04 4.92229457E+00 3.16826710E+00-	3.27931884E-03 6.64306396E-06	3
2649	-6.12806624E-09 2.11265971E-12 2.91222592E+04	2.05193346E+00 2.99687009E+04	4
2650	H2O L 5/89H 2 O 1 0 OG	200.000 6000.00 1000.00	1
2651	0.26770389E+01 0.29731816E-02-0.77376889E-06	0.94433514E-10-0.42689991E-14	2
2652	-0.29885894E+05 0.68825500E+01 0.41986352E+01-	0.20364017E-02 0.65203416E-05	3
2653	-0.54879269E-08 0.17719680E-11-0.30293726E+05-	0.84900901E+00-0.29084817E+05	4
2654	OH IU3/03O 1 H 1 0 OG	200.000 6000.00 1000.00	1
2655	2.83853033E+00 1.10741289E-03-2.94000209E-07	4.20698729E-11-2.42289890E-15	2
2656	3.69780808E+03 5.84494652E+00 3.99198424E+00-	2.40106655E-03 4.61664033E-06	3
2657	-3.87916306E-09 1.36319502E-12 3.36889836E+03-	1.03998477E-01 4.48613328E+03	4
2658	OHV 121286O 1H 1 G	0300.00 5000.00 1000.00	1
2659	0.02882730E+02 0.10139743E-02-0.02276877E-05	0.02174683E-09-0.05126305E-14	2
2660	5.02650000E+04 0.05595712E+02 0.03637266E+02	0.01850910E-02-0.16761646E-05	3

2661	0.02387202E-07-0.08431442E-11	5.00213000E+04	0.13588605E+01	4
2662	H2O2	T 8/03H 20 2 0	OG 200.000 6000.00 1000.00	1
2663	4.57977305E+00	4.05326003E-03-1.29844730E-06	1.98211400E-10-1.13968792E-14	2
2664	-1.80071775E+04	6.64970694E-01 4.31515149E+00	-8.47390622E-04 1.76404323E-05	3
2665	-2.26762944E-08	9.08950158E-12-1.77067437E+04	3.27373319E+00-1.63425145E+04	4
2666	HO2	T 1/09H 10 2 0	OG 200.000 5000.00 1000.00	1
2667	4.17228741E+00	1.88117627E-03-3.46277286E-07	1.94657549E-11 1.76256905E-16	2
2668	3.10206839E+01	2.95767672E+00 4.30179807E+00	-4.74912097E-03 2.11582905E-05	3
2669	-2.42763914E-08	9.29225225E-12 2.64018485E+02	3.71666220E+00 1.47886045E+03	4
2670	CO	RUS 79C 10 1 0	OG 200.000 6000.00 1000.00	1
2671	0.30484859E+01	0.13517281E-02-0.48579405E-06	0.78853644E-10-0.46980746E-14	2
2672	-0.14266117E+05	0.60170977E+01 0.35795335E+01	-0.61035369E-03 0.10168143E-05	3
2673	0.90700586E-09-0.90442449E-12	-0.14344086E+05	0.35084093E+01-0.13293628E+05	4
2674	CO2	L 7/88C 10 2 0	OG 200.000 6000.00 1000.00	1
2675	0.46365111E+01	0.27414569E-02-0.99589759E-06	0.16038666E-09-0.91619857E-14	2
2676	-0.49024904E+05-0.19348955E+01	0.23568130E+01	0.89841299E-02-0.71220632E-05	3
2677	0.24573008E-08-0.14288548E-12	-0.48371971E+05	0.99009035E+01-0.47328105E+05	4
2678	HOCO	T05/06H 1 C 1 O 2	OG 200.000 6000.00 1000.00	1
2679	5.39206152E+00	4.11221455E-03-1.48194900E-06	2.39875460E-10-1.43903104E-14	2
2680	-2.38606717E+04-2.23529091E+00	2.92207919E+00	7.62453859E-03 3.29884437E-06	3
2681	-1.07135205E-08	5.11587057E-12-2.30281524E+04	1.12925886E+01-2.18076591E+04	4
2682	CH4	G 8/99C 1 H 4 0	OG 200.000 6000.00 1000.00	1
2683	1.65326226E+00	1.00263099E-02-3.31661238E-06	5.36483138E-10-3.14696758E-14	2
2684	-1.00095936E+04	9.90506283E+00 5.14911468E+00	-1.36622009E-02 4.91453921E-05	3
2685	-4.84246767E-08	1.66603441E-11-1.02465983E+04	-4.63848842E+00-8.97226656E+03	4
2686	CH3	IU0702C 1 H 3 0	OG 200.000 6000.00 1000.00	1
2687	0.29781206E+01	0.57978520E-02-0.19755800E-05	0.30729790E-09-0.17917416E-13	2
2688	0.16509513E+05	0.47224799E+01 0.36571797E+01	0.21265979E-02 0.54583883E-05	3
2689	-0.66181003E-08	0.24657074E-11 0.16422716E+05	0.16735354E+01 0.17643935E+05	4
2690	CH2	IU3/03C 1 H 2 0	OG 200.000 6000.00 1000.00	1
2691	3.14631886E+00	3.03671259E-03-9.96474439E-07	1.50483580E-10-8.57335515E-15	2
2692	4.60412605E+04	4.72341711E+00 3.71757846E+00	1.27391260E-03 2.17347251E-06	3
2693	-3.48858500E-09	1.65208866E-12 4.58723866E+04	1.75297945E+00 4.70504920E+04	4
2694	CH2(S)	IU6/03C 1 H 2 0	OG 200.000 6000.00 1000.00	1
2695	3.13501686E+00	2.89593926E-03-8.16668090E-07	1.13572697E-10-6.36262835E-15	2
2696	5.05040504E+04	4.06030621E+00 4.19331325E+00	-2.33105184E-03 8.15676451E-06	3
2697	-6.62985981E-09	1.93233199E-12 5.03662246E+04	-7.46734310E-01 5.15727280E+04	4
2698	C	L 7/88C 1 0 0	OG 200.000 6000.00 1000.00	1
2699	0.26055830E+01-0.19593434E-03	0.10673722E-06-0.16423940E-10	0.81870580E-15	2
2700	0.85411742E+05	0.41923868E+01 0.25542395E+01	-0.32153772E-03 0.73379223E-06	3
2701	-0.73223487E-09	0.26652144E-12 0.85442681E+05	0.45313085E+01 0.86195097E+05	4
2702	CH	IU3/03C 1 H 1 0	OG 200.000 6000.00 1000.00	1
2703	0.25209369E+01	0.17653639E-02-0.46147660E-06	0.59289675E-10-0.33474501E-14	2
2704	0.70946769E+05	0.74051829E+01 0.34897583E+01	0.32432160E-03-0.16899751E-05	3
2705	0.31628420E-08-0.14061803E-11	0.70612646E+05	0.20842841E+01 0.71658188E+05	4
2706	CHV	073003C 1H 1	G 0300.00 5000.00 1000.00	1
2707	0.02196223E+02	0.02340381E-01-0.07058201E-05	0.09007582E-09-0.03855040E-13	2
2708	0.10419559E+06	0.09178373E+02 0.03200202E+02	0.02072875E-01-0.05134431E-04	3
2709	0.05733890E-07-0.01955533E-10	0.10393714E+06	0.03331587E+02	4
2710	CH3O2H	A 7/05C 1 H 4 O 2	OG 200.000 6000.00 1000.00	1
2711	7.76538058E+00	8.61499712E-03-2.98006935E-06	4.68638071E-10-2.75339255E-14	2
2712	-1.82979984E+04-1.43992663E+01	2.90540897E+00	1.74994735E-02 5.28243630E-06	3
2713	-2.52827275E-08	1.34368212E-11-1.68894632E+04	1.13741987E+01-1.52423685E+04	4
2714	CH3O2	H 3C 10 2	OG 300.000 5000.000 1374.000	11
2715	6.47970487E+00	7.44401080E-03-2.52348555E-06	3.89577296E-10-2.25182399E-14	2
2716	-1.56285441E+03-8.19477074E+00	1.97339205E+00	1.53542340E-02-6.37314891E-06	3
2717	3.19930565E-10	2.82193915E-13 2.54278835E+02	1.69194215E+01	4
2718	CH2O2H	9/ 1/12 C 1H 3O 2	OG 300.000 5000.000 1410.000	21
2719	9.24697852E+00	4.60845541E-03-1.53501472E-06	2.34434830E-10-1.34573106E-14	2
2720	4.11529953E+03-2.11503248E+01	2.88976454E+00	2.09465776E-02-1.75190772E-05	3
2721	7.27819787E-09-1.18912344E-12	6.12390620E+03	1.23802076E+01	4
2722	CH3OH	T06/02C 1H 4 O 1	OG 200.000 6000.00 1000.00	1
2723	3.52726795E+00	1.03178783E-02-3.62892944E-06	5.77448016E-10-3.42182632E-14	2
2724	-2.60028834E+04	5.16758693E+00 5.65851051E+00	-1.62983419E-02 6.91938156E-05	3
2725	-7.58372926E-08	2.80427550E-11-2.56119736E+04	-8.97330508E-01-2.41746056E+04	4
2726	CH3O	IU1/03C 1 H 3 O 1	OG 200.000 6000.00 1000.00	1
2727	4.75779238E+00	7.44142474E-03-2.69705176E-06	4.38090504E-10-2.63537098E-14	2
2728	3.78111940E+02-1.96680028E+00	3.71180502E+00	-2.80463306E-03 3.76550971E-05	3
2729	-4.73072089E-08	1.86588420E-11 1.29569760E+03	6.57240864E+00 2.52571660E+03	4
2730	CH2OH	IU2/03C 1 H 3 O 1	OG 200.000 6000.00 1000.00	1
2731	5.09314370E+00	5.94761260E-03-2.06497460E-06	3.23008173E-10-1.88125902E-14	2
2732	-4.03409640E+03-1.84691493E+00	4.47834367E+00	-1.35070310E-03 2.78484980E-05	3
2733	-3.64869060E-08	1.47907450E-11-3.50072890E+03	3.30913500E+00-2.04462770E+03	4

2734	CH2O	T 5/11H	2C	1O	1	OG	200.000	6000.00	1000.00	1	
2735	3.16952665E+00	6.19320560E-03	-2.25056366E-06	3.65975660E-10	-2.20149458E-14					2	
2736	-1.45486831E+04	6.04207898E+00	4.79372312E+00	-9.90833322E-03	3.73219990E-05					3	
2737	-3.79285237E-08	1.31772641E-11	-1.43791953E+04	6.02798058E-01	-1.31293365E+04					4	
2738	HCO	T 5/03C	1H	1O	1	OG	200.000	6000.00	1000.00	1	
2739	3.92001542E+00	2.52279324E-03	-6.71004164E-07	1.05615948E-10	-7.43798261E-15					2	
2740	3.65342928E+03	3.58077056E+00	4.23754610E+00	-3.32075257E-03	1.40030264E-05					3	
2741	-1.34239995E-08	4.37416208E-12	3.87241185E+03	3.30834869E+00	5.08749163E+03					4	
2742	HCOH	MAR94 C	1H	2O	1	OG	300.	5000.	1398.	1	
2743	9.18749272E+00	1.52011152E-03	-6.27603516E-07	1.09727989E-10	-6.89655128E-15					2	
2744	7.81364593E+03	-2.73434214E+01	-2.82157421E+00	3.57331702E-02	-3.80861580E-05					3	
2745	1.86205951E-08	-3.45957838E-12	1.12956672E+04	3.48487757E+01						4	
2746	HO2CHO	6/26/95 THERMC	1H	2O	3	OG	300.000	5000.000	1378.00	21	
2747	9.87503878E+00	4.64663708E-03	-1.67230522E-06	2.68624413E-10	-1.59595232E-14					2	
2748	-3.80502496E+04	-2.24939155E+01	2.42464726E+00	2.19706380E-02	-1.68705546E-05					3	
2749	6.25612194E-09	-9.11645843E-13	-3.54828006E+04	1.75027796E+01						4	
2750	HOCH2O2H	9/ 1/12	C	1H	4O	3	OG	300.000	5000.000	1398.000	21
2751	1.24531886E+01	7.18221110E-03	-2.47029548E-06	3.85611737E-10	-2.24774193E-14					2	
2752	-4.24862928E+04	-3.58745197E+01	5.35189713E-01	3.73266553E-02	-3.15299511E-05					3	
2753	1.30352583E-08	-2.11473264E-12	-3.86609415E+04	2.71776082E+01						4	
2754	HOCH2O2	9/ 1/12	C	1H	3O	3	OG	300.000	5000.000	1377.000	21
2755	1.16406115E+01	5.72826040E-03	-2.05362036E-06	3.29070695E-10	-1.95188360E-14					2	
2756	-2.53505769E+04	-3.07332064E+01	2.82068616E+00	2.47857094E-02	-1.66186399E-05					3	
2757	4.79633095E-09	-4.28087766E-13	-2.22077036E+04	1.70599803E+01						4	
2758	OCH2O2H	7/21/14 THERMC	1H	3O	3	OG	300.000	5000.000	1418.000	31	
2759	1.29622491E+01	4.21948855E-03	-1.54275194E-06	2.50413077E-10	-1.49855537E-14					2	
2760	-1.81326406E+04	-3.87016356E+01	4.46349361E-01	3.63049606E-02	-3.26130978E-05					3	
2761	1.37050551E-08	-2.20872791E-12	-1.41972598E+04	2.72960376E+01						4	
2762	HOCH2O	2/16/99 THERMC	1H	3O	2	OG	300.000	5000.000	1452.000	11	
2763	6.39521515E+00	7.43673043E-03	-2.50422354E-06	3.84879712E-10	-2.21778689E-14					2	
2764	-2.41108840E+04	-6.63865583E+00	4.11183145E+00	7.53850697E-03	3.77337370E-06					3	
2765	-5.38746005E-09	1.45615887E-12	-2.28023001E+04	7.46807254E+00						4	
2766	O2CHO	6/26/95 THERMC	1H	1O	3	OG	300.000	5000.000	1368.00	11	
2767	7.24075139E+00	4.63312951E-03	-1.63693995E-06	2.59706693E-10	-1.52964699E-14					2	
2768	-1.87027618E+04	-6.49547212E+00	3.96059309E+00	1.06002279E-02	-5.25713351E-06					3	
2769	1.01716726E-09	-2.87487602E-14	-1.73599383E+04	1.17807483E+01						4	
2770	HOCHO	L 8/88H	2C	1O	2	OG	200.000	6000.00	1000.00	1	
2771	0.46138316E+01	0.64496364E-02	-0.22908251E-05	0.36716047E-09	-0.21873675E-13					2	
2772	-0.47514850E+05	0.84788383E+00	0.38983616E+01	-0.35587795E-02	0.35520538E-04					3	
2773	-0.43849959E-07	0.17107769E-10	-0.46770609E+05	0.73495397E+01	-0.45531246E+05					4	
2774	OCHO	ATCT/AC	1O	2H	1	OG	200.000	6000.000	1000.00	1	
2775	4.14394211E+00	5.59738818E-03	-1.99794019E-06	3.16179193E-10	-1.85614483E-14					2	
2776	-1.72459887E+04	5.07778617E+00	4.68825921E+00	-4.14871834E-03	2.55066010E-05					3	
2777	-2.84473900E-08	1.04422559E-11	-1.69867041E+04	4.28426480E+00	-1.55992356E+04					4	
2778	C2H6	G 8/88C	2H	6	0	OG	200.000	6000.00	1000.00	1	
2779	4.04666411E+00	1.53538802E-02	-5.47039485E-06	8.77826544E-10	-5.23167531E-14					2	
2780	-1.24473499E+04	-9.68698313E-01	4.29142572E+00	-5.50154901E-03	5.99438458E-05					3	
2781	-7.08466469E-08	2.68685836E-11	-1.15222056E+04	2.66678994E+00	-1.00849652E+04					4	
2782	C2H5	8/ 4/ 4 THERMC	2H	5	0	OG	300.000	5000.000	1387.000	11	
2783	5.88784390E+00	1.03076793E-02	-3.46844396E-06	5.32499257E-10	-3.06512651E-14					2	
2784	1.15065499E+04	-8.49651771E+00	1.32730217E+00	1.76656753E-02	-6.14926558E-06					3	
2785	-3.01143466E-10	4.38617775E-13	1.34284028E+04	1.71789216E+01						4	
2786	C2H5O2H	9/ 1/12	C	2H	6O	2	OG	300.000	5000.000	1390.000	31
2787	1.04823538E+01	1.34779879E-02	-4.62179078E-06	7.18618519E-10	-4.17307436E-14					2	
2788	-2.46578171E+04	-2.84294243E+01	1.83755328E+00	3.38053586E-02	-2.37548140E-05					3	
2789	9.31974865E-09	-1.58003428E-12	-2.15814086E+04	1.80977584E+01						4	
2790	C2H5O2	9/ 1/12	C	2H	5O	2	OG	300.000	5000.000	1389.000	21
2791	9.50282570E+00	1.20429839E-02	-4.09491581E-06	6.33049241E-10	-3.66133788E-14					2	
2792	-7.37069391E+03	-2.21717130E+01	3.90351912E+00	2.22599212E-02	-1.01610079E-05					3	
2793	1.71709751E-09	1.88166738E-14	-5.09654081E+03	8.98722750E+00						4	
2794	C2H4	8/12/15	C	2H	4	OG	300.000	5000.000	1392.000	01	
2795	5.07061289E+00	9.11140768E-03	-3.10506692E-06	4.80733851E-10	-2.78321396E-14					2	
2796	3.66391217E+03	-6.64501414E+00	4.81118223E-01	1.83778060E-02	-9.99633565E-06					3	
2797	2.73211039E-09	-3.01837289E-13	5.44386648E+03	1.85867157E+01						4	
2798	C2H3	8/12/15	C	2H	3	OG	300.000	5000.000	1400.000	01	
2799	4.99675415E+00	6.55838271E-03	-2.20921909E-06	3.39300272E-10	-1.95316926E-14					2	
2800	3.34604382E+04	-3.01451097E+00	1.25545094E+00	1.57481597E-02	-1.12218328E-05					3	
2801	4.50915682E-09	-7.74861577E-13	3.47435574E+04	1.69664043E+01						4	
2802	CHOCHO	C	2H	2O	2	OG	300.000	5000.000	1386.000	11	
2803	9.75438561E+00	4.97645947E-03	-1.74410483E-06	2.75586994E-10	-1.61969892E-14					2	
2804	-2.95832896E+04	-2.61878329E+01	1.88105120E+00	2.36386368E-02	-1.83443295E-05					3	
2805	6.84842963E-09	-9.92733674E-13	-2.69280190E+04	1.59154793E+01						4	
2806	C2H3OOH	4/18/ 8 THERMC	2H	4O	2	OG	300.000	5000.000	1397.000	21	

2807	1.15749951E+01	8.09909174E-03-2.81808668E-06	4.42697954E-10-2.58998042E-14	2
2808	-8.84852664E+03-3.43859117E+01	1.35644398E+00	3.37002447E-02-2.75988500E-05	3
2809	1.14222854E-08-1.89488886E-12-5.49996692E+03	1.98354466E+01		4
2810	C2H3OO	H 3C 2O 2 G	298.150 2000.000 1000.00	1
2811	6.04483828E+00	1.45511127E-02-7.50974622E-06	1.83488280E-09-1.66689681E-13	2
2812	1.01699244E+04-3.71144913E+00	1.09784776E+00	2.95333237E-02-2.27744360E-05	3
2813	7.20559155E-09-3.07929092E-13	1.13996101E+04	2.13563583E+01	4
2814	CHCHO	H 2C 2O 1 G	298.150 2000.000 1000.00	1
2815	4.92632910E+00	9.71712147E-03-5.54855980E-06	1.53068537E-09-1.64742462E-13	2
2816	2.89499494E+04	5.27874677E-01	2.33256751E+00	3
2817	5.15124155E-10	1.03836514E-12	2.96585452E+04	4
2818	C2H2	G 1/91C 2 H 2 0 0 G	200.000 6000.00 1000.00	1
2819	4.65878489E+00	4.88396667E-03-1.60828888E-06	2.46974544E-10-1.38605959E-14	2
2820	2.57594042E+04-3.99838194E+00	8.08679682E-01	2.33615762E-02-3.55172234E-05	3
2821	2.80152958E-08-8.50075165E-12	2.64289808E+04	1.39396761E+01	4
2822	C2H	T 5/10C 2 H 1 0 0 G	200.000 6000.00 1000.00	1
2823	3.66270248E+00	3.82492252E-03-1.36632500E-06	2.13455040E-10-1.23216848E-14	2
2824	6.71683790E+04	3.92205792E+00	2.89867676E+00	3
2825	2.89484755E-08-1.07502351E-11	6.70616050E+04	6.18547632E+00	4
2826	H2CC	L12/89H 2C 2 0 0G	200.000 6000.000 1000.000	1
2827	0.42780340E+01	0.47562804E-02-0.16301009E-05	0.25462806E-09-0.14886379E-13	2
2828	0.48316688E+05	0.64023701E+00	0.32815483E+01	3
2829	-0.12104432E-08	0.98189545E-12	0.48621794E+05	4
2830	C2H5OH	8/12/15 C 2H 6O 1 0G	300.000 5000.000 1402.000	21
2831	8.14483865E+00	1.28314052E-02-4.29052743E-06	6.55971721E-10-3.76506611E-14	2
2832	-3.24005526E+04-1.86241126E+01	2.15805861E-01	2.95228396E-02-1.68271048E-05	3
2833	4.49484797E-09-4.02451543E-13-2.94851823E+04		2.45725052E+01	4
2834	C2H5O	8/12/15 C 2H 5O 1 0G	300.000 5000.000 1467.000	11
2835	8.19120635E+00	1.10391986E-02-3.75270536E-06	5.80275784E-10-3.35735146E-14	2
2836	-5.66847208E+03-1.90131344E+01	2.90353584E+00	1.77256708E-02-2.69624757E-06	3
2837	-3.45830533E-09	1.25224784E-12-3.28930290E+03	1.13545591E+01	4
2838	PC2H4OH	8/12/15 C 2H 5O 1 0G	300.000 5000.000 1395.000	21
2839	8.06750150E+00	1.06143554E-02-3.57999360E-06	5.50363760E-10-3.17051769E-14	2
2840	-6.92747939E+03-1.53833428E+01	2.59479867E+00	2.27100669E-02-1.39473846E-05	3
2841	4.70095591E-09-6.90044236E-13-4.91486975E+03		1.43240718E+01	4
2842	SC2H4OH	8/12/15 C 2H 5O 1 0G	300.000 5000.000 1385.000	21
2843	8.15007136E+00	1.02549305E-02-3.40137764E-06	5.17509965E-10-2.96128942E-14	2
2844	-1.05014386E+04-1.73134615E+01	1.46281093E+00	2.39193995E-02-1.30667185E-05	3
2845	3.10615465E-09-1.85896007E-13-8.00790323E+03		1.92547092E+01	4
2846	O2C2H4OH	9/ 1/12 THERMC 2H 5O 3 0G	300.000 5000.000 1506.000	41
2847	1.27503881E+01	1.11514325E-02-3.83473891E-06	5.98155829E-10-3.48372108E-14	2
2848	-2.52770876E+04-3.54317608E+01	7.04009800E+00	1.59564166E-02	3
2849	-7.05197355E-09	2.08266026E-12-2.24524432E+04	-1.75361758E+00	4
2850	C2H4O2H	9/ 1/12 C 2H 5O 2 0G	300.000 5000.000 1389.000	31
2851	1.00590614E+01	1.13378955E-02-3.89403387E-06	6.06090687E-10-3.52212353E-14	2
2852	4.24048653E+02-2.32086536E+01	2.75788364E+00	2.88271987E-02-2.08302264E-05	3
2853	8.47401397E-09-1.48617610E-12	3.00153893E+03	1.59921711E+01	4
2854	C2H4O1-2	L 8/88C 2 H 4 O 1 0 G	200.000 6000.00 1000.00	1
2855	0.54887641E+01	0.12046190E-01-0.43336931E-05	0.70028311E-09-0.41949088E-13	2
2856	-0.91804251E+04-0.70799605E+01	0.37590532E+01	-0.94412180E-02	3
2857	-0.10080788E-06	0.40039921E-10-0.75608143E+04	0.78497475E+01-0.63304657E+04	4
2858	C2H3O1-2	A 1/05C 2 H 3 O 1 0 G	200.000 6000.00 1000.00	1
2859	5.60158035E+00	9.17613962E-03-3.28028902E-06	5.27903888E-10-3.15362241E-14	2
2860	1.71446252E+04-5.47228512E+00	3.58349017E+00	-6.02275805E-03	3
2861	-8.18540707E-08	3.30444505E-11	1.85681353E+04	4
2862	CH3CHO	L 8/88C 2 H 4 O 1 0 G	200.000 6000.00 1000.00	1
2863	0.54041108E+01	0.11723059E-01-0.42263137E-05	0.68372451E-09-0.40984863E-13	2
2864	-0.22593122E+05-0.34807917E+01	0.47294595E+01	-0.31932858E-02	3
2865	-0.57458611E-07	0.21931112E-10-0.21572878E+05	0.41030159E+01-0.19987949E+05	4
2866	CH3CO	IU2/03C 2 H 3 O 1 0 G	200.000 6000.00 1000.00	1
2867	0.53137165E+01	0.91737793E-02-0.33220386E-05	0.53947456E-09-0.32452368E-13	2
2868	-0.36450414E+04-0.16757558E+01	0.40358705E+01	0.87729487E-03	3
2869	-0.39247565E-07	0.15296869E-10-0.26820738E+04	0.78617682E+01-0.12388039E+04	4
2870	CH2CHO	T03/10C 2 H 3 O 1 0 G	200.000 6000.00 1000.00	1
2871	6.53928338E+00	7.80238629E-03-2.76413612E-06	4.42098906E-10-2.62954290E-14	2
2872	-1.18858659E+03-8.72091393E+00	2.79502600E+00	1.01099472E-02	3
2873	-3.10303145E-08	1.39436139E-11	1.62944975E+02	4
2874	O2CH2CHO	BOZ 03C 2H 3O 3 0G	300.000 5000.000 1393.000	01
2875	1.11807543E+01	9.14479256E-03-3.15089833E-06	4.91944238E-10-2.86639180E-14	2
2876	-1.55790331E+04-2.87892740E+01-1.29465843E+00		4.44936393E-02-4.26577074E-05	3
2877	2.07391950E-08-3.96828771E-12-1.18275628E+04		3.60778797E+01	4
2878	HO2CH2CO	BOZ 03C 2H 3O 3 0G	300.000 5000.000 1386.000	01
2879	1.04146322E+01	1.12680116E-02-5.17494839E-06	1.00333285E-09-6.68165911E-14	2

2880	-1.40955672E+04-2.27894400E+01	2.22681686E+00	3.56781380E-02-3.26401909E-05	3
2881	1.47651988E-08-2.64794380E-12-1.18735095E+04	1.91581197E+01		4
2882	C2H3OH 2/ 3/ 9 THERMC 2H 40 1 OG	300.000 5000.000 1410.000		11
2883	8.32598158E+00 8.03387281E-03-2.63928405E-06	3.98410726E-10-2.26551155E-14		2
2884	-1.83221436E+04-2.02080305E+01-1.27972260E-01	3.38506073E-02-3.30644935E-05		3
2885	1.64858739E-08-3.19935455E-12-1.59914544E+04	2.30438601E+01		4
2886	C2H2OH H 3C 2O 1 OG	300.000 5000.000 1401.000		11
2887	8.20268447E+00 5.92989165E-03-1.99194448E-06	3.05794341E-10-1.76114732E-14		2
2888	1.24881328E+04-1.89670436E+01 6.41642616E-01	2.61903633E-02-2.30385370E-05		3
2889	1.02804704E-08-1.81971416E-12 1.48276951E+04	2.06750999E+01		4
2890	CH2CO H 2C 2O 1 OG	300.00 5000.00 1000.00		1
2891	5.35869367E+00 6.95641586E-03-2.64802637E-06	4.65067592E-10-3.08641820E-14		2
2892	-7.90294013E+03-3.98525731E+00 1.81422511E+00	1.99008590E-02-2.21416008E-05		3
2893	1.45028521E-08-3.98877068E-12-7.05394926E+03	1.36079359E+01		4
2894	HCCO T 4/09H 1 C 2 O 1 O G	200.000 6000.00 1000.00		1
2895	5.91479333E+00 3.71408730E-03-1.30137010E-06	2.06473345E-10-1.21476759E-14		2
2896	1.93596301E+04-5.50567269E+00 1.87607969E+00	2.21205418E-02-3.58869325E-05		3
2897	3.05402541E-08-1.01281069E-11 2.01633840E+04	1.36968290E+01 2.14444387E+04		4
2898	HCCOH T12/09C 2 H 2 O 1 O G	200.000 6000.00 1000.00		1
2899	6.37509678E+00 5.49429011E-03-1.88136576E-06	2.93803536E-10-1.71771901E-14		2
2900	8.93277676E+03-8.24498007E+00 2.05541154E+00	2.52003372E-02-3.80821654E-05		3
2901	3.09890632E-08-9.89799902E-12 9.76872113E+03	1.22271534E+01 1.12217316E+04		4
2902	CH3CO3H 6/26/95 THERMC 2H 40 3 OG	300.000 5000.000 1391.000		31
2903	1.25060485E+01 9.47789695E-03-3.30402246E-06	5.19630793E-10-3.04233568E-14		2
2904	-4.59856703E+04-3.79195947E+01 2.24135876E+00	3.37963514E-02-2.53887482E-05		3
2905	9.67583587E-09-1.49266157E-12-4.24677831E+04	1.70668133E+01		4
2906	CH3CO3 4/ 3/ 0 THERMC 2H 30 3 OG	300.000 5000.000 1391.000		21
2907	1.12522498E+01 8.33652672E-03-2.89014530E-06	4.52781734E-10-2.64354456E-14		2
2908	-2.60238584E+04-2.96370457E+01 3.60373432E+00	2.70080341E-02-2.08293438E-05		3
2909	8.50541104E-09-1.43846110E-12-2.34205171E+04	1.12014914E+01		4
2910	CH3CO2 2/14/95 THERMC 2H 30 2 OG	300.000 5000.000 1395.000		11
2911	8.54059736E+00 8.32951214E-03-2.84722010E-06	4.41927196E-10-2.56373394E-14		2
2912	-2.97290678E+04-2.03883545E+01 1.37440768E+00	2.49115604E-02-1.74308894E-05		3
2913	6.24799508E-09-9.09516835E-13-2.72330150E+04	1.81405454E+01		4
2914	CH3OCH3 2/11/14 THERMC 2H 60 1 OG	300.000 5000.000 1999.000		21
2915	6.03232751E+00 1.56155270E-02-5.50761030E-06	8.75666140E-10-5.17180562E-14		2
2916	-2.52690354E+04-8.25885183E+00 2.05597390E+00	2.07019456E-02-5.00382376E-06		3
2917	-1.62279885E-09 6.84330155E-13-2.35494445E+04	1.45029944E+01		4
2918	CH3OCH2 2/11/14 THERMC 2H 50 1 OG	300.000 5000.000 1395.000		11
2919	6.62621974E+00 1.22219496E-02-4.12416696E-06	6.34127512E-10-3.65317390E-14		2
2920	-3.33965890E+03-8.95305753E+00 1.58874948E+00	2.24414123E-02-1.19434933E-05		3
2921	3.37160213E-09-4.15077249E-13-1.37208255E+03	1.87548958E+01		4
2922	CHOCHO C 2H 2O 2 G	300.00 4000.00 1000.00		1
2923	.872506895E+01 .633096819E-02-.235574814E-05	.389782853E-09-.237486912E-13		2
2924	-.291024131E+05-.203903909E+02 .468412461E+01	.478012819E-03 .426390768E-04		3
2925	-.579018239E-07 .231669328E-10-.271985007E+05	.451187184E+01		4
2926	CH2OHCHO C 2H 4O 2 G	300.00 4000.00 1000.00		1
2927	.691088832E+01 .123280849E-01-.438373062E-05	.703055164E-09-.419009846E-13		2
2928	-.400211587E+05-.696132551E+01 .614926095E+01-	.596828114E-02 .596003337E-04		3
2929	-.716663578E-07 .274014411E-10-.388356849E+05	.186644598E+01		4
2930	O2C2H4O2H C 2H 5O 4 G	300.00 4000.00 1387.00		1
2931	.145471032E+02 .123393823E-01-.427259469E-05	.668763337E-09-.390196721E-13		2
2932	-.196338761E+05-.408784236E+02 .590031872E+01	.305658528E-01-.185905950E-04		3
2933	.567871605E-08-.702799577E-12-.163916571E+05	.633051038E+01		4
2934	HO2CH2CHO C 2H 4O 3 G	300.00 4000.00 1000.00		1
2935	.127662941E+02 .102143437E-01-.363547001E-05	.583491588E-09-.347179974E-13		2
2936	-.753528536E+05-.396511752E+02 .280443702E+01	.210851644E-01 .335863233E-04		3
2937	-.702669107E-07 .326849274E-10-.720649998E+05	.151180675E+02		4
2938	CH3OCH2OH 2/12/14 THERMC 2H 60 3 OG	300.000 5000.000 1404.000		31
2939	1.28159161E+01 1.34818095E-02-4.50397729E-06	6.88229286E-10-3.94883680E-14		2
2940	-4.06745921E+04-3.78047802E+01 1.05786981E+00	4.36787095E-02-3.46383899E-05		3
2941	1.44808830E-08-2.46100643E-12-3.68851076E+04	2.43391936E+01		4
2942	CH3OCH2O2 2/12/14 THERMC 2H 50 3 OG	300.000 5000.000 1441.000		21
2943	1.19179361E+01 1.19412867E-02-3.93526185E-06	5.95756132E-10-3.39597705E-14		2
2944	-2.34231833E+04-3.20096863E+01 3.39930541E+00	3.09460407E-02-1.92548181E-05		3
2945	5.76033887E-09-6.16081571E-13-2.04433218E+04	1.39429608E+01		4
2946	CH2OCH2O2H 2/12/14 THERMC 2H 50 3 OG	300.000 5000.000 1418.000		21
2947	1.23892901E+01 1.11758961E-02-3.59249095E-06	5.34196366E-10-3.00536541E-14		2
2948	-1.80551598E+04-3.29576862E+01 1.62245477E-01	4.76101093E-02-4.52046954E-05		3
2949	2.18379311E-08-4.11295947E-12-1.46498100E+04	2.98253164E+01		4
2950	O2CH2OCH2O2H 2/12/14 ERM C 2H 5O 5 OG	300.000 5000.000 1433.000		31
2951	1.77378326E+01 1.13589899E-02-3.67382539E-06	5.49255712E-10-3.10405899E-14		2
2952	-3.82903058E+04-5.66609932E+01 2.39977678E+00	5.39881943E-02-4.87969524E-05		3

2953	2.19792134E-08-3.86106979E-12-3.37824638E+04	2.30683371E+01	4
2954	HO2CH2OCHO 2/12/14 THERMC 2H 40 4 OG	300.000 5000.000 1386.000	31
2955	1.57136128E+01 9.64430166E-03-3.44136025E-06	5.49722196E-10-3.25360322E-14	2
2956	-6.29409094E+04-5.29505242E+01 1.21909586E+00	4.28858235E-02-3.17634222E-05	3
2957	1.11542676E-08-1.49753153E-12-5.79287926E+04	2.49759193E+01	4
2958	OCH2OCHO 5/29/14 THERMC 2H 30 3 OG	300.000 5000.000 1523.000	21
2959	1.24013200E+01 7.83738243E-03-2.82992688E-06	4.55558739E-10-2.71061389E-14	2
2960	-4.68453470E+04-3.78084549E+01 1.89539692E+00	2.74118545E-02-1.36476090E-05	3
2961	1.26325603E-09 5.17970476E-13-4.27879440E+04	2.02333278E+01	4
2962	HOCH2OCO 5/29/14 THERMC 2H 30 3 OG	300.000 5000.000 1443.000	11
2963	1.11498410E+01 9.34736520E-03-3.35541548E-06	5.38037115E-10-3.19260183E-14	2
2964	-4.75012119E+04-2.95983867E+01 5.95255071E+00	8.42196282E-03 1.36741678E-05	3
2965	-1.46786275E-08 3.84143533E-12-4.44470269E+04	2.85657217E+00	4
2966	CH3OCH2O 5/15/14 THERMC 2H 50 2 OG	300.000 5000.000 1523.000	31
2967	9.81288609E+00 1.21313106E-02-4.30285768E-06	6.84443177E-10-4.03862658E-14	2
2968	-2.50760742E+04-2.51866352E+01 5.63414373E+00	8.92830283E-03 1.37225633E-05	3
2969	-1.40497059E-08 3.54625624E-12-2.22825214E+04	1.93588846E+00	4
2970	CH3OCHO T 6/08C 2 H 4 O 2 0 G	200.000 6000.00 1000.00	1
2971	6.33360880E+00 1.34851485E-02-4.84305805E-06	7.81719241E-10-4.67917447E-14	2
2972	-4.68316521E+04-6.91542601E+00 5.96757028E+00	-9.38085425E-03 7.07648417E-05	3
2973	-8.29932227E-08 3.13522917E-11-4.55713267E+04	7.50341113E-01-4.37330508E+04	4
2974	CH3OCO 5/ 8/ 3 THERMC 2H 30 2 OG	300.000 5000.000 1601.000	21
2975	9.73659803E+00 7.42432713E-03-2.65641779E-06	4.25031143E-10-2.51824924E-14	2
2976	-2.36015721E+04-2.36353471E+01 4.16215406E+00	1.38037511E-02-3.08486109E-07	3
2977	-4.56430814E-09 1.46909632E-12-2.10130301E+04	8.64301044E+00	4
2978	CH2OCHO 4/15/ 8 THERMC 2H 30 2 OG	300.000 5000.000 1442.000	21
2979	1.00960096E+01 7.19887066E-03-2.59813465E-06	4.18110812E-10-2.48723387E-14	2
2980	-2.36389018E+04-2.71144175E+01 2.31031671E+00	1.80474065E-02-2.71519637E-06	3
2981	-4.60918579E-09 1.70037078E-12-2.02910878E+04	1.71549722E+01	4
2982	C3H8 8/12/15 C 3H 8 0 OG	300.000 5000.000 1390.000	21
2983	9.15541310E+00 1.72574139E-02-5.85614868E-06	9.04190155E-10-5.22523772E-14	2
2984	-1.75762439E+04-2.77418510E+01 2.40878470E-01	3.39548599E-02-1.60930874E-05	3
2985	2.83480628E-09 2.78195172E-14-1.40362853E+04	2.16500800E+01	4
2986	NC3H7O2H 8/12/15 C 3H 80 2 OG	300.000 5000.000 1392.000	41
2987	1.42246236E+01 1.74340964E-02-5.97063522E-06	9.27753851E-10-5.38585168E-14	2
2988	-2.88159737E+04-4.74357865E+01 1.35815897E+00	4.56683952E-02-2.91646368E-05	3
2989	9.41701313E-09-1.22337394E-12-2.41528416E+04	2.23322825E+01	4
2990	NC3H7O2 8/12/15 C 3H 70 2 OG	300.000 5000.000 1390.000	31
2991	1.32753283E+01 1.61303126E-02-5.52348308E-06	8.58197168E-10-4.98172586E-14	2
2992	-1.16032968E+04-4.15091215E+01 2.13311681E+00	3.96692045E-02-2.37570127E-05	3
2993	6.96020417E-09-7.82576856E-13-7.46687112E+03	1.92444565E+01	4
2994	IC3H7O2H 8/12/15 C 3H 80 2 OG	300.000 5000.000 1405.000	41
2995	1.44896107E+01 1.68268026E-02-5.67601391E-06	8.72850837E-10-5.02993991E-14	2
2996	-3.06478491E+04-5.01352281E+01 1.77384705E+00	4.75813498E-02-3.43745304E-05	3
2997	1.31405381E-08-2.06922904E-12-2.63458844E+04	1.77669753E+01	4
2998	IC3H7O2 8/12/15 C 3H 70 2 OG	300.000 5000.000 1407.000	31
2999	1.35268120E+01 1.54306581E-02-5.17464218E-06	7.92548669E-10-4.55415379E-14	2
3000	-1.33946348E+04-4.40461451E+01 2.58517502E+00	4.16107259E-02-2.92193877E-05	3
3001	1.08614807E-08-1.66312005E-12-9.67013161E+03	1.44731300E+01	4
3002	NC3H7O 8/12/15 C 3H 70 1 OG	300.000 5000.000 1386.000	21
3003	1.15279177E+01 1.53775991E-02-5.23946272E-06	8.11382512E-10-4.69927603E-14	2
3004	-9.85099867E+03-3.54233008E+01 2.57486880E+00	3.07100600E-02-1.20048836E-05	3
3005	3.40807108E-12 7.25275283E-13-6.20913350E+03	1.45966401E+01	4
3006	IC3H7O 8/12/15 C 3H 70 1 OG	300.000 5000.000 1527.000	21
3007	1.19648494E+01 1.42943974E-02-4.71413211E-06	7.14027066E-10-4.07161162E-14	2
3008	-1.17519389E+04-3.88860959E+01 2.36108410E+00	3.45650027E-02-1.94579631E-05	3
3009	4.71536901E-09-2.64704937E-13-8.28791395E+03	1.33112436E+01	4
3010	C3H6OOH1-2 9/ 1/12 C 3H 70 2 OG	300.000 5000.000 1387.000	41
3011	1.38088686E+01 1.43845650E-02-4.74440961E-06	7.19308280E-10-4.10654123E-14	2
3012	-5.14352831E+03-4.20210765E+01 2.83631132E+00	3.88229894E-02-2.47944364E-05	3
3013	7.85644898E-09-9.58634300E-13-1.26002528E+03	1.72549973E+01	4
3014	C3H6OOH1-3 9/ 1/12 C 3H 70 2 OG	300.000 5000.000 1401.000	41
3015	1.39130757E+01 1.40218463E-02-4.55921149E-06	6.84182417E-10-3.87696213E-14	2
3016	-3.65650518E+03-4.21532559E+01 1.74271107E+00	4.53733504E-02-3.57580373E-05	3
3017	1.48540053E-08-2.49981756E-12 2.32580844E+02	2.20973041E+01	4
3018	C3H6OOH2-1 9/ 1/12 C 3H 70 2 OG	300.000 5000.000 1393.000	41
3019	1.36645362E+01 1.54329764E-02-5.29285952E-06	8.23001262E-10-4.77931121E-14	2
3020	-5.58295862E+03-4.28758364E+01 2.38465746E+00	4.42928555E-02-3.50977087E-05	3
3021	1.53695144E-08-2.81167824E-12-1.80979612E+03	1.69923285E+01	4
3022	C3H6OOH1-2O2 9/ 1/12 C 3H 70 4 OG	300.000 5000.000 1404.000	51
3023	1.91044980E+01 1.44076100E-02-4.72127814E-06	7.12631642E-10-4.05578490E-14	2
3024	-2.50270510E+04-6.63747978E+01 3.99085043E+00	5.31865338E-02-4.28597948E-05	3
3025	1.77187019E-08-2.92768695E-12-2.02143526E+04	1.34150719E+01	4

3026	C3H60OH1-302	9/ 1/12	C	3H	70	4	0G	300.000	5000.000	1416.000	51
3027	1.81661664E+01	1.47644887E-02-4.74842743E-06						7.06972467E-10-3.98305587E-14			2
3028	-2.26256376E+04-5.93719393E+01	5.56933350E+00						4.68523421E-02-3.58917784E-05			3
3029	1.43314525E-08-2.29776083E-12-1.86065694E+04							7.18655005E+00			4
3030	C3H60OH2-102	9/ 1/12	C	3H	70	4	0G	300.000	5000.000	1404.000	51
3031	1.91044980E+01	1.44076100E-02-4.72127814E-06						7.12631642E-10-4.05578490E-14			2
3032	-2.50270510E+04-6.63747978E+01	3.99085043E+00						5.31865338E-02-4.28597948E-05			3
3033	1.77187019E-08-2.92768695E-12-2.02143526E+04							1.34150719E+01			4
3034	C3KET12	10/17/12	C	3H	60	3	0G	300.000	5000.000	1385.000	41
3035	1.70187760E+01	1.32097361E-02-4.67054741E-06						7.41411770E-10-4.36869787E-14			2
3036	-4.23572589E+04-5.92615939E+01	1.03882879E+00						5.34180080E-02-4.47684141E-05			3
3037	1.94651680E-08-3.45055244E-12-3.70308881E+04							2.56511209E+01			4
3038	C3KET13	10/17/12	C	3H	60	3	0G	300.000	5000.000	1508.000	41
3039	1.73612692E+01	1.32330813E-02-4.75332110E-06						7.62529227E-10-4.52613717E-14			2
3040	-4.06248060E+04-6.17768199E+01	4.74956819E+00						3.14080991E-02-6.83838427E-06			3
3041	-5.67123901E-09	2.27686972E-12-3.51924570E+04						9.83753744E+00			4
3042	C3H51-2,30OH	8/26/3	THRMC	3H	70	4	0G	300.000	5000.000	1386.000	61
3043	2.12378169E+01	1.39519596E-02-4.94539222E-06						7.86381389E-10-4.63925564E-14			2
3044	-1.92864584E+04-7.69636561E+01	2.55619708E+00						6.13504487E-02-5.23205391E-05			3
3045	2.28208029E-08-4.02231508E-12-1.31353414E+04							2.21043799E+01			4
3046	C3H52-1,30OH	8/26/3	THRMC	3H	70	4	0G	300.000	5000.000	1379.000	61
3047	2.02817964E+01	1.48155431E-02-5.25503386E-06						8.35963453E-10-4.93308915E-14			2
3048	-1.80085066E+04-7.22688262E+01	4.12253742E+00						5.19553611E-02-3.83733727E-05			3
3049	1.45851637E-08-2.29820536E-12-1.22759164E+04							1.48367359E+01			4
3050	C3H501-20OH-3	10/13	THERC	3H	60	3	0G	300.000	5000.000	1432.000	31
3051	1.57042382E+01	1.30255692E-02-4.23544254E-06						6.35555595E-10-3.60110207E-14			2
3052	-2.77269333E+04-5.51895464E+01-3.25001215E+00							6.65787151E-02-6.18859778E-05			3
3053	2.84638649E-08-5.08511634E-12-2.22371240E+04							4.30381280E+01			4
3054	C3H501-30OH-2	10/13	THERC	3H	60	3	0G	300.000	5000.000	1434.000	21
3055	1.44493479E+01	1.36372560E-02-4.25836513E-06						6.20006211E-10-3.43451580E-14			2
3056	-2.77372360E+04-5.06099103E+01-4.43959178E+00							7.16532928E-02-7.15032351E-05			3
3057	3.51737842E-08-6.63682938E-12-2.27250412E+04							4.56394038E+01			4
3058	C3H601-2	A01/05C	3 H	6 O	1	0	G	200.000	6000.000	1000.000	1
3059	8.01491079E+00	1.73919953E-02-6.26027968E-06						1.01188256E-09-6.06239111E-14			2
3060	-1.51980838E+04-1.88279964E+01	3.42806676E+00						6.25176642E-03	6.13196311E-05		3
3061	-8.60387185E-08	3.51371393E-11-1.28446646E+04						1.04244994E+01-1.11564001E+04			4
3062	C3H601-3	A11/04C	3 H	6 O	1	0	G	200.000	6000.000	1000.000	1
3063	6.80716906E+00	1.88824545E-02-6.79082475E-06						1.09713919E-09-6.57154952E-14			2
3064	-1.36547629E+04-1.35382154E+01	5.15283752E+00-1.86401716E-02						1.29980652E-04			3
3065	-1.58629974E-07	6.20668783E-11-1.13243512E+04						4.73561224E+00-9.75233898E+03			4
3066	C3H6	8/12/15	C	3H	6	0	0G	298.000	6000.000	1000.000	01
3067	6.59032304E+00	1.52592866E-02-5.30369441E-06						8.35510888E-10-4.91215549E-14			2
3068	-2.47481113E+02-1.15748238E+01-1.54606737E+00							4.36553128E-02-5.61392417E-05			3
3069	4.98421927E-08-1.84798923E-11	2.07056233E+03						2.99232495E+01			4
3070	C3H5-A	8/12/15	C	3H	5	0	0G	298.000	6000.000	1000.000	01
3071	7.37604097E+00	1.23449782E-02-4.26463882E-06						6.69045835E-10-3.92202554E-14			2
3072	1.77332960E+04-1.61758204E+01-3.32899442E+00							5.38423469E-02-7.65500752E-05			3
3073	6.35512285E-08-2.14283003E-11	2.03420628E+04						3.68038362E+01			4
3074	C3H5-S	8/12/15	C	3H	5	0	0G	300.000	5000.000	1390.000	11
3075	7.95954498E+00	1.11163183E-02-3.75197834E-06						5.77246260E-10-3.32768957E-14			2
3076	2.80567891E+04-1.79800372E+01	1.61793372E+00						2.44803904E-02-1.41856503E-05			3
3077	4.16402233E-09-4.90904795E-13	3.04291037E+04						1.66341443E+01			4
3078	C3H5-T	8/12/15	C	3H	5	0	0G	300.000	5000.000	1376.000	11
3079	7.69949212E+00	1.17803985E-02-4.07791749E-06						6.38119222E-10-3.72229675E-14			2
3080	2.61747145E+04-1.68305890E+01	2.29256998E+00						1.98527646E-02-6.42635654E-06			3
3081	-5.90016395E-10	5.05491095E-13	2.85773377E+04					1.39407124E+01			4
3082	CC3H6	C	3H	6 O	0	0	G	200.000	6000.000	1000.	1
3083	6.21663437E+00	1.65393591E-02-5.90075838E-06						9.48095199E-10-5.65661522E-14			2
3084	2.95937491E+03-1.36041009E+01	2.83278674E+00-5.21028618E-03						9.29583210E-05			3
3085	-1.22753194E-07	4.99191366E-11	5.19520048E+03					1.08306333E+01	6.41047999E+03		4
3086	C3H5O	KPS12	C	3H	50	1	0G	300.000	5000.000	1402.000	01
3087	1.02638186E+01	1.17609932E-02-3.89837957E-06						5.92650815E-10-3.38867417E-14			2
3088	7.25938472E+03-2.75108651E+01	8.24068673E-01						3.46749909E-02-2.51786795E-05			3
3089	9.56781953E-09-1.48085302E-12	1.04203725E+04						2.28283070E+01			4
3090	CH2CHOCH2	8/ 8/15	C	3H	50	1	0G	300.000	5000.000	1384.000	21
3091	1.20076931E+01	1.05055204E-02-3.69920541E-06						5.85629983E-10-3.44431587E-14			2
3092	6.97311613E+03-3.75189859E+01	1.15350351E+00						3.51253596E-02-2.50071619E-05			3
3093	9.00715632E-09-1.32376643E-12	1.08300872E+04						2.10606652E+01			4
3094	CH3CHCHO	C	3H	50	1	0	G	300.000	5000.000	1424.000	21
3095	1.06781476E+01	1.12805711E-02-3.89010759E-06						6.07617268E-10-3.54120848E-14			2
3096	-7.73234209E+03-3.24971238E+01	1.47166733E+00						2.69251618E-02-1.00248013E-05			3
3097	-1.13421435E-09	1.03416658E-12-4.04142023E+03						1.88722472E+01			4
3098	RALD3BG	C	3H	50	1	G		300.00	4000.00	1366.00	1

3099	.979372730E+01	.168079281E-01-	.684815970E-05	.118460585E-08-	.738195109E-13								2
3100	-.875662870E+04-	.294639062E+02	.667614768E+01	.261082031E-02	.280410577E-04								3
3101	-.226802600E-07	.516442572E-11-	.510504908E+04-	.439698728E+01									4
3102	RALD3BG	C	3H	50	1	OG	300.000	5000.000	1424.000				21 !
	CH3CHCHO												
3103	1.06781476E+01	1.12805711E-02-	3.89010759E-06	6.07617268E-10-	3.54120848E-14								2
3104	-7.73234209E+03-	3.24971238E+01	1.47166733E+00	2.69251618E-02-	1.00248013E-05								3
3105	-1.13421435E-09	1.03416658E-12-	4.04142023E+03	1.88722472E+01									4
3106	AC4H7OOH	6/17/13	THERMC	4H	80	2	OG	300.000	5000.000	1395.000			41
3107	1.47661443E+01	2.12235231E-02-	7.09403390E-06	1.08423759E-09-	6.22145708E-14								2
3108	-1.35617411E+04-	4.77449138E+01	1.33470633E+00	5.27831440E-02-	3.58861360E-05								3
3109	1.32495013E-08-	2.06619289E-12-	8.87891782E+03	2.43857336E+01									4
3110	C3H6OH1-2	9/ 1/12	C	3H	70	1	OG	300.000	5000.000	1395.000			31
3111	1.00338281E+01	1.60227373E-02-	5.41658448E-06	8.34191172E-10-	4.81215988E-14								2
3112	-1.27912397E+04-	2.39034395E+01	5.05207596E-01	3.63869988E-02-	2.15530901E-05								3
3113	6.45584786E-09-	7.71267046E-13-	9.26980840E+03	2.79804349E+01									4
3114	CH3CHCO	03/03/95	THERMC	3H	40	1	OG	300.000	5000.000	1400.00			41
3115	1.00219123E+01	9.56966300E-03-	3.26221644E-06	5.05231706E-10-	2.92593257E-14								2
3116	-1.42482738E+04-	2.77829973E+01	1.48380119E+00	3.22203013E-02-	2.70250033E-05								3
3117	1.20499164E-08-	2.18365931E-12-	1.15276540E+04	1.71552068E+01									4
3118	AC3H5OOH	GOLDSMITH	C	3H	60	2	OG	298.0	6000.0	1000.000			31
3119	1.20838649E+01	1.47946591E-02-	5.13212591E-06	8.07504999E-10-	4.74394983E-14								2
3120	-1.02184463E+04-	3.36434791E+01	3.18124993E+00	4.35233041E-02-	5.16277353E-05								3
3121	4.32011427E-08-	1.57714983E-11-	7.63521503E+03	1.21725683E+01									4
3122	C3H6OH2-1	8/ 9/ 4	THERMC	3H	70	1	OG	300.000	5000.000	1392.000			31
3123	1.12222277E+01	1.36444398E-02-	4.51406709E-06	7.10523275E-10-	4.22690392E-14								2
3124	-1.75350136E+04-	3.18911926E+01	1.09670360E+00	3.80727565E-02-	2.75022497E-05								3
3125	1.07477493E-08-	1.74895773E-12-	1.40764487E+04	2.22475799E+01									4
3126	HOC3H6O2	9/ 1/12	C	3H	70	3	OG	300.000	5000.000	1407.000			41
3127	1.56948113E+01	1.57703692E-02-	5.30501726E-06	8.14307835E-10-	4.68666193E-14								2
3128	-3.24540840E+04-	5.06084117E+01	2.84960487E+00	4.77244552E-02-	3.60392974E-05								3
3129	1.43479922E-08-	2.33507634E-12-	2.82106103E+04	1.76478537E+01									4
3130	SC3H5OH	2/ 3/ 9	C	3H	60	1	OG	300.000	5000.000	1404.000			21
3131	1.11222064E+01	1.27745410E-02-	4.25315532E-06	6.48216484E-10-	3.71190850E-14								2
3132	-2.36690795E+04-	3.41335182E+01-	3.53977226E-02	4.34969453E-02-	3.74479918E-05								3
3133	1.70906074E-08-	3.13775054E-12-	2.02502608E+04	2.41528201E+01									4
3134	IC3H5OH	8/ 1/95	THERMC	3H	60	1	OG	300.000	5000.000	1374.00			21
3135	1.07381025E+01	1.31698194E-02-	4.41529622E-06	6.77009837E-10-	3.89608901E-14								2
3136	-2.47298321E+04-	3.13634050E+01	1.58376391E+00	3.16215366E-02-	1.73664942E-05								3
3137	4.18927663E-09-	2.79899620E-13-	2.12643496E+04	1.88313766E+01									4
3138	C3H5OH	T06/10C	3 H	6 O	1	0 G	200.000	6000.00	1000.00				1
3139	8.72477114E+00	1.63942712E-02-	5.90852993E-06	9.53262253E-10-	5.70318010E-14								2
3140	-1.90496618E+04-	1.97198674E+01	3.15011905E+00	1.28538274E-02	4.28438434E-05								3
3141	-6.67818707E-08	2.80408237E-11-	1.66413668E+04	1.35066359E+01-	1.48710589E+04								4
3142	CH2CCH2OH	9/ 8/95	THERMC	3H	50	1	OG	300.000	5000.000	1372.00			21
3143	9.70702027E+00	1.13972660E-02-	3.77993962E-06	5.75209277E-10-	3.29229125E-14								2
3144	1.93212884E+03-	2.25012933E+01	2.88422544E+00	2.42428071E-02-	1.14152268E-05								3
3145	1.71775334E-09	1.42177454E-13	1.17935615E+04	1.52102335E+01									4
3146	C3H4-P	T 2/90H	4 C	3	0	0 G	200.000	6000.00	1000.00				1
3147	0.60252400E+01	0.11336542E-01-	0.40223391E-05	0.64376063E-09-	0.38299635E-13								2
3148	0.19620942E+05-	0.86043785E+01	0.26803869E+01	0.15799651E-01	0.25070596E-05								3
3149	-0.13657623E-07	0.66154285E-11	0.20802374E+05	0.98769351E+01	0.22302059E+05								4
3150	C3H4-A	L 8/89C	3 H	4	0	0 G	200.000	6000.00	1000.00				1
3151	0.63168722E+01	0.11133728E-01-	0.39629378E-05	0.63564238E-09-	0.37875540E-13								2
3152	0.20117495E+05-	0.10995766E+02	0.26130445E+01	0.12122575E-01	0.18539880E-04								3
3153	-0.34525149E-07	0.15335079E-10	0.21541567E+05	0.10226139E+02	0.22962267E+05								4
3154	C3H3	T 7/11C	3 H	3	0	0 G	200.000	6000.00	1000.000				1
3155	7.14221719E+00	7.61902211E-03-	2.67460030E-06	4.24914904E-10-	2.51475443E-14								2
3156	3.95709594E+04-	1.25848690E+01	1.35110873E+00	3.27411291E-02-	4.73827407E-05								3
3157	3.76310220E-08-	1.18541128E-11	4.07679941E+04	1.52058598E+01	4.22762135E+04								4
3158	CC3H4	T12/81C	3H	4	0	OG	300.000	5000.00	1000.00				1
3159	0.66999931E+01	0.10357372E-01-	0.34551167E-05	0.50652949E-09-	0.26682276E-13								2
3160	0.30199051E+05-	0.13378770E+02-	0.24621047E-01	0.23197215E-01-	0.18474357E-05								3
3161	-0.15927593E-07	0.86846155E-11	0.32334137E+05	0.22729762E+02	0.3332728 E+05								4
3162	C3H2	T12/00C	3 H	2	0	0 G	200.000	6000.00	1000.00				1
3163	6.67324762E+00	5.57728845E-03-	1.99180164E-06	3.20289156E-10-	1.91216272E-14								2
3164	7.57571184E+04-	9.72894405E+00	2.43417332E+00	1.73013063E-02-	1.18294047E-05								3
3165	1.02756396E-09	1.62626314E-12	7.69074892E+04	1.21012230E+01	7.83005132E+04								4
3166	H2CCC(S)	OC	3H	2	0	OG	200.000	5000.000	1500.00				0 1
3167	0.64888762E+01	0.53112789E-02-	0.17809490E-05	0.27252642E-09-	0.15619590E-13								2
3168	0.63661864E+05-	0.10064283E+02	0.37229726E+01	0.92589854E-02-	0.23006191E-05								3
3169	-0.10200808E-08	0.45374357E-12	0.64877289E+05	0.56865936E+01									4
3170	C3H2 (S)	OC	3H	2	0	OG	200.000	5000.000	900.00				0 1

3171	0.77642570E+01	0.47112774E-02	-0.16170637E-05	0.25472406E-09	-0.15038572E-13	2					
3172	0.66849672E+05	-0.15098549E+02	0.52976482E+01	0.16987466E-01	-0.24266517E-04	3					
3173	0.18653681E-07	-0.55763001E-11	0.67240466E+05	-0.37540041E+01		4					
3174	C3H2C	OC	3H	2	0	OG	200.000	5000.000	1500.00	0	1
3175	0.65632680E+01	0.52363256E-02	-0.17544830E-05	0.26866106E-09	-0.15428509E-13	2					
3176	0.56514618E+05	-0.12000607E+02	0.11295888E+01	0.17287401E-01	-0.11366823E-04	3					
3177	0.34569296E-08	-0.36615951E-12	0.58419080E+05	0.17331448E+02		4					
3178	PC3H4OH-2	4/ 2/13	THERMC	3H	50	1	OG	300.000	5000.000	1403.000	21
3179	1.07164095E+01	1.06066461E-02	-3.51374060E-06	5.33713932E-10	-3.04901511E-14	2					
3180	4.98486803E+03	-2.98329329E+01	1.42757363E+00	3.64825569E-02	-3.18007132E-05	3					
3181	1.46914605E-08	-2.72331227E-12	7.80342663E+03	1.85890339E+01		4					
3182	SC3H4OH	3/28/13	C	3H	50	1	OG	300.000	5000.000	1407.000	21
3183	1.20968484E+01	9.43976596E-03	-3.10773897E-06	4.69609188E-10	-2.67165710E-14	2					
3184	-3.85854894E+02	-3.76795997E+01	1.72870561E+00	4.41015870E-02	-4.72013860E-05	3					
3185	2.52073596E-08	-5.13375710E-12	2.22720503E+03	1.43928257E+01		4					
3186	C3H3O	2/17/14	CZHOUH	3C	30	1	G	298.150	2000.000	1000.00	1
3187	4.19355696E+00	1.95625103E-02	-1.22336450E-05	3.90615061E-09	-5.08539231E-13	2					
3188	3.14931737E+04	5.03216224E+00	8.75023836E-01	3.51184068E-02	-3.89901356E-05	3					
3189	2.40255750E-08	-6.10883631E-12	3.20427921E+04	2.04717253E+01		4					
3190	C3H3O2H	1/31/13	C	3H	40	2	OG	300.000	5000.000	1385.000	31
3191	1.38152174E+01	8.62174763E-03	-3.06710006E-06	4.88874247E-10	-2.88888385E-14	2					
3192	6.29182941E+03	-4.39151257E+01	1.09787313E+00	4.22717882E-02	-3.83969355E-05	3					
3193	1.77405069E-08	-3.27674312E-12	1.03592314E+04	2.30651783E+01		4					
3194	C2HCHO	1/31/13	C	3H	20	1	OG	300.000	5000.000	2012.000	11
3195	7.99952054E+00	7.07825497E-03	-2.63086819E-06	4.33073185E-10	-2.62003284E-14	2					
3196	8.71863156E+03	-1.57226237E+01	4.20776611E+00	1.34382727E-02	-5.15442099E-06	3					
3197	-2.24570818E-11	2.74111284E-13	1.02117375E+04	5.43871873E+00		4					
3198	C2H5CHO	8/12/15	C	3H	60	1	OG	300.000	5000.000	1449.000	21
3199	1.06224453E+01	1.35569132E-02	-4.60754771E-06	7.12755462E-10	-4.12631683E-14	2					
3200	-2.78692266E+04	-3.16628752E+01	2.18895588E+00	2.58289987E-02	-6.04170058E-06	3					
3201	-3.70702654E-09	1.57131095E-12	-2.42671146E+04	1.61496330E+01		4					
3202	C2H5CO	A10/04C	3 H	5	0	1	O G	200.000	6000.00	1000.00	1
3203	6.52325448E+00	1.54211952E-02	-5.50898157E-06	8.85889862E-10	-5.28846399E-14	2					
3204	-7.19631634E+03	-5.19862218E+00	6.25722402E+00	-9.17612184E-03	7.61190493E-05	3					
3205	-9.05514997E-08	3.46198215E-11	-5.91616484E+03	2.23330599E+00	-3.94851891E+03	4					
3206	CH2CH2CHO		C	3H	50	1	OG	300.000	5000.000	1437.000	21
3207	1.00673122E+01	1.14971005E-02	-3.90137798E-06	6.03029101E-10	-3.48958224E-14	2					
3208	-2.75080876E+03	-2.58818404E+01	2.55799036E+00	2.23391941E-02	-4.89741478E-06	3					
3209	-3.58874384E-09	1.47175030E-12	4.53127696E+02	1.67016285E+01		4					
3210	C2H3CHO	KPS12	C	3H	40	1	OG	300.000	5000.000	1398.000	01
3211	9.99155394E+00	9.82348001E-03	-3.31203088E-06	5.09524422E-10	-2.93821890E-14	2					
3212	-1.25303509E+04	-2.85168883E+01	7.33844455E-01	3.17482671E-02	-2.29599468E-05	3					
3213	8.42104232E-09	-1.23613478E-12	-9.38473548E+03	2.10308851E+01		4					
3214	C2H3CO	KPS12	C	3H	30	1	OG	300.000	5000.000	1395.000	01
3215	8.86032735E+00	8.48985205E-03	-2.90350080E-06	4.50763986E-10	-2.61524281E-14	2					
3216	7.73489171E+03	-2.06978792E+01	1.65335195E+00	2.57402596E-02	-1.89009911E-05	3					
3217	7.29174972E-09	-1.16083226E-12	1.02020654E+04	1.78705872E+01		4					
3218	CH3COCH3	8/12/15	C	3H	60	1	OG	300.000	5000.000	1394.000	21
3219	8.87619308E+00	1.45700263E-02	-4.84823280E-06	7.38614777E-10	-4.22831194E-14	2					
3220	-3.06046242E+04	-2.12730484E+01	2.20008426E+00	2.74019559E-02	-1.31342003E-05	3					
3221	2.57150371E-09	-6.21509091E-14	-2.79933966E+04	1.55883508E+01		4					
3222	CH3COCH2	2/14/13	THERMC	3H	50	1	OG	300.000	5000.000	1387.000	21
3223	1.09524298E+01	1.11458668E-02	-3.86262877E-06	6.05088857E-10	-3.53293362E-14	2					
3224	-9.60833727E+03	-3.15622776E+01	1.13381826E+00	3.25095045E-02	-2.10424651E-05	3					
3225	6.64421151E-09	-8.12618901E-13	-6.04868361E+03	2.17158655E+01		4					
3226	CH3COCH2O2	2/14/13	THERMC	3H	50	3	OG	300.000	5000.000	1397.000	31
3227	1.65756401E+01	1.06465489E-02	-3.61368681E-06	5.59053564E-10	-3.23832271E-14	2					
3228	-2.42541401E+04	-5.45304899E+01	1.19378141E+00	4.98027161E-02	-4.17999508E-05	3					
3229	1.74527607E-08	-2.88198761E-12	-1.93244224E+04	2.67877493E+01		4					
3230	CH3COCH2O	2/ 8/13	THERMC	3H	50	2	OG	300.000	5000.000	2002.000	21
3231	9.84061707E+00	1.59181106E-02	-5.85164644E-06	9.56160073E-10	-5.75477263E-14	2					
3232	-2.11214823E+04	-2.12330791E+01	5.85960137E+00	1.78954926E-02	7.41506398E-07	3					
3233	-5.40032753E-09	1.47393197E-12	-1.90714739E+04	2.70987883E+00		4					
3234	C3KET21	2/14/13	THERMC	3H	60	3	OG	300.000	5000.000	1394.000	41
3235	1.75768076E+01	1.20311704E-02	-4.11633942E-06	6.40149366E-10	-3.72127562E-14	2					
3236	-4.15502347E+04	-6.09097100E+01	-8.74352903E-01	6.12501498E-02	-5.51474542E-05	3					
3237	2.48491014E-08	-4.42613472E-12	-3.58060819E+04	3.59306224E+01		4					
3238	NC4H10	8/12/15	C	4H	10	0	OG	300.000	5000.000	1392.000	31
3239	1.24923813E+01	2.15951935E-02	-7.34277611E-06	1.13529859E-09	-6.56730149E-14	2					
3240	-2.17598985E+04	-4.41546866E+01	-9.20862487E-02	4.69703816E-02	-2.54761945E-05	3					
3241	6.35894738E-09	-5.16005946E-13	-1.69556758E+04	2.49101571E+01		4					
3242	PC4H9	8/12/15	C	4H	9	0	OG	300.000	5000.000	1393.000	31
3243	1.18547949E+01	1.96962095E-02	-6.71054229E-06	1.03891144E-09	-6.01513573E-14	2					

3244	3.38182243E+03-3.72343446E+01	4.09644702E-01	4.29511341E-02-2.36582809E-05	3	
3245	6.15744917E-09-5.64300671E-13	7.74319150E+03	2.55312526E+01	4	
3246	SC4H9	8/12/15	C 4H 9 0 OG	300.000 5000.000 1682.000	31
3247	9.25139144E+00	2.24301385E-02-7.82648592E-06	1.23559460E-09-7.26249864E-14	2	
3248	3.11148804E+03-2.16080436E+01	9.42662332E-01	3.77414530E-02-1.58911963E-05	3	
3249	1.75489317E-09	2.89725750E-13	6.20542636E+03	2.42126605E+01	4
3250	PC4H9O		C 4H 90 1 OG	300.000 5000.000 1396.000	31
3251	1.53371588E+01	1.92789649E-02-6.56856538E-06	1.01724003E-09-5.89183466E-14	2	
3252	-1.41958782E+04-5.45071855E+01	1.84659093E+00	4.61054365E-02-2.44856516E-05	3	
3253	5.11293268E-09-1.07538298E-13	9.09206746E+03	1.95237441E+01	4	
3254	SC4H9O		C 4H 90 1 OG	300.000 5000.000 1411.000	31
3255	1.52130012E+01	1.90029969E-02-6.39004701E-06	9.80774402E-10-5.64493733E-14	2	
3256	-1.59888805E+04-5.43195369E+01	2.01772535E+00	4.70083969E-02-2.74726645E-05	3	
3257	7.36290028E-09-6.30414237E-13	-1.11892176E+04	1.74371746E+01	4	
3258	PC4H9O2	8/12/15	C 4H 90 2 OG	300.000 5000.000 1391.000	41
3259	1.66120049E+01	2.04752336E-02-7.01415262E-06	1.09010510E-09-6.32913959E-14	2	
3260	-1.57901735E+04-5.79272276E+01	1.80541406E+00	5.26493060E-02-3.30870383E-05	3	
3261	1.04593484E-08-1.32305701E-12	-1.03866773E+04	2.24829685E+01	4	
3262	SC4H9O2		C 4H 90 2 OG	300.000 5000.000 1403.000	41
3263	1.68209433E+01	1.98834074E-02-6.71755569E-06	1.03411636E-09-5.96371075E-14	2	
3264	-1.75815350E+04-5.95731156E+01	2.27751066E+00	5.44334651E-02-3.82988187E-05	3	
3265	1.42447767E-08-2.18864515E-12	-1.25909100E+04	1.83237264E+01	4	
3266	PC4H9O2H	8/12/15	C 4H 100 2 OG	300.000 5000.000 1393.000	51
3267	1.75610913E+01	2.17832847E-02-7.46366287E-06	1.16012068E-09-6.73630029E-14	2	
3268	-3.30036118E+04-6.38547212E+01	1.04177717E+00	5.85996659E-02-3.84212378E-05	3	
3269	1.28728231E-08-1.75491358E-12	-2.70744200E+04	2.55179528E+01	4	
3270	SC4H9O2H		C 4H 100 2 OG	300.000 5000.000 1402.000	51
3271	1.78075939E+01	2.12546017E-02-7.20960281E-06	1.11291271E-09-6.43060022E-14	2	
3272	-3.48455718E+04-6.58011470E+01	1.44010868E+00	6.05300206E-02-4.36262678E-05	3	
3273	1.66226146E-08-2.61556930E-12	-2.92631492E+04	2.17354113E+01	4	
3274	C4H8OOH1-2		C 4H 90 2 OG	300.000 5000.000 1389.000	51
3275	1.67810269E+01	1.99677597E-02-6.85257220E-06	1.06628911E-09-6.19616154E-14	2	
3276	-9.14762760E+03-5.68667893E+01	2.91878364E+00	4.86143951E-02-2.81342168E-05	3	
3277	7.64456491E-09-7.32889491E-13	-3.94464787E+03	1.89326241E+01	4	
3278	C4H8OOH1-3		C 4H 90 2 OG	300.000 5000.000 1396.000	51
3279	1.61247782E+01	2.02420980E-02-6.88631475E-06	1.06534945E-09-6.16599545E-14	2	
3280	-9.16802012E+03-5.26575415E+01	2.46292502E+00	4.70131194E-02-2.42145198E-05	3	
3281	4.65407810E-09	1.62198662E-14-3.95787917E+03	2.24569578E+01	4	
3282	C4H8OOH1-4		C 4H 90 2 OG	300.000 5000.000 1393.000	51
3283	1.69217927E+01	1.99305696E-02-6.85727522E-06	1.06879474E-09-6.21774931E-14	2	
3284	-7.87920857E+03-5.76630146E+01	1.35984095E+00	5.52812385E-02-3.75640846E-05	3	
3285	1.32624209E-08-1.93623296E-12	-2.34455867E+03	2.63197893E+01	4	
3286	C4H8OOH2-1		C 4H 90 2 OG	300.000 5000.000 1404.000	51
3287	1.77648250E+01	1.87777052E-02-6.36410476E-06	9.81958228E-10-5.67252066E-14	2	
3288	-9.93851667E+03-6.28169590E+01	2.32205003E+00	5.55032280E-02-3.97237996E-05	3	
3289	1.47353739E-08-2.22481777E-12	-4.67331585E+03	1.98332327E+01	4	
3290	C4H8OOH2-3		C 4H 90 2 OG	300.000 5000.000 1403.000	51
3291	1.70353922E+01	1.92729887E-02-6.50684653E-06	1.00126173E-09-5.77270961E-14	2	
3292	-1.09437234E+04-5.87403112E+01	3.30289851E+00	5.08231524E-02-3.39615358E-05	3	
3293	1.17622237E-08-1.66012808E-12	-6.13671017E+03	1.51726178E+01	4	
3294	C4H8OOH2-4		C 4H 90 2 OG	300.000 5000.000 1403.000	51
3295	1.72354039E+01	1.91946365E-02-6.49946502E-06	1.00210964E-09-5.78559962E-14	2	
3296	-9.71158144E+03-5.98986150E+01	1.82672511E+00	5.69912331E-02-4.24389492E-05	3	
3297	1.67119278E-08-2.70635765E-12	-4.54629884E+03	2.22051948E+01	4	
3298	C4H8O1-2		C 4H 80 1 OG	300.000 5000.000 1463.000	21
3299	1.41886108E+01	1.63162740E-02-5.16581368E-06	7.60173986E-10-4.24548403E-14	2	
3300	-2.02839382E+04-5.12817914E+01	-4.29657099E+00	6.75906816E-02-5.89614134E-05	3	
3301	2.59401158E-08-4.45926746E-12	-1.48799944E+04	4.47755567E+01	4	
3302	C4H8O1-3		C 4H 80 1 OG	300.000 5000.000 1447.000	11
3303	1.32076917E+01	1.77467973E-02-5.69933762E-06	8.47771212E-10-4.77345874E-14	2	
3304	-2.11717546E+04-4.78386420E+01	-5.37284363E+00	6.62224444E-02-5.35318273E-05	3	
3305	2.19451842E-08-3.54479816E-12	-1.54144887E+04	4.98345472E+01	4	
3306	C4H8O1-4		C 4H 80 1 OG	300.000 5000.000 1484.000	01
3307	1.22763349E+01	1.89105920E-02-6.09113637E-06	9.08066245E-10-5.12149503E-14	2	
3308	-2.92260872E+04-4.41235671E+01	-7.78117916E+00	6.98405060E-02-5.45315920E-05	3	
3309	2.13029617E-08-3.24666872E-12	-2.28996340E+04	6.17620955E+01	4	
3310	C4H8O2-3		C 4H 80 1 OG	300.000 5000.000 1403.000	21
3311	1.06341771E+01	2.41442268E-02-1.13123977E-05	2.25480711E-09-1.54043041E-13	2	
3312	-2.10383343E+04-3.36763636E+01	-4.48183187E+00	6.89313360E-02-6.15371646E-05	3	
3313	2.73743747E-08-4.85890996E-12	-1.68924193E+04	4.38882874E+01	4	
3314	C4H8OOH1-2O2		C 4H 90 4 OG	300.000 5000.000 1400.000	61
3315	2.15734750E+01	2.04528589E-02-6.99497777E-06	1.08597818E-09-6.30071127E-14	2	
3316	-2.88428166E+04-7.84560716E+01	3.02241018E+00	6.53862812E-02-4.89645658E-05	3	

3317	1.90437784E-08-3.02309317E-12-2.25805572E+04	2.05729328E+01	4
3318	C4H8OOH1-3O2 C 4H 90 4 OG	300.000 5000.000 1400.000	61
3319	2.15734750E+01 2.04528589E-02-6.99497777E-06	1.08597818E-09-6.30071127E-14	2
3320	-2.88428166E+04-7.84560716E+01 3.02241018E+00	6.53862812E-02-4.89645658E-05	3
3321	1.90437784E-08-3.02309317E-12-2.25805572E+04	2.05729328E+01	4
3322	C4H8OOH1-4O2 C 4H 90 4 OG	300.000 5000.000 1387.000	71
3323	2.26393370E+01 1.98017374E-02-6.92349554E-06	1.09100182E-09-6.39617643E-14	2
3324	-2.75442161E+04-8.40747892E+01 2.91974455E+00	6.34948347E-02-4.29699499E-05	3
3325	1.42283155E-08-1.84506244E-12-2.04867301E+04	2.26279495E+01	4
3326	C4H8OOH2-1O2 C 4H 90 4 OG	300.000 5000.000 1400.000	61
3327	2.15734750E+01 2.04528589E-02-6.99497777E-06	1.08597818E-09-6.30071127E-14	2
3328	-2.88428166E+04-7.84560716E+01 3.02241018E+00	6.53862812E-02-4.89645658E-05	3
3329	1.90437784E-08-3.02309317E-12-2.25805572E+04	2.05729328E+01	4
3330	C4H8OOH2-3O2 C 4H 90 4 OG	300.000 5000.000 1408.000	61
3331	2.19463055E+01 1.97307584E-02-6.65765380E-06	1.02424556E-09-5.90486257E-14	2
3332	-3.07772334E+04-8.12053531E+01 3.34683971E+00	6.67468082E-02-5.25088611E-05	3
3333	2.14288389E-08-3.53381793E-12-2.47340662E+04	1.73189003E+01	4
3334	C4H8OOH2-4O2 C 4H 90 4 OG	300.000 5000.000 1400.000	61
3335	2.15734750E+01 2.04528589E-02-6.99497777E-06	1.08597818E-09-6.30071127E-14	2
3336	-2.88428166E+04-7.84560716E+01 3.02241018E+00	6.53862812E-02-4.89645658E-05	3
3337	1.90437784E-08-3.02309317E-12-2.25805572E+04	2.05729328E+01	4
3338	C4H71-2,4OOH C 4H 90 4 OG	300.000 5000.000 1398.000	71
3339	2.18629952E+01 1.99359398E-02-6.85103949E-06	1.06712096E-09-6.20561893E-14	2
3340	-2.10042547E+04-7.80706874E+01 2.99387028E+00	6.52913914E-02-4.87958562E-05	3
3341	1.88107554E-08-2.95256716E-12-1.46021097E+04	2.27763716E+01	4
3342	C4H72-1,3OOH C 4H 90 4 OG	300.000 5000.000 1395.000	71
3343	2.14626449E+01 2.02946207E-02-6.97889021E-06	1.08750673E-09-6.32605387E-14	2
3344	-2.22196721E+04-7.60671568E+01 3.85542428E+00	6.05523559E-02-4.18122063E-05	3
3345	1.46680029E-08-2.07881996E-12-1.60359412E+04	1.87734959E+01	4
3346	C4H72-1,4OOH C 4H 90 4 OG	300.000 5000.000 1387.000	71
3347	2.10228668E+01 2.10127561E-02-7.30349553E-06	1.14623341E-09-6.70076491E-14	2
3348	-2.02908167E+04-7.29927491E+01 3.41714555E+00	5.89885977E-02-3.76843121E-05	3
3349	1.18450422E-08-1.46347291E-12-1.38437952E+04	2.27094787E+01	4
3350	C4H71-2,3OOH C 4H 90 4 OG	300.000 5000.000 1406.000	71
3351	2.22828679E+01 1.92253507E-02-6.52860872E-06	1.00881573E-09-5.83408336E-14	2
3352	-2.29719991E+04-8.11231836E+01 3.30790561E+00	6.66513240E-02-5.21744859E-05	3
3353	2.10434152E-08-3.42495389E-12-1.67536738E+04	1.95806784E+01	4
3354	C4H701-3OOH-4 C 4H 80 3 OG	300.000 5000.000 1418.000	31
3355	1.87250111E+01 1.88463312E-02-6.40165949E-06	9.89754621E-10-5.72727585E-14	2
3356	-3.29825730E+04-7.18225468E+01-5.40949665E+00	8.05102667E-02-6.64646030E-05	3
3357	2.73711905E-08-4.44856733E-12-2.53005240E+04	5.56327196E+01	4
3358	C4H701-3OOH-2 C 4H 80 3 OG	300.000 5000.000 1425.000	31
3359	1.97110479E+01 1.79060432E-02-6.05724664E-06	9.34110479E-10-5.39628469E-14	2
3360	-3.52532541E+04-7.83129016E+01-4.68244067E+00	8.03419743E-02-6.67264700E-05	3
3361	2.74081300E-08-4.41623778E-12-2.75307409E+04	5.04193128E+01	4
3362	C4H701-2OOH-4 C 4H 80 3 OG	300.000 5000.000 1417.000	41
3363	1.96187267E+01 1.77382423E-02-6.03563743E-06	9.34268374E-10-5.41073277E-14	2
3364	-3.21917914E+04-7.50295988E+01-3.06056578E+00	7.52777235E-02-6.16382083E-05	3
3365	2.51520765E-08-4.05109146E-12-2.49310387E+04	4.48871201E+01	4
3366	C4H701-4OOH-2 C 4H 80 3 OG	300.000 5000.000 1470.000	21
3367	1.74906412E+01 1.87794733E-02-6.05491558E-06	9.03185679E-10-5.09571870E-14	2
3368	-4.22716632E+04-6.51860330E+01-5.17426936E+00	7.89225917E-02-6.62654132E-05	3
3369	2.77698767E-08-4.54377840E-12-3.53780833E+04	5.35508489E+01	4
3370	C4H701-2OOH-3 C 4H 80 3 OG	300.000 5000.000 1435.000	41
3371	1.83476383E+01 1.72627711E-02-5.53440131E-06	8.21396496E-10-4.61479654E-14	2
3372	-3.29223599E+04-6.69919656E+01-9.44964311E-01	7.31026695E-02-6.71227799E-05	3
3373	3.12252290E-08-5.67206759E-12-2.74510619E+04	3.25427282E+01	4
3374	C4H702-3OOH-1 C 4H 80 3 OG	300.000 5000.000 1424.000	41
3375	2.03028185E+01 1.69331534E-02-5.71128715E-06	8.79005552E-10-5.07088176E-14	2
3376	-3.43451470E+04-7.95919117E+01-3.04171082E+00	7.75254740E-02-6.55776743E-05	3
3377	2.74944445E-08-4.52476822E-12-2.70343494E+04	4.33136810E+01	4
3378	C4H72-1OOH C 4H 80 2 OG	300.000 5000.000 1381.000	41
3379	1.80122740E+01 1.70340943E-02-5.89884086E-06	9.23962123E-10-5.39539803E-14	2
3380	-1.74585465E+04-6.55209757E+01 1.29755275E+00	5.59252255E-02-4.08890003E-05	3
3381	1.54880526E-08-2.42412478E-12-1.16046928E+04	2.43621382E+01	4
3382	NC4KET12 C 4H 80 3 OG	300.000 5000.000 1389.000	51
3383	2.17577434E+01 1.64473301E-02-5.79961988E-06	9.19149624E-10-5.41037382E-14	2
3384	-4.47115295E+04-8.37725285E+01-7.24231793E-01	7.26648886E-02-6.04779190E-05	3
3385	2.54348857E-08-4.30152907E-12-3.72936909E+04	3.56276963E+01	4
3386	NC4KET13 C 4H 80 3 OG	300.000 5000.000 1411.000	51
3387	1.93085398E+01 1.73455091E-02-5.85046818E-06	9.00297947E-10-5.19274609E-14	2
3388	-4.51023813E+04-7.04869509E+01 3.31775682E+00	5.28482064E-02-3.43211665E-05	3
3389	1.04562704E-08-1.12796519E-12-3.94868388E+04	1.58443308E+01	4

3390	NC4KET14	C	4H	80	3	OG	300.000	5000.000	1385.000	51	
3391	1.89231898E+01	1.82270124E-02	-6.27434124E-06	9.78729382E-10	-5.69844333E-14					2	
3392	-4.32508875E+04	-6.78717188E+01	2.92378737E+00	5.07578011E-02	-2.88360718E-05					3	
3393	6.64649914E-09	-2.83907499E-13	-3.72946444E+04	1.96328202E+01						4	
3394	NC4KET21	C	4H	80	3	OG	300.000	5000.000	1389.000	51	
3395	2.10786402E+01	1.61788162E-02	-5.53076294E-06	8.59641186E-10	-4.99535144E-14					2	
3396	-4.57563821E+04	-7.88014765E+01	-3.88449068E-01	6.92735051E-02	-5.58731127E-05					3	
3397	2.25791086E-08	-3.63900158E-12	-3.86875801E+04	3.52948090E+01						4	
3398	NC4KET23	C	4H	80	3	OG	300.000	5000.000	1411.000	51	
3399	1.76877593E+01	1.84820224E-02	-6.18384585E-06	9.45792334E-10	-5.42981801E-14					2	
3400	-4.78594254E+04	-6.06681612E+01	3.56926969E+00	5.20285891E-02	-3.64134216E-05					3	
3401	1.32007682E-08	-1.93576774E-12	-4.30650503E+04	1.48669401E+01						4	
3402	NC4KET24	C	4H	80	3	OG	300.000	5000.000	1394.000	51	
3403	1.74146206E+01	1.92744267E-02	-6.57971403E-06	1.02023879E-09	-5.91418353E-14					2	
3404	-4.60663138E+04	-5.80320911E+01	3.12062686E+00	5.01343936E-02	-3.10194950E-05					3	
3405	9.36512355E-09	-1.07548923E-12	-4.08644270E+04	1.96071994E+01						4	
3406	C4H71-3OOH	C	4H	80	2	OG	300.000	5000.000	1392.000	41	
3407	1.92985494E+01	1.54534427E-02	-5.25460431E-06	8.13772446E-10	-4.71689947E-14					2	
3408	-1.85003480E+04	-7.49926639E+01	-1.50977396E+00	6.85369305E-02	-5.75193633E-05					3	
3409	2.43179107E-08	-4.09788488E-12	-1.18018961E+04	3.50420113E+01						4	
3410	C4H71-3,4OOH	C	4H	90	4	OG	300.000	5000.000	1400.000	71	
3411	2.18394783E+01	1.98802807E-02	-6.81505369E-06	1.05975117E-09	-6.15560073E-14					2	
3412	-2.09468667E+04	-7.79984909E+01	2.56890026E+00	6.71962184E-02	-5.16999792E-05					3	
3413	2.05770379E-08	-3.32914310E-12	-1.45125600E+04	2.46332539E+01						4	
3414	C4H72-3,4OOH	C	4H	90	4	OG	300.000	5000.000	1395.000	71	
3415	2.14626449E+01	2.02946207E-02	-6.97889021E-06	1.08750673E-09	-6.32605387E-14					2	
3416	-2.22196721E+04	-7.60671568E+01	3.85542428E+00	6.05523559E-02	-4.18122063E-05					3	
3417	1.46680029E-08	-2.07881996E-12	-1.60359412E+04	1.87734959E+01						4	
3418	HO2CH2CHO	9/ 8/14	C	2H	40	3	OG	300.000	5000.000	1391.000	31
3419	1.51554685E+01	7.57240000E-03	-2.72693024E-06	4.38217189E-10	-2.60434287E-14					2	
3420	-3.41419680E+04	-5.01255068E+01	-1.32768631E+00	5.21618601E-02	-4.97327645E-05					3	
3421	2.31272366E-08	-4.20787867E-12	-2.90608844E+04	3.61860491E+01						4	
3422	IC4H10	8/12/15	C	4H	10	0	OG	300.000	5000.000	1397.000	31
3423	1.26422737E+01	2.14133551E-02	-7.26711536E-06	1.12207226E-09	-6.48434177E-14					2	
3424	-2.28293782E+04	-4.66059659E+01	-1.07413829E+00	5.24618320E-02	-3.42407949E-05					3	
3425	1.18817533E-08	-1.73238254E-12	-1.79218932E+04	2.74851665E+01						4	
3426	IC4H9	8/12/15	C	4H	9	0	OG	300.000	5000.000	1397.000	31
3427	1.23261837E+01	1.92057770E-02	-6.52063623E-06	1.00704497E-09	-5.82038734E-14					2	
3428	2.50995714E+03	-4.13478742E+01	1.20802408E-01	4.73187324E-02	-3.16440251E-05					3	
3429	1.14229699E-08	-1.74784642E-12	6.84032915E+03	2.44291032E+01						4	
3430	TC4H9	8/12/15	C	4H	9	0	OG	300.000	5000.000	1380.000	31
3431	1.02682832E+01	2.09965262E-02	-7.14945754E-06	1.10648358E-09	-6.40498314E-14					2	
3432	1.57542675E+02	-3.00960941E+01	1.05841769E+00	3.41133739E-02	-9.03156779E-06					3	
3433	-2.95313136E-09	1.41436845E-12	4.22699258E+03	2.23965051E+01						4	
3434	TC4H9O	T08/04C	4 H	9 O	1	OG	200.000	6000.000	1000.000	1	
3435	1.27371509E+01	2.33707342E-02	-8.50516678E-06	1.38519973E-09	-8.34398061E-14					2	
3436	-1.66940150E+04	-4.53156321E+01	2.77057100E+00	2.68033175E-02	4.12718360E-05					3	
3437	-7.22054739E-08	3.02642276E-11	-1.27079262E+04	1.21532856E+01	-1.04543262E+04					4	
3438	IC4H9O	A08/04C	4 H	9 O	1	OG	200.000	6000.000	1000.000	1	
3439	1.16309708E+01	2.47981574E-02	-9.01550536E-06	1.46714720E-09	-8.83214518E-14					2	
3440	-1.37854612E+04	-3.81956151E+01	3.80297372E+00	1.56874209E-02	6.81105412E-05					3	
3441	-9.83346774E-08	3.95261902E-11	-1.00832243E+04	9.78963305E+00	-7.82602559E+03					4	
3442	IC4H8O	9/ 1/12	C	4H	80	1	OG	300.000	5000.000	1394.000	21
3443	1.40433578E+01	2.05733637E-02	-9.09519220E-06	1.73417298E-09	-1.14908544E-13					2	
3444	-3.62275308E+04	-6.90009668E+01	-5.02573822E+00	7.51340960E-02	-6.88668822E-05					3	
3445	3.12223247E-08	-5.60128818E-12	-3.07481413E+04	2.96284295E+01						4	
3446	IC3H7CHO	2/22/96	THERMC	4H	80	1	OG	300.000	5000.000	1391.000	31
3447	1.37501656E+01	1.83126722E-02	-6.28572629E-06	9.78250756E-10	-5.68538653E-14					2	
3448	-3.26936771E+04	-4.77270548E+01	-2.73021382E-01	4.89696307E-02	-3.12770049E-05					3	
3449	1.00052945E-08	-1.27512074E-12	-2.76054737E+04	2.83451139E+01						4	
3450	IC3H7CO	2/22/96	THERMC	4H	70	1	OG	300.000	5000.000	1390.000	31
3451	1.33305736E+01	1.61873930E-02	-5.56711402E-06	8.67575951E-10	-5.04696549E-14					2	
3452	-1.37307001E+04	-4.33958746E+01	5.03452639E-01	4.41607510E-02	-2.82139091E-05					3	
3453	8.93548675E-09	-1.11327422E-12	-9.07755468E+03	2.61991461E+01						4	
3454	IC3H6CHO	2/22/96	THERMC	4H	70	1	OG	300.000	5000.000	1390.000	31
3455	1.33102250E+01	1.62097959E-02	-5.57575891E-06	8.69003718E-10	-5.05554202E-14					2	
3456	-7.62177931E+03	-4.25050854E+01	5.21481767E-01	4.43114357E-02	-2.86617314E-05					3	
3457	9.30319894E-09	-1.20761563E-12	-2.99677086E+03	2.68182130E+01						4	
3458	TC3H6CHO	2/22/96	THERMC	4H	70	1	OG	300.000	5000.000	1389.000	21
3459	1.31013047E+01	1.66391865E-02	-5.68457623E-06	8.81808351E-10	-5.11290161E-14					2	
3460	-1.30638647E+04	-4.42705813E+01	1.87052762E+00	4.14869677E-02	-2.66815701E-05					3	
3461	9.01531610E-09	-1.27870633E-12	-8.97730744E+03	1.66174178E+01						4	
3462	IC3H5CHO	C	4H	60	1	OG	300.000	5000.000	1396.000	21	

3463	1.33892118E+01	1.39115420E-02-4.75820958E-06	7.38736618E-10-4.28606559E-14	2
3464	-1.97917448E+04-4.60146004E+01	1.09372823E+00	4.43315368E-02-3.41918451E-05	3
3465	1.39369607E-08-2.33791460E-12-1.56745978E+04	1.94458467E+01		4
3466	TC3H6O2CHO 8/ 2/95 THERMC 4H 70 3 OG	300.000	5000.000 1386.00	41
3467	1.85534443E+01	1.68774389E-02-5.90752965E-06	9.31518085E-10-5.46345187E-14	2
3468	-2.85447191E+04-6.82486667E+01	2.17883383E+00	5.41595832E-02-3.83435886E-05	3
3469	1.38308104E-08-2.04190147E-12-2.27394154E+04	2.00751264E+01		4
3470	IC3H5O2HCHO 8/2/95 THERMC 4H 70 3 OG	300.000	5000.000 1387.00	51
3471	2.06288832E+01	1.48625539E-02-5.25305276E-06	8.33772951E-10-4.91277401E-14	2
3472	-2.27589076E+04-7.82962888E+01	2.05984770E+00	5.82331716E-02-4.37672100E-05	3
3473	1.63249918E-08-2.43462051E-12-1.63496250E+04	2.13687921E+01		4
3474	TC3H6O2HCO 8/ 2/95 THERMC 4H 70 3 OG	300.000	5000.000 1387.00	51
3475	2.06472678E+01	1.48526500E-02-5.25104875E-06	8.33619219E-10-4.91256069E-14	2
3476	-2.88719869E+04-7.95951389E+01	2.03864428E+00	5.80421003E-02-4.32123528E-05	3
3477	1.58792094E-08-2.32209543E-12-2.24284673E+04	2.03680990E+01		4
3478	TC3H6OCHO 8/25/95 THERMC 4H 70 2 OG	300.000	5000.000 1394.00	31
3479	1.70371287E+01	1.54400645E-02-5.28332886E-06	8.21085347E-10-4.76898429E-14	2
3480	-2.75871941E+04-6.37271230E+01	3.70830259E-01	5.38475661E-02-3.82477565E-05	3
3481	1.32882237E-08-1.79228730E-12-2.18391262E+04	2.58142112E+01		4
3482	IC3H6CO 03/03/95 THERMC 4H 60 1 OG	300.000	5000.000 1397.00	41
3483	1.32548232E+01	1.40142787E-02-4.78910215E-06	7.42924342E-10-4.30737566E-14	2
3484	-2.00529779E+04-4.44810221E+01	2.28039055E+00	4.17016989E-02-3.25089661E-05	3
3485	1.37243419E-08-2.40573132E-12-1.63939712E+04	1.38187714E+01		4
3486	IC3H5CO C 4H 50 1 OG	300.000	5000.000 1396.000	21
3487	1.29634401E+01	1.17954996E-02-4.04361488E-06	6.28771516E-10-3.65209867E-14	2
3488	-8.26519462E+02-4.20562575E+01	1.87306990E+00	3.95188508E-02-3.11404053E-05	3
3489	1.28844447E-08-2.18165308E-12	2.85270691E+03	1.68774016E+01	4
3490	IC3H4CHO-A C 4H 50 1 OG	300.000	5000.000 1392.000	11
3491	1.41736959E+01	1.09161978E-02-3.69020878E-06	5.69228087E-10-3.29023246E-14	2
3492	-1.92867979E+03-5.02663740E+01	7.64345054E-01	4.45242412E-02-3.61033720E-05	3
3493	1.48295287E-08-2.43809290E-12	2.44732544E+03	2.08541848E+01	4
3494	SC4H7OH-I L 2/00C 4H 80 1 OG	300.000	5000.000 1395.000	31
3495	1.30299481E+01	1.83782479E-02-6.18529878E-06	9.49578099E-10-5.46526348E-14	2
3496	-3.10723026E+04-4.22891828E+01	2.70103499E+00	4.17950180E-02-2.67860575E-05	3
3497	9.38191037E-09-1.41171285E-12-2.73561190E+04	1.35316306E+01		4
3498	IC4H9O2 9/ 1/12 C 4H 90 2 OG	300.000	5000.000 1432.000	41
3499	1.78793870E+01	1.82474607E-02-6.01252193E-06	9.11106794E-10-5.20018932E-14	2
3500	-1.74569774E+04-6.61552973E+01	1.77219624E+00	5.34032789E-02-3.31041810E-05	3
3501	9.24465657E-09-8.01706642E-13-1.17768774E+04	2.09581481E+01		4
3502	TC4H9O2 9/ 1/12 C 4H 90 2 OG	300.000	5000.000 1380.000	41
3503	1.80863238E+01	1.99282971E-02-6.98287309E-06	1.10171726E-09-6.46381057E-14	2
3504	-2.04420664E+04-6.97533212E+01	2.63892371E+00	5.44717499E-02-3.75504698E-05	3
3505	1.40479250E-08-2.27968600E-12-1.47598933E+04	1.40325533E+01		4
3506	IC4H8O2H-I 9/ 1/12 C 4H 90 2 OG	300.000	5000.000 1414.000	51
3507	1.83915486E+01	1.73042831E-02-5.66841018E-06	8.55414265E-10-4.86781778E-14	2
3508	-9.48569748E+03-6.67673286E+01	1.86432620E-01	6.26430177E-02-4.83690886E-05	3
3509	1.88657148E-08-2.91189385E-12-3.59086611E+03	2.97635367E+01		4
3510	IC4H8O2H-T 9/ 1/12 C 4H 90 2 OG	300.000	5000.000 1413.000	51
3511	1.69753885E+01	1.85198010E-02-6.09075415E-06	9.21673609E-10-5.25502501E-14	2
3512	-1.14812757E+04-5.88259039E+01	3.84374544E+00	4.36800978E-02-2.07599526E-05	3
3513	2.51709167E-09	5.41306513E-13-6.50766215E+03	1.34244877E+01	4
3514	TC4H8O2H-I 9/ 1/12 C 4H 90 2 OG	300.000	5000.000 1379.000	51
3515	1.81415374E+01	1.94699499E-02-6.82750014E-06	1.07773311E-09-6.32519099E-14	2
3516	-1.23570939E+04-6.63491602E+01	3.54378349E+00	5.25201369E-02-3.69898493E-05	3
3517	1.44634925E-08-2.47536050E-12-6.98183185E+03	1.27623539E+01		4
3518	CC4H8O 9/ 1/12 C 4H 80 1 OG	300.000	5000.000 1431.000	11
3519	1.51841776E+01	1.64656666E-02-5.33483091E-06	7.98149768E-10-4.51160381E-14	2
3520	-3.33923434E+04-7.43746988E+01-6.56746688E+00	7.87298554E-02-7.33065478E-05		3
3521	3.40602701E-08-6.15674656E-12-2.71582518E+04	3.80875851E+01		4
3522	IC4H8OOH-IO2 9/ 1/12 C 4H 90 4 OG	300.000	5000.000 1367.000	61
3523	2.24664901E+01	2.09351287E-02-7.44324128E-06	1.18589255E-09-7.00546897E-14	2
3524	-2.94495457E+04-8.54241451E+01	4.23354857E+00	5.63088857E-02-3.15672522E-05	3
3525	7.79536931E-09-6.21665008E-13-2.22782534E+04	1.52623111E+01		4
3526	IC4H8OOH-TO2 9/ 1/12 C 4H 90 4 OG	300.000	5000.000 1385.000	61
3527	2.32464612E+01	1.88384513E-02-6.40938087E-06	9.92649459E-10-5.75275879E-14	2
3528	-3.16533132E+04-8.88301710E+01	3.36413530E+00	6.93742776E-02-5.70416393E-05	3
3529	2.46040165E-08-4.32848680E-12-2.51137558E+04	1.65767339E+01		4
3530	TC4H8OOH-IO2 9/ 1/12 C 4H 90 4 OG	300.000	5000.000 1385.000	61
3531	2.32464612E+01	1.88384513E-02-6.40938087E-06	9.92649459E-10-5.75275879E-14	2
3532	-3.16533132E+04-8.88301710E+01	3.36413530E+00	6.93742776E-02-5.70416393E-05	3
3533	2.46040165E-08-4.32848680E-12-2.51137558E+04	1.65767339E+01		4
3534	IC4KETII 7/19/ 0 THERMC 4H 80 3 OG	300.000	5000.000 1387.000	51
3535	1.95143059E+01	1.82377395E-02-6.38908606E-06	1.00801571E-09-5.91440350E-14	2

3536	-4.46884836E+04	-7.17167584E+01	1.15501614E+00	6.10622345E-02	-4.49711323E-05	3
3537	1.70514654E-08	-2.65948602E-12	-3.82747956E+04	2.69612235E+01		4
3538	IC4KETIT	7/19/ 0	THERMC	4H	80 3 OG	300.000 5000.000 1388.000 51
3539	2.09369850E+01	1.71090955E-02	-6.01892169E-06	9.52353863E-10	-5.59926176E-14	2
3540	-4.77819819E+04	-8.27717611E+01	1.14243741E+00	6.33840797E-02	-4.73084738E-05	3
3541	1.77145373E-08	-2.67265475E-12	-4.09366796E+04	2.34844867E+01		4
3542	TIC4H7Q2-I	5/ 6/96	THERMC	4H	90 4 OG	300.000 5000.000 1400.000 71
3543	2.33848631E+01	1.87070035E-02	-6.44021945E-06	1.00428123E-09	-5.84468189E-14	2
3544	-2.61180902E+04	-8.76610135E+01	4.48426361E+00	6.61225007E-02	-5.27349018E-05	3
3545	2.18215585E-08	-3.66788946E-12	-1.98906586E+04	1.26719614E+01		4
3546	IIC4H7Q2-I	7/15/96	THERMC	4H	90 4 OG	300.000 5000.000 1394.000 71
3547	2.30500244E+01	1.92149194E-02	-6.66622576E-06	1.04495725E-09	-6.10370520E-14	2
3548	-2.32086881E+04	-8.39949885E+01	4.93055661E+00	6.05819201E-02	-4.23665566E-05	3
3549	1.49122008E-08	-2.10978665E-12	-1.68415495E+04	1.36228018E+01		4
3550	IIC4H7Q2-T	7/15/96	THERMC	4H	90 4 OG	300.000 5000.000 1377.000 71
3551	2.15070321E+01	2.05359839E-02	-7.12383399E-06	1.11655053E-09	-6.52112103E-14	2
3552	-2.51117508E+04	-7.43379783E+01	8.16274487E+00	4.34463050E-02	-1.76972456E-05	3
3553	4.88790666E-10	9.03915465E-13	-1.96501749E+04	2.62067299E-01		4
3554	IC4H7OOH	4/15/15	C	4H	80 2 OG	300.000 5000.000 1386.000 41
3555	1.82897194E+01	1.67815784E-02	-5.80668193E-06	9.08949180E-10	-5.30513302E-14	2
3556	-1.82046522E+04	-6.72111342E+01	1.31851762E-01	6.19561224E-02	-4.99343877E-05	3
3557	2.09628211E-08	-3.59717924E-12	-1.21399925E+04	2.93905962E+01		4
3558	IC4H9O2H	9/ 1/12	C	4H	100 2 OG	300.000 5000.000 1402.000 51
3559	1.91651624E+01	1.93678648E-02	-6.41984435E-06	9.76947752E-10	-5.59299558E-14	2
3560	-3.48790978E+04	-7.42063787E+01	-5.47969191E-01	6.57428787E-02	-4.70123149E-05	3
3561	1.65991096E-08	-2.27331437E-12	-2.82180462E+04	3.12961385E+01		4
3562	TC4H9O2H	9/ 1/12	C	4H	100 2 OG	300.000 5000.000 1382.000 51
3563	1.90926853E+01	2.12697804E-02	-7.46252626E-06	1.17841127E-09	-6.91795087E-14	2
3564	-3.77278405E+04	-7.61321196E+01	4.45573540E-01	6.66153523E-02	-5.20932123E-05	3
3565	2.22301799E-08	-4.00189859E-12	-3.12260714E+04	2.37278262E+01		4
3566	IC4H8	8/12/15	C	4H	8 0 OG	300.000 5000.000 1392.000 21
3567	1.11444028E+01	1.81609265E-02	-6.17791116E-06	9.55481871E-10	-5.52826092E-14	2
3568	-7.84024684E+03	-3.68508829E+01	5.72478139E-02	4.17768938E-02	-2.49095729E-05	3
3569	7.54294402E-09	-9.23202212E-13	-3.72166259E+03	2.35698905E+01		4
3570	IC4H7	8/12/15	C	4H	7 0 OG	300.000 5000.000 1384.000 11
3571	1.18999143E+01	1.51569859E-02	-5.09995449E-06	7.83722199E-10	-4.51660275E-14	2
3572	1.00363555E+04	-4.02286635E+01	-2.29578762E-01	4.17842986E-02	-2.66885700E-05	3
3573	8.42205744E-09	-1.03175361E-12	1.43946680E+04	2.54797645E+01		4
3574	IC4H7-I1	5/13/15	C	4H	7 0 OG	300.000 5000.000 1396.000 21
3575	1.11158752E+01	1.55127192E-02	-5.23769366E-06	8.05998394E-10	-4.64703390E-14	2
3576	2.19488297E+04	-3.41440480E+01	9.12464579E-01	3.88654394E-02	-2.57575714E-05	3
3577	9.07760026E-09	-1.33946902E-12	2.55635553E+04	2.08634918E+01		4
3578	IC4H7O2	L 2/00C	4H	70 2 OG		300.000 5000.000 1404.000 31
3579	1.45791608E+01	1.62136068E-02	-5.26957103E-06	7.90454323E-10	-4.47755051E-14	2
3580	-1.20848042E+03	-4.56459433E+01	1.43532045E+00	4.89026570E-02	-3.63600970E-05	3
3581	1.41906420E-08	-2.24557878E-12	3.09284623E+03	2.41320196E+01		4
3582	IC4H6OOH-I	L 2/00C	4H	70 2 OG		300.000 5000.000 1398.000 31
3583	1.73601429E+01	1.42046196E-02	-4.65348263E-06	7.02209785E-10	-3.99552775E-14	2
3584	-1.07509366E+03	-6.12822377E+01	6.06669321E+00	3.94950065E-02	-2.52721718E-05	3
3585	7.84485641E-09	-8.98876886E-13	2.87448422E+03	-3.78377026E-01		4
3586	CCYCCOOC-T1	THERMC	4H	70 2 OG		300.000 5000.000 1394.000 11
3587	1.68269657E+01	1.64471921E-02	-5.63767184E-06	8.78001611E-10	-5.10959632E-14	2
3588	-3.65710841E+03	-6.74096786E+01	-5.29767923E+00	6.65082201E-02	-4.67054235E-05	3
3589	1.51029775E-08	-1.74322091E-12	3.97935712E+03	5.16412476E+01		4
3590	C2CYCOOC-I1	7/14	C	4H	70 2 OG	300.000 5000.000 1388.000 21
3591	1.89745085E+01	1.50113808E-02	-5.30728309E-06	8.42454740E-10	-4.96392976E-14	2
3592	-6.93111358E+03	-9.08581019E+01	-2.04718031E+00	7.26608379E-02	-6.82960279E-05	3
3593	3.27505762E-08	-6.23802161E-12	-3.71475599E+02	1.92056057E+01		4
3594	IC4H7O	4/ 3/ 0	THERMC	4H	70 1 OG	300.000 5000.000 1386.000 21
3595	1.33457615E+01	1.61218588E-02	-5.44376403E-06	8.38199374E-10	-4.83608280E-14	2
3596	6.11443644E+02	-4.36818838E+01	1.74700687E+00	4.07783436E-02	-2.44750243E-05	3
3597	7.06502958E-09	-7.51570589E-13	4.86979233E+03	1.94535999E+01		4
3598	CVCYCCOC	L 2/00C	4H	60 1 OG		300.000 5000.000 1397.000 1
3599	1.14363523E+01	1.63250968E-02	-5.57146218E-06	8.63795613E-10	-5.00701899E-14	2
3600	-5.44653450E+03	-3.87179379E+01	-2.45566808E+00	4.88377067E-02	-3.46186324E-05	3
3601	1.26590643E-08	-1.88737988E-12	-6.43460880E+02	3.58434061E+01		4
3602	CCYC2OCO	L 2/00C	4H	70 2 OG		300.000 5000.000 1401.000 21
3603	1.64352871E+01	1.65843210E-02	-5.71790511E-06	8.92586562E-10	-5.19865043E-14	2
3604	-1.60938498E+04	-5.96946106E+01	-2.97381263E+00	6.75615160E-02	-5.79901709E-05	3
3605	2.55213006E-08	-4.49991674E-12	-9.93607156E+03	4.25127997E+01		4
3606	CCYCCOOC-I2	L 2/00C	4H	70 2 OG		300.000 5000.000 1398.000 11
3607	1.63388791E+01	1.65879474E-02	-5.61829108E-06	8.67331033E-10	-5.01476782E-14	2
3608	6.66946988E+03	-6.40322040E+01	-4.55772603E+00	7.10221387E-02	-6.05228430E-05	3

3609	2.61773944E-08-4.51390528E-12	1.32922215E+04	4.60828737E+01		4
3610	CHOIC3H6O	L 2/00C	4H 70 2 OG	300.000 5000.000 1386.000	31
3611	1.55511970E+01	1.67360034E-02-5.73573457E-06	8.92095191E-10-5.18351848E-14		2
3612	-2.50674335E+04-5.23215658E+01	2.55559437E-01	5.22086026E-02-3.72283766E-05		3
3613	1.36714420E-08-2.05638885E-12	-1.97284649E+04	2.99210251E+01		4
3614	IC3H5OOCH2	L 2/00C	4H 70 2 OG	300.000 5000.000 1410.000	41
3615	5.05335676E+00	3.62904388E-02-1.54012992E-05	2.74341619E-09-1.74718602E-13		2
3616	4.08326144E+03-2.55389509E+00	-1.26548168E+00	-3.61337863E-03 7.31803998E-05		3
3617	-5.49845697E-08	1.20447492E-11	1.33108969E+04	5.33428723E+01	4
3618	CCYCCO-T1	L 2/00C	3H 50 1 OG	300.000 5000.000 1389.000	11
3619	1.03394781E+01	1.15180335E-02-3.87496644E-06	5.95744364E-10-3.43539552E-14		2
3620	7.17658970E+03-2.89687593E+01	-1.39311392E+00	3.81789194E-02-2.62316288E-05		3
3621	8.74877238E-09-1.11296763E-12	1.12534953E+04	3.41877003E+01		4
3622	IC4H8OH-IT	C	4H 90 1 OG	300.000 5000.000 1391.000	41
3623	1.29136746E+01	2.06583409E-02-6.98445966E-06	1.07562552E-09-6.20443876E-14		2
3624	-1.81394866E+04-3.84972088E+01	3.05275715E+00	3.93926461E-02-1.90686417E-05		3
3625	3.86408022E-09-1.48005244E-13	-1.42263749E+04	1.60840537E+01		4
3626	IC4H8OH-TI	C	4H 90 1 OG	300.000 5000.000 1402.000	41
3627	1.46323607E+01	1.88895981E-02-6.30561450E-06	9.62474230E-10-5.51640163E-14		2
3628	-1.87976018E+04-4.93218793E+01	2.33169342E+00	5.13017040E-02-4.02698872E-05		3
3629	1.75150405E-08-3.16001727E-12	-1.48318978E+04	1.55368130E+01		4
3630	IC4H7OH	C	4H 80 1 OG	300.000 5000.000 1398.000	31
3631	1.23304221E+01	1.83885172E-02-6.06721733E-06	9.19054723E-10-5.24036171E-14		2
3632	-2.59452023E+04-3.67418286E+01	2.04124240E+00	4.14387207E-02-2.55228632E-05		3
3633	8.28133017E-09-1.10654457E-12	-2.22709637E+04	1.88699473E+01		4
3634	IC4H8OH	2/14/95 THERMC	4H 90 1 OG	300.000 5000.000 1376.000	41
3635	1.25605997E+01	2.10637488E-02-7.15019648E-06	1.10439262E-09-6.38428695E-14		2
3636	-1.86203249E+04-3.67889430E+01	3.29612707E+00	3.47649647E-02-1.02505618E-05		3
3637	-2.04641931E-09	1.18879408E-12-1.45627247E+04	1.58606320E+01		4
3638	IC4H6OH	C	4H 70 1 OG	300.000 5000.000 1402.000	21
3639	1.53490714E+01	1.38856699E-02-4.56427754E-06	6.90418690E-10-3.93540403E-14		2
3640	-1.20164758E+04-5.55975530E+01	-1.46664187E+00	6.03351671E-02-5.43112644E-05		3
3641	2.49299933E-08-4.52282491E-12	-6.95012413E+03	3.20768458E+01		4
3642	TQJC4H8OH	C	4H 90 3 OG	300.000 5000.000 1415.000	51
3643	2.29681617E+01	1.65162786E-02-5.50247318E-06	8.39335285E-10-4.81030625E-14		2
3644	-4.10051460E+04-9.34897892E+01	-6.43419503E-01	8.49131517E-02-8.17210578E-05		3
3645	3.90979927E-08-7.27092842E-12	-3.42375932E+04	2.84394025E+01		4
3646	TQC4H8OI	C	4H 90 3 OG	300.000 5000.000 1411.000	51
3647	2.13200701E+01	1.80489663E-02-6.06124072E-06	9.29740751E-10-5.34977374E-14		2
3648	-3.12966663E+04-8.20046659E+01	7.45747835E-02	7.46499596E-02-6.42255048E-05		3
3649	2.80908988E-08-4.87692045E-12	-2.47182737E+04	2.94511549E+01		4
3650	QC4H7OHP	C	4H 90 3 OG	300.000 5000.000 1416.000	61
3651	2.43481084E+01	1.50316366E-02-5.01788017E-06	7.66774357E-10-4.40093220E-14		2
3652	-3.31922320E+04-9.68211106E+01	-1.27864186E+00	8.94492926E-02-8.78565423E-05		3
3653	4.22110919E-08-7.83450876E-12	-2.58975226E+04	3.53963909E+01		4
3654	TQC4H7OHI	L 2/00C	4H 90 3 OG	300.000 5000.000 1404.000	61
3655	2.08281225E+01	1.81675094E-02-6.12943202E-06	9.43194119E-10-5.43937008E-14		2
3656	-3.37386684E+04-7.74823720E+01	2.55843807E+00	6.37086077E-02-4.97169945E-05		3
3657	1.99225109E-08-3.21373436E-12	-2.77526909E+04	1.95001368E+01		4
3658	CCY(CCO)COH	C	4H 80 2 OG	300.000 5000.000 1412.000	31
3659	1.91884885E+01	1.56255714E-02-5.22569800E-06	7.99171074E-10-4.58832445E-14		2
3660	-4.71120302E+04-7.84579023E+01	-7.10048774E+00	9.53371808E-02-9.78701612E-05		3
3661	4.90005646E-08-9.41685766E-12	-3.98987202E+04	5.60924667E+01		4
3662	C2CY(COC)OH	C	4H 80 2 OG	300.000 5000.000 1393.000	31
3663	1.56829970E+01	1.92910506E-02-6.63718495E-06	1.03441014E-09-6.01715267E-14		2
3664	-4.10598236E+04-5.85686221E+01	5.92324183E-01	5.52429007E-02-4.02419018E-05		3
3665	1.57152217E-08-2.57388393E-12	-3.58241476E+04	2.23378086E+01		4
3666	IQJC4H8OH	L 2/00C	4H 90 3 OG	300.000 5000.000 1410.000	51
3667	2.11752212E+01	1.75144254E-02-5.73227292E-06	8.63386596E-10-4.90282414E-14		2
3668	-3.98881576E+04-8.19187015E+01	1.81448831E+00	7.47452750E-02-7.10895172E-05		3
3669	3.44973679E-08-6.54646593E-12	-3.44023586E+04	1.77380434E+01		4
3670	IC3H6OHCHO	C	4H 80 2 OG	300.000 5000.000 1393.000	41
3671	1.60254376E+01	1.85402212E-02-6.36973877E-06	9.91732739E-10-5.76472640E-14		2
3672	-5.50198923E+04-5.83074874E+01	1.84080874E+00	5.29601347E-02-3.94261774E-05		3
3673	1.59063430E-08-2.69565279E-12	-5.01437169E+04	1.75482756E+01		4
3674	IQC4H8OT	C	4H 90 3 OG	300.000 5000.000 1405.000	51
3675	2.04823628E+01	1.82966721E-02-6.04413378E-06	9.16380548E-10-5.22866551E-14		2
3676	-2.94287153E+04-7.53563247E+01	3.72211529E+00	6.42864861E-02-5.52809053E-05		3
3677	2.50036630E-08-4.53471908E-12	-2.43110525E+04	1.21981167E+01		4
3678	IQC4H7OHT	C	4H 90 3 OG	300.000 5000.000 1413.000	61
3679	2.19945886E+01	1.62011186E-02-5.23758492E-06	7.81898296E-10-4.41125515E-14		2
3680	-3.07383725E+04-8.16613568E+01	3.58900054E+00	7.25591129E-02-7.14080484E-05		3
3681	3.55250907E-08-6.84991795E-12	-2.57241250E+04	1.23766657E+01		4

3682	CCY(CCOC)OH	L 2/00C	4H	80	2	OG	300.000	5000.000	1404.000	21	
3683	1.43404718E+01	1.98311504E-02	-6.60657660E-06	1.00779570E-09	-5.77614335E-14					2	
3684	-4.30959414E+04	-5.30535015E+01	-2.84914896E+00	6.23736856E-02	-4.70326536E-05					3	
3685	1.84908286E-08	-2.94976027E-12	-3.74257004E+04	3.83163588E+01						4	
3686	CH2COHCH2OOH	C	3H	60	3	OG	300.000	5000.000	1398.000	41	
3687	1.87971268E+01	1.12783442E-02	-3.90789058E-06	6.12064651E-10	-3.57305453E-14					2	
3688	-3.61154867E+04	-6.94914300E+01	-3.89823383E-01	7.01531131E-02	-7.42036788E-05					3	
3689	3.84181056E-08	-7.63555985E-12	-3.07879938E+04	2.86873505E+01						4	
3690	TC3H6OH	8/ 9/ 4 THERMC	3H	70	1	OG	300.000	5000.000	1392.000	31	
3691	1.12222277E+01	1.36444398E-02	-4.51406709E-06	7.10523275E-10	-4.22690392E-14					2	
3692	-1.75350136E+04	-3.18911926E+01	1.09670360E+00	3.80727565E-02	-2.75022497E-05					3	
3693	1.07477493E-08	-1.74895773E-12	-1.40764487E+04	2.22475799E+01						4	
3694	TQC4H7OHIO2	C	4H	90	5	OG	300.000	5000.000	1402.000	71	
3695	2.82564819E+01	1.66969871E-02	-5.67314614E-06	8.78350442E-10	-5.09090253E-14					2	
3696	-5.66017464E+04	-1.15147927E+02	3.17336206E+00	7.94005900E-02	-6.51165712E-05					3	
3697	2.62035931E-08	-4.13406290E-12	-4.84943162E+04	1.77867184E+01						4	
3698	TQC4H7OHTO2	C	4H	90	5	OG	300.000	5000.000	1402.000	71	
3699	2.82564819E+01	1.66969871E-02	-5.67314614E-06	8.78350442E-10	-5.09090253E-14					2	
3700	-5.66017464E+04	-1.15147927E+02	3.17336206E+00	7.94005900E-02	-6.51165712E-05					3	
3701	2.62035931E-08	-4.13406290E-12	-4.84943162E+04	1.77867184E+01						4	
3702	TQC4H7OHIO-I	C	4H	90	5	OG	300.000	5000.000	1384.000	71	
3703	2.88466964E+01	1.66289773E-02	-5.74301906E-06	8.98791324E-10	-5.24794891E-14					2	
3704	-4.69249234E+04	-1.19117836E+02	6.09881562E+00	6.93745451E-02	-5.12049498E-05					3	
3705	1.81276221E-08	-2.46329781E-12	-3.91393707E+04	2.93862639E+00						4	
3706	TQC4H7OHIO-P	C	4H	90	5	OG	300.000	5000.000	1400.000	81	
3707	2.81439191E+01	1.63524649E-02	-5.54998081E-06	8.58603978E-10	-4.97359401E-14					2	
3708	-4.84502814E+04	-1.11572783E+02	3.36947511E+00	7.96855226E-02	-6.74365765E-05					3	
3709	2.82233283E-08	-4.65270820E-12	-4.05567534E+04	1.92726029E+01						4	
3710	IC3H5COHQ	C	4H	80	3	OG	300.000	5000.000	1504.000	51	
3711	2.07387831E+01	1.58360934E-02	-5.27614462E-06	8.05932218E-10	-4.62682425E-14					2	
3712	-4.41821241E+04	-7.94239893E+01	2.64360992E+00	5.72485066E-02	-3.95907807E-05					3	
3713	1.27775635E-08	-1.47241476E-12	-3.80099993E+04	1.77322273E+01						4	
3714	CH2CQCOHQ	7/ 1/14	C	3H	60	5	OG	300.000	5000.000	1418.000	61
3715	3.86574091E+01	4.83815026E-04	-2.10413843E-07	3.81490832E-11	-2.46187754E-15					2	
3716	-6.56392184E+04	-1.61083579E+02	-1.61171759E+01	1.78866440E-01	-2.16751308E-04					3	
3717	1.15450289E-07	-2.27163078E-11	-5.21165145E+04	1.14441286E+02						4	
3718	IC3H5Q	C	3H	60	2	OG	300.000	5000.000	1397.000	31	
3719	1.43424294E+01	1.28053632E-02	-4.40584813E-06	6.86848148E-10	-3.99675209E-14					2	
3720	-1.65261025E+04	-4.89934539E+01	1.32903007E+00	4.49170722E-02	-3.51235127E-05					3	
3721	1.41982181E-08	-2.33335008E-12	-1.21898396E+04	2.02696565E+01						4	
3722	CH3COCHO	C	3H	40	2	OG	300.000	5000.000	1381.000	21	
3723	1.14371190E+01	1.06773624E-02	-3.68967757E-06	5.77006752E-10	-3.36532201E-14					2	
3724	-3.78079398E+04	-3.25054087E+01	2.08731049E+00	3.09032484E-02	-1.98794164E-05					3	
3725	6.26174519E-09	-7.69945504E-13	-3.43989451E+04	1.82839639E+01						4	
3726	IC3H5OCH2	6/ 2/14 CZHOH	7C	40	1	G	298.150	2000.000	1000.00	1	
3727	6.64731727E+00	3.08190709E-02	-1.73209320E-05	5.01099629E-09	-6.00089387E-13					2	
3728	1.70679921E+03	-5.91214819E+00	-2.14798958E+00	7.00225553E-02	-8.21595440E-05					3	
3729	5.22589946E-08	-1.34176532E-11	3.26474773E+03	3.55145589E+01						4	
3730	IC4H7OOCH3	C	5H	100	2	OG	300.000	5000.000	1386.000	51	
3731	1.95896715E+01	2.31057369E-02	-8.02911330E-06	1.25969946E-09	-7.36169360E-14					2	
3732	-1.80069088E+04	-7.34192482E+01	1.26784161E+00	6.82442475E-02	-5.30807931E-05					3	
3733	2.27496198E-08	-4.11475065E-12	-1.16767937E+04	2.44900544E+01						4	
3734	IC4H7OOIC4H7	C	8H	140	2	OG	300.000	5000.000	1390.000	71	
3735	2.80447245E+01	3.27505220E-02	-1.13220177E-05	1.77027767E-09	-1.03211988E-13					2	
3736	-1.72683337E+04	-1.15134796E+02	-2.07881710E-01	1.04075647E-01	-8.33973077E-05					3	
3737	3.60897624E-08	-6.47906520E-12	-7.79062693E+03	3.50446555E+01						4	
3738	C4H8-1	C	4H	8	0	OG	300.000	5000.000	1388.000	21	
3739	1.10189295E+01	1.82714177E-02	-6.21801907E-06	9.62038611E-10	-5.56791341E-14					2	
3740	-5.80998818E+03	-3.47942287E+01	1.62599556E-01	4.01052746E-02	-2.18038592E-05					3	
3741	5.47070727E-09	-4.54073315E-13	-1.65402601E+03	2.48169258E+01						4	
3742	C4H8-2	8/12/15	C	4H	8	0	OG	300.000	5000.000	1383.000	21
3743	1.08652083E+01	1.84123129E-02	-6.26886673E-06	9.70205962E-10	-5.61638967E-14					2	
3744	-7.09625867E+03	-3.51547481E+01	1.30795510E+00	3.53136624E-02	-1.51866126E-05					3	
3745	1.64112363E-09	3.44257620E-13	-3.19767852E+03	1.81594717E+01						4	
3746	C4H71-1	C	4H	7	0	OG	300.000	5000.000	1390.000	21	
3747	1.10531750E+01	1.55668782E-02	-5.25853044E-06	8.09627095E-10	-4.67015477E-14					2	
3748	2.39455759E+04	-3.31548457E+01	8.97231085E-01	3.77003788E-02	-2.33194855E-05					3	
3749	7.38468124E-09	-9.50027900E-13	2.76498158E+04	2.19835413E+01						4	
3750	C4H71-2	C	4H	7	0	OG	300.000	5000.000	1381.000	21	
3751	1.07105686E+01	1.63539126E-02	-5.63688038E-06	8.79591989E-10	-5.12098725E-14					2	
3752	2.21011255E+04	-3.15300308E+01	1.56405993E+00	3.32162309E-02	-1.59178310E-05					3	
3753	2.92637814E-09	-3.02645386E-14	2.57966120E+04	1.93052496E+01						4	
3754	C4H71-3	1/13/16	C	4H	7	0	OG	300.000	5000.000	1367.000	11

3755	1.16977564E+01	1.53404517E-02	-5.16928607E-06	7.95431212E-10	-4.58914150E-14	2					
3756	1.07395001E+04	-3.82992966E+01	9.40350126E-01	3.56830321E-02	-1.74384567E-05	3					
3757	2.78964567E-09	1.78068599E-13	1.49303203E+04	2.11349333E+01		4					
3758	C4H71-4	C	4H	7	0	OG	300.000	5000.000	1389.000	21	
3759	1.03875084E+01	1.63677264E-02	-5.58416036E-06	8.65388736E-10	-5.01415385E-14	2					
3760	1.93282846E+04	-2.86081068E+01	5.36903096E-01	3.66356251E-02	-2.07814610E-05	3					
3761	5.74895154E-09	-6.05742821E-13	2.30645349E+04	2.53369983E+01		4					
3762	C4H72-2	8/12/15	C	4H	7	0	OG	300.000	5000.000	1378.000	21
3763	1.05359634E+01	1.65535631E-02	-5.71669066E-06	8.93155269E-10	-5.20432637E-14	2					
3764	2.08161211E+04	-3.11046229E+01	2.46499885E+00	2.94957335E-02	-1.08904521E-05	3					
3765	9.17747264E-11	5.46417906E-13	2.42904093E+04	1.44728237E+01		4					
3766	C4H71-O	4/ 3/ 0	THERMC	4H	70	1	OG	300.000	5000.000	1395.000	21
3767	1.53137780E+01	1.43427017E-02	-4.81625517E-06	7.39574839E-10	-4.26140814E-14	2					
3768	-7.29342884E+02	-5.52937859E+01	-1.60619192E+00	5.58562682E-02	-4.35595767E-05	3					
3769	1.70589279E-08	-2.65635180E-12	4.85090326E+03	3.47112559E+01		4					
3770	PC4H8OH-2	C	4H	90	1	OG	300.000	5000.000	1396.000	41	
3771	1.47198620E+01	1.93691825E-02	-6.59356634E-06	1.02018538E-09	-5.90410746E-14	2					
3772	-1.53023402E+04	-4.85296396E+01	1.89476538E+00	4.87803114E-02	-3.26702980E-05	3					
3773	1.17119949E-08	-1.77100238E-12	-1.07455371E+04	2.06226225E+01		4					
3774	SC4H8OH-1	C	4H	90	1	OG	300.000	5000.000	1405.000	41	
3775	1.50517242E+01	1.84748629E-02	-6.15327969E-06	9.38017339E-10	-5.37214281E-14	2					
3776	-1.71974443E+04	-5.03733848E+01	1.78282749E+00	5.18872497E-02	-3.89600849E-05	3					
3777	1.57818686E-08	-2.64133852E-12	-1.28305019E+04	2.00308244E+01		4					
3778	SC4H8OH-3	C	4H	90	1	OG	300.000	5000.000	1403.000	41	
3779	1.42453780E+01	1.89491000E-02	-6.27403528E-06	9.52692609E-10	-5.44157896E-14	2					
3780	-1.81803642E+04	-4.56206494E+01	1.93185505E+00	4.79506224E-02	-3.23719194E-05	3					
3781	1.16232751E-08	-1.72498918E-12	-1.39431370E+04	2.03995003E+01		4					
3782	C4H71-3OH	C	4H	80	1	OG	300.000	5000.000	1385.000	31	
3783	1.42401634E+01	1.83038695E-02	-6.37213444E-06	1.00099740E-09	-5.85511411E-14	2					
3784	-2.68183960E+04	-4.83949774E+01	7.16707858E-02	5.04772909E-02	-3.50356983E-05	3					
3785	1.30539199E-08	-2.07783174E-12	-2.16983717E+04	2.82072724E+01		4					
3786	C4H71-4OH	C	4H	80	1	OG	300.000	5000.000	1396.000	31	
3787	1.33437331E+01	1.82063693E-02	-6.15150719E-06	9.47318576E-10	-5.46543216E-14	2					
3788	-2.48479001E+04	-4.27998774E+01	-2.12276307E-01	4.86358034E-02	-3.17241965E-05	3					
3789	1.04986646E-08	-1.39007078E-12	-2.00365173E+04	3.04092052E+01		4					
3790	C4H71-1OH	C	4H	80	1	OG	300.000	5000.000	1402.000	31	
3791	1.42586569E+01	1.71932504E-02	-5.74956414E-06	8.79089774E-10	-5.04586493E-14	2					
3792	-2.78051048E+04	-4.96581579E+01	-4.65981165E-01	5.56573217E-02	-4.50578305E-05	3					
3793	1.93726056E-08	-3.38967639E-12	-2.31007894E+04	2.79744544E+01		4					
3794	C4H71-2OH	C	4H	80	1	OG	300.000	5000.000	1404.000	31	
3795	1.50658194E+01	1.65276030E-02	-5.52197706E-06	8.43591643E-10	-4.83870716E-14	2					
3796	-2.99737946E+04	-5.53405024E+01	-1.28560619E+00	6.35758020E-02	-5.85328191E-05	3					
3797	2.80452715E-08	-5.32187122E-12	-2.51538600E+04	2.93802791E+01		4					
3798	C4H72-1OH	C	4H	80	1	OG	300.000	5000.000	1367.000	31	
3799	1.32893235E+01	1.93843938E-02	-6.80733358E-06	1.07559847E-09	-6.31698641E-14	2					
3800	-2.58627911E+04	-4.34782359E+01	2.94637661E+00	3.45852975E-02	-1.10024787E-05	3					
3801	-1.33281467E-09	9.54964043E-13	-2.12241816E+04	1.55037145E+01		4					
3802	C4H72-2OH	C	4H	80	1	OG	300.000	5000.000	1402.000	31	
3803	1.49411596E+01	1.66289929E-02	-5.55627511E-06	8.48898851E-10	-4.86949390E-14	2					
3804	-3.12496851E+04	-5.51730870E+01	-1.84033728E-01	5.90104774E-02	-5.22507028E-05	3					
3805	2.44135801E-08	-4.56518659E-12	-2.66717960E+04	2.36075268E+01		4					
3806	SQC4H8OP	C	4H	90	3	OG	300.000	5000.000	1421.000	51	
3807	2.02482113E+01	1.90403096E-02	-6.41818812E-06	9.86791658E-10	-5.68666168E-14	2					
3808	-2.70686177E+04	-7.43734665E+01	3.92966105E+00	5.67740736E-02	-3.88077818E-05	3					
3809	1.31554059E-08	-1.72822772E-12	-2.14649445E+04	1.32313419E+01		4					
3810	PQC4H8OS	C	4H	90	3	OG	300.000	5000.000	1403.000	51	
3811	1.99993833E+01	1.96391125E-02	-6.70755815E-06	1.04036085E-09	-6.03187960E-14	2					
3812	-2.71257575E+04	-7.31284601E+01	2.68979886E+00	6.10664073E-02	-4.46910607E-05	3					
3813	1.68939056E-08	-2.59692346E-12	-2.12460925E+04	1.94271757E+01		4					
3814	PQC4H7OHS-3	C	4H	90	3	OG	300.000	5000.000	1404.000	61	
3815	1.89703648E+01	1.96512375E-02	-6.61522830E-06	1.01590849E-09	-5.84889733E-14	2					
3816	-2.92876345E+04	-6.40682635E+01	3.14058820E+00	5.94343278E-02	-4.55414505E-05	3					
3817	1.85507067E-08	-3.10109441E-12	-2.40765022E+04	1.99412365E+01		4					
3818	NC4KET12OH	C	4H	80	2	OG	300.000	5000.000	1384.000	41	
3819	1.68650782E+01	1.83319076E-02	-6.41389893E-06	1.01105283E-09	-5.92858731E-14	2					
3820	-5.27353126E+04	-5.97188408E+01	5.20269850E-01	5.40316915E-02	-3.57074151E-05	3					
3821	1.18022134E-08	-1.57485744E-12	-4.67781081E+04	2.89999061E+01		4					
3822	SQC4H7OHS-4	C	4H	90	3	OG	300.000	5000.000	1414.000	61	
3823	2.06664415E+01	1.78772156E-02	-5.93193686E-06	9.02005813E-10	-5.15691990E-14	2					
3824	-3.04132233E+04	-7.44595459E+01	3.37952725E+00	6.50949152E-02	-5.59109752E-05	3					
3825	2.496444089E-08	-4.44896795E-12	-2.51501593E+04	1.58596901E+01		4					
3826	SQC4H8OS	C	4H	90	3	OG	300.000	5000.000	1424.000	51	
3827	2.05363895E+01	1.85261859E-02	-6.18257770E-06	9.44045247E-10	-5.41390400E-14	2					

3828	-2.90453556E+04-7.66224497E+01	3.45579406E+00	6.10420456E-02-4.64106547E-05	3
3829	1.80687264E-08-2.81124474E-12-2.34835698E+04	1.39991890E+01		4
3830	NC4KET23OH 7/27/15 C 4H 80 2 OG	300.000 5000.000 1386.000		41
3831	1.54636087E+01 1.92120108E-02-6.64681122E-06	1.03988604E-09-6.06552757E-14		2
3832	-5.57292725E+04-5.19147488E+01 1.64761234E+00	4.74122084E-02-2.72508571E-05		3
3833	7.25755846E-09-6.68682869E-13-5.04946247E+04	2.37800424E+01		4
3834	C4H7O2-1 9/ 8/14 C 4H 70 1 OG	300.000 5000.000 1684.000		21
3835	1.12685690E+01 2.01724820E-02-7.41925667E-06	1.21275519E-09-7.30115348E-14		2
3836	2.13876442E+03-3.15208064E+01 5.16434924E+00	2.53427725E-02-1.39669041E-06		3
3837	-6.00013944E-09 1.76696879E-12 5.03210693E+03	4.37441148E+00		4
3838	C4H6-1 L10/93C 4.H 6. 0. 0.G	200.000 6000.000 1000.		1
3839	7.81179394E+00 1.79733772E-02-6.61044149E-06	1.05501491E-09-6.19297169E-14		2
3840	1.61770171E+04-1.59658015E+01 2.42819263E+00	2.49821955E-02 6.27370548E-06		3
3841	-2.61747866E-08 1.26585079E-11 1.80248564E+04	1.36683982E+01 1.98688798E+04		4
3842	AC3H5OCH2 9/ 8/14 C 4H 70 1 OG	300.000 5000.000 1397.000		31
3843	1.19880368E+01 1.70263516E-02-5.78617265E-06	8.94150465E-10-5.16994613E-14		2
3844	3.48367473E+03-3.35860630E+01 1.20089076E+00	4.24760987E-02-2.94114641E-05		3
3845	1.11824860E-08-1.81309530E-12 7.26792055E+03	2.43628654E+01		4
3846	C5H10-2 9/ 8/14 C 5H 10 0 OG	300.000 5000.000 1385.000		31
3847	1.39425521E+01 2.28734997E-02-7.77800113E-06	1.20284861E-09-6.95972140E-14		2
3848	-1.12165700E+04-4.95379542E+01 5.90528835E-01	4.85275113E-02-2.43231598E-05		3
3849	4.86096027E-09-1.13099201E-13-5.99777644E+03	2.41816377E+01		4
3850	CC5H10 9/ 8/14 C 5H 10 0 OG	300.000 5000.000 1394.000		31
3851	1.44242929E+01 2.26454984E-02-7.73646334E-06	1.19999861E-09-6.95711276E-14		2
3852	-1.14981027E+04-5.30391197E+01-9.64397004E-01	5.68482691E-02-3.66324275E-05		3
3853	1.23008921E-08-1.71392531E-12-5.93502026E+03	3.02998433E+01		4
3854	C6H10D24 C 6H 10 0 OG	300.000 5000.000 1393.000		31
3855	1.67662657E+01 2.32109616E-02-7.93355119E-06	1.23101995E-09-7.13892514E-14		2
3856	-2.93324539E+03-6.44104411E+01-3.63783422E-01	6.36719104E-02-4.53090160E-05		3
3857	1.73368393E-08-2.79133016E-12 3.04087286E+03	2.75469470E+01		4
3858	C5H91-3 9/ 8/14 C 5H 9 0 OG	300.000 5000.000 1390.000		21
3859	1.39593933E+01 2.09180210E-02-7.14307074E-06	1.10781333E-09-6.42268160E-14		2
3860	7.02651017E+03-5.03103610E+01-4.68159636E-01	5.13472600E-02-3.05648794E-05		3
3861	8.82809744E-09-9.61458255E-13 1.23781446E+04	2.83587835E+01		4
3862	C5H92-4 9/ 8/14 C 5H 9 0 OG	300.000 5000.000 1384.000		21
3863	1.35637956E+01 2.11621316E-02-7.20826071E-06	1.11611006E-09-6.46370085E-14		2
3864	5.82258629E+03-4.87323606E+01 2.55028348E-01	4.69860501E-02-2.40447582E-05		3
3865	4.89006694E-09-1.15557679E-13 1.09775103E+04	2.46226810E+01		4
3866	C5H92-5 9/ 8/14 C 5H 9 0 OG	300.000 5000.000 1386.000		31
3867	1.32988753E+01 2.09845923E-02-7.14999241E-06	1.10717347E-09-6.41183619E-14		2
3868	1.39270369E+04-4.32758927E+01 9.96363945E-01	4.49148898E-02-2.30951498E-05		3
3869	5.01698735E-09-2.38646470E-13 1.87161506E+04	2.45616052E+01		4
3870	C5H91-4 9/ 8/14 C 5H 9 0 OG	300.000 5000.000 1387.000		31
3871	1.29229725E+01 2.10931621E-02-7.14227112E-06	1.10137556E-09-6.35983966E-14		2
3872	1.38192408E+04-4.00293126E+01 1.58797615E+00	4.01577239E-02-1.50062687E-05		3
3873	-3.94608061E-10 1.02064182E-12 1.84683983E+04	2.34273438E+01		4
3874	C5H91-5 9/ 8/14 C 5H 9 0 OG	300.000 5000.000 1391.000		31
3875	1.37334869E+01 2.07003006E-02-7.06962737E-06	1.09638953E-09-6.35591113E-14		2
3876	1.51176253E+04-4.50794850E+01 2.07676634E-01	4.96049077E-02-3.00621602E-05		3
3877	9.19962077E-09-1.13246061E-12 2.01251866E+04	2.85856261E+01		4
3878	C5H9O2-4 9/ 8/14 C 5H 90 1 OG	300.000 5000.000 1376.000		31
3879	1.73707371E+01 2.09044827E-02-7.30723872E-06	1.15106814E-09-6.74601377E-14		2
3880	-5.48020434E+03-6.50109045E+01 3.38899911E+00	4.71704753E-02-2.40389823E-05		3
3881	4.99166621E-09-2.03242522E-13 1.15232772E+02	1.25183625E+01		4
3882	SC3H5OCH2-1 C 4H 70 1 OG	300.000 5000.000 1382.000		31
3883	1.47022035E+01 1.55342107E-02-5.45701052E-06	8.62544885E-10-5.06734446E-14		2
3884	1.81294800E+03-5.05120353E+01 2.35694446E-01	4.67367652E-02-3.04880689E-05		3
3885	9.75216148E-09-1.23281228E-12 7.11668364E+03	2.81378517E+01		4
3886	NC4KET21OH C 4H 80 2 OG	300.000 5000.000 1507.000		41
3887	1.52252911E+01 1.86615017E-02-6.30658772E-06	9.72355897E-10-5.61770184E-14		2
3888	-5.34759661E+04-5.00397269E+01 5.46677192E+00	3.01119974E-02-2.59548850E-06		3
3889	-7.61700554E-09 2.55573161E-12-4.89909104E+04	6.33307684E+00		4
3890	C2H5CHOHCO C 4H 70 2 OG	300.000 5000.000 1389.000		41
3891	1.82917246E+01 1.48007410E-02-5.24974573E-06	8.35220286E-10-4.92942253E-14		2
3892	-3.36703722E+04-7.12363783E+01-2.44749259E+00	6.46308488E-02-5.10457937E-05		3
3893	1.99850773E-08-3.12214490E-12-2.66670442E+04	3.95566556E+01		4
3894	CH3COCOCH3 C 4H 70 2 OG	300.000 5000.000 1395.000		41
3895	1.65624631E+01 1.59037217E-02-5.54554278E-06	8.72274939E-10-5.10735025E-14		2
3896	-3.65884887E+04-6.10833920E+01-1.65607674E+00	6.08409982E-02-4.85215440E-05		3
3897	1.97794382E-08-3.26305133E-12-3.05158227E+04	3.58911868E+01		4
3898	C2H4COCH2OH C 4H 70 2 OG	300.000 5000.000 1462.000		41
3899	1.40828195E+01 1.76833414E-02-6.09759192E-06	9.52794521E-10-5.55571628E-14		2
3900	-3.37518398E+04-4.08944306E+01 7.98874348E+00	1.41152447E-02 1.86299924E-05		3

3901	-1.99223089E-08	5.12983835E-12	-2.98706372E+04	-1.87192030E+00	4						
3902	CH3COHCO	9/24/15	C	3H	40	2	OG	300.000	5000.000	1410.000	21
3903	1.50110709E+01	7.26697312E-03	-2.42872486E-06	3.71246886E-10	-2.13068531E-14	2					
3904	-3.87354954E+04	-5.41005540E+01	8.25855205E-01	5.22217422E-02	-5.66992291E-05	3					
3905	2.94815948E-08	-5.81714952E-12	-3.50157127E+04	1.78488731E+01		4					
3906	CH2COHCHO	9/24/15	C	3H	40	2	OG	300.000	5000.000	1406.000	21
3907	1.40200417E+01	7.95092924E-03	-2.63244516E-06	3.99896432E-10	-2.28538120E-14	2					
3908	-3.76808145E+04	-4.80457990E+01	5.76639663E-02	5.16589617E-02	-5.49773816E-05	3					
3909	2.83487148E-08	-5.57464421E-12	-3.39594513E+04	2.29757289E+01		4					
3910	NC4KET13OH-2		C	4H	80	4	OG	300.000	5000.000	1395.000	61
3911	2.25434165E+01	1.76377030E-02	-6.14926113E-06	9.67201484E-10	-5.66321794E-14	2					
3912	-6.59724022E+04	-8.48522697E+01	2.13332105E+00	6.69840817E-02	-5.19672275E-05	3					
3913	2.03864253E-08	-3.22074763E-12	-5.90962942E+04	2.40964870E+01		4					
3914	NC4KET24OH-1		C	4H	80	4	OG	300.000	5000.000	1672.000	61
3915	1.76639507E+01	2.38921914E-02	-8.87612081E-06	1.46065294E-09	-8.83476797E-14	2					
3916	-6.36561283E+04	-5.60405234E+01	7.17383002E+00	3.72830917E-02	-7.30000099E-06	3					
3917	-5.42423663E-09	1.94298976E-12	-5.91469605E+04	3.98040888E+00		4					
3918	NC4KET24OH-3		C	4H	80	4	OG	300.000	5000.000	1392.000	61
3919	2.02237496E+01	1.94540798E-02	-6.73928381E-06	1.05529414E-09	-6.15931037E-14	2					
3920	-6.68651215E+04	-6.99676945E+01	2.60979522E+00	6.11530456E-02	-4.50409252E-05	3					
3921	1.73313054E-08	-2.75573967E-12	-6.07708447E+04	2.44892030E+01		4					
3922	C4H6OHOH1-4-3		C	4H	80	3	OG	300.000	5000.000	1398.000	51
3923	2.15163584E+01	1.55811846E-02	-5.27569793E-06	8.14810620E-10	-4.71424652E-14	2					
3924	-3.74825726E+04	-8.24101150E+01	-1.90016482E+00	7.72727339E-02	-6.79667571E-05	3					
3925	2.98158102E-08	-5.16343458E-12	-3.01649655E+04	4.06810164E+01		4					
3926	C4H6OHOH2-2-1		C	4H	80	3	OG	300.000	5000.000	1396.000	51
3927	2.16656460E+01	1.59965487E-02	-5.52214578E-06	8.62740322E-10	-5.02768063E-14	2					
3928	-4.14875437E+04	-8.39377540E+01	4.72576793E-02	7.85787048E-02	-7.68006410E-05	3					
3929	3.79206120E-08	-7.33203833E-12	-3.51140091E+04	2.80064858E+01		4					
3930	C4H6OHOH1-3-4		C	4H	80	3	OG	300.000	5000.000	1391.000	51
3931	1.93445152E+01	1.82185729E-02	-6.34491630E-06	9.97097673E-10	-5.83420009E-14	2					
3932	-3.79952136E+04	-6.88144861E+01	9.44277749E-01	6.34330602E-02	-4.99455695E-05	3					
3933	2.05720571E-08	-3.48143957E-12	-3.17827282E+04	2.92923796E+01		4					
3934	C4H6OHOH1-2-3		C	4H	80	3	OG	300.000	5000.000	1403.000	51
3935	2.32793098E+01	1.38280934E-02	-4.61330737E-06	7.05319574E-10	-4.05174739E-14	2					
3936	-4.26348237E+04	-9.51979841E+01	-2.88475927E+00	9.16099207E-02	-9.37152074E-05	3					
3937	4.66406895E-08	-8.92736049E-12	-3.52899912E+04	3.92851633E+01		4					
3938	HOCH2CHO	9/24/15	C	2H	40	2	OG	300.000	5000.000	1680.000	21
3939	7.99598542E+00	1.20664034E-02	-4.43693399E-06	7.25167046E-10	-4.36535460E-14	2					
3940	-4.09020567E+04	-1.33754312E+01	4.35084369E+00	1.50412895E-02	-5.95083030E-07	3					
3941	-3.75736217E-09	1.09353598E-12	-3.91654526E+04	8.09610238E+00		4					
3942	C4H71-4OOH		C	4H	80	2	OG	300.000	5000.000	1392.000	41
3943	1.59871304E+01	1.86028119E-02	-6.40003189E-06	9.97531711E-10	-5.80334203E-14	2					
3944	-1.70152141E+04	-5.46227137E+01	1.31653247E+00	5.16546159E-02	-3.47310922E-05	3					
3945	1.20405755E-08	-1.71650639E-12	-1.17754576E+04	2.46384545E+01		4					
3946	C4H71-4O2	9/25/15	C	4H	70	2	OG	300.000	5000.000	1390.000	31
3947	1.50240251E+01	1.72860962E-02	-5.94297061E-06	9.25861430E-10	-5.38461748E-14	2					
3948	1.92460667E+02	-4.85941022E+01	2.09042625E+00	4.57130080E-02	-2.94815830E-05	3					
3949	9.69604853E-09	-1.30061388E-12	4.88932667E+03	2.15456077E+01		4					
3950	C4H61-3OOH4		C	4H	70	2	OG	300.000	5000.000	1391.000	31
3951	1.55818475E+01	1.69176098E-02	-5.84009100E-06	9.12401042E-10	-5.31699330E-14	2					
3952	1.20753065E+01	-5.36683745E+01	1.00320366E+00	4.99893791E-02	-3.43100656E-05	3					
3953	1.20104294E-08	-1.71132691E-12	5.17744264E+03	2.49842453E+01		4					
3954	C4H601-3OOH4		C	4H	70	3	OG	300.000	5000.000	1386.000	41
3955	1.95456291E+01	1.60358540E-02	-5.61768950E-06	8.86341914E-10	-5.20072732E-14	2					
3956	-1.12679434E+04	-6.99490153E+01	3.83045773E+00	5.07388403E-02	-3.42226447E-05	3					
3957	1.13486298E-08	-1.48529245E-12	-5.61786232E+03	1.51509867E+01		4					
3958	C4H6O2-1OOH4		C	4H	70	3	OG	300.000	5000.000	1364.000	41
3959	2.05164800E+01	1.55727845E-02	-5.54197222E-06	8.83592649E-10	-5.22241946E-14	2					
3960	-9.30030707E+03	-7.46630628E+01	5.38344712E+00	4.47089832E-02	-2.43630482E-05	3					
3961	5.07835349E-09	-1.20805939E-13	-3.40711224E+03	8.84731441E+00		4					
3962	HOCH2COCH2		C	3H	50	2	OG	300.000	5000.000	1363.000	31
3963	1.27106963E+01	1.15513960E-02	-3.95951917E-06	6.16237371E-10	-3.58328248E-14	2					
3964	-2.71538154E+04	-3.67129478E+01	4.98634970E+00	2.51766916E-02	-1.10893306E-05	3					
3965	1.12011467E-09	2.89491135E-13	-2.40047973E+04	6.38258616E+00		4					
3966	HOCH2CO	9/25/15	C	2H	30	2	OG	300.000	5000.000	1487.000	21
3967	9.43496508E+00	7.68897340E-03	-2.74959280E-06	4.39772312E-10	-2.60488233E-14	2					
3968	-2.29700136E+04	-2.04618579E+01	5.12916864E+00	9.07172819E-03	6.49228146E-06	3					
3969	-8.56591893E-09	2.31070825E-12	-2.06151607E+04	5.73007596E+00		4					
3970	HOCHCHO	9/25/15	C	2H	30	2	OG	300.000	5000.000	1680.000	21
3971	9.99251726E+00	7.77560619E-03	-2.94238616E-06	4.90136333E-10	-2.98979778E-14	2					
3972	-2.20440827E+04	-2.73957153E+01	5.42856274E-01	2.95295948E-02	-2.08315490E-05	3					
3973	6.72777461E-09	-8.06116446E-13	-1.89378452E+04	2.31681075E+01		4					

3974	PC3H4OH-3	9/25/15	C	3H	50	1	OG	300.000	5000.000	1378.000	11
3975											2
3976											3
3977											4
3978	PC3H4OH-1	9/25/15	C	3H	50	1	OG	300.000	5000.000	1403.000	21
3979											2
3980											3
3981											4
3982	CH3COCHOH	9/25/15	C	3H	50	2	OG	300.000	5000.000	1378.000	31
3983											2
3984											3
3985											4
3986	SC2H2OH	9/25/15	C	2H	30	1	OG	300.000	5000.000	1410.000	11
3987											2
3988											3
3989											4
3990	PC4H8OH-1		C	4H	90	1	OG	300.000	5000.000	1392.000	41
3991											2
3992											3
3993											4
3994	PC4H8OH-3		C	4H	90	1	OG	300.000	5000.000	1398.000	41
3995											2
3996											3
3997											4
3998	C4H7O1-4	9/ 8/14	C	4H	70	1	OG	300.000	5000.000	1388.000	21
3999											2
4000											3
4001											4
4002	PC4H8OH-4		C	4H	90	1	OG	300.000	5000.000	1401.000	41
4003											2
4004											3
4005											4
4006	SC4H8OH-2		C	4H	90	1	OG	300.000	5000.000	1395.000	41
4007											2
4008											3
4009											4
4010	CH2COHCO	9/25/15	C	3H	30	2	OG	300.000	5000.000	1411.000	11
4011											2
4012											3
4013											4
4014	C4H72-202	9/29/15	C	4H	70	2	OG	300.000	5000.000	1390.000	31
4015											2
4016											3
4017											4
4018	C4H71-102	9/29/15	C	4H	70	2	OG	300.000	5000.000	1390.000	31
4019											2
4020											3
4021											4
4022	C4H71-202	9/29/15	C	4H	70	2	OG	300.000	5000.000	1394.000	31
4023											2
4024											3
4025											4
4026	C3H6OH1-1	10/ 2/15	C	3H	70	1	OG	300.000	5000.000	1388.000	31
4027											2
4028											3
4029											4
4030	PC4H8OH-202		C	4H	90	3	OG	300.000	5000.000	1407.000	51
4031											2
4032											3
4033											4
4034	SC4H8OH-102		C	4H	90	3	OG	300.000	5000.000	1405.000	51
4035											2
4036											3
4037											4
4038	C4H71-300CH3		C	5H	100	2	OG	300.000	5000.000	1387.000	51
4039											2
4040											3
4041											4
4042	C4H72-100CH3		C	5H	100	2	OG	300.000	5000.000	1382.000	51
4043											2
4044											3
4045											4
4046	C4H6		C	4H	6	0	OG	300.000	5000.000	1388.000	11

4047	1.01064561E+01	1.46248415E-02	-5.01373934E-06	7.79510645E-10	-4.52675769E-14	2
4048	9.96133753E+03	-2.97310638E+01	1.01356056E+00	3.35722771E-02	-1.96279376E-05	3
4049	5.74803850E-09	-6.75029065E-13	1.33956759E+04	1.99957382E+01		4
4050	C4H612	A 8/83C	4H 6 0 0G	300.000	5000.000 1374.000	11
4051	1.14059885E+01	1.31489843E-02	-4.43542071E-06	6.83028825E-10	-3.94289265E-14	2
4052	1.42427294E+04	-3.69674067E+01	9.45515689E-01	3.46162239E-02	-1.98590697E-05	3
4053	5.02139421E-09	-3.67977164E-13	1.81439079E+04	2.02191143E+01		4
4054	C4H6-2	A 8/83C	4H 6 0 0G	300.000	5000.000 1377.000	21
4055	9.60305554E+00	1.48972169E-02	-5.16751230E-06	8.09757170E-10	-4.72817668E-14	2
4056	1.24831314E+04	-2.87129792E+01	1.97152408E+00	2.76790997E-02	-1.13396645E-05	3
4057	1.02970745E-09	2.75290944E-13	1.57283766E+04	1.42147356E+01		4
4058	C4H5-I	H6W/94C	4H 5 0 0G	300.000	3000.00 1000.00	1
4059	0.10229092E+02	0.94850138E-02	-0.90406445E-07	-0.12596100E-08	0.24781468E-12	2
4060	0.34642812E+05	-0.28564529E+02	-0.19932900E-01	0.38005672E-01	-0.27559450E-04	3
4061	0.77835551E-08	0.40209383E-12	0.37496223E+05	0.24394241E+02		4
4062	C4H5-N	H6W/94C	4H 5 0 0G	300.000	3000.00 1000.00	1
4063	0.98501978E+01	0.10779008E-01	-0.13672125E-05	-0.77200535E-09	0.18366314E-12	2
4064	0.38840301E+05	-0.26001846E+02	0.16305321E+00	0.39830137E-01	-0.34000128E-04	3
4065	0.15147233E-07	-0.24665825E-11	0.41429766E+05	0.23536163E+02		4
4066	C4H5	H6W/94C	4H 5 0 0G	300.000	3000.00 1000.00	1 !
	lumped C4H5-N					
4067	0.98501978E+01	0.10779008E-01	-0.13672125E-05	-0.77200535E-09	0.18366314E-12	2
4068	0.38840301E+05	-0.26001846E+02	0.16305321E+00	0.39830137E-01	-0.34000128E-04	3
4069	0.15147233E-07	-0.24665825E-11	0.41429766E+05	0.23536163E+02		4
4070	C4H5-2	H6W/94C	4H 5 0 0G	300.000	5000.000 1385.000	11
4071	1.03230828E+01	1.17625574E-02	-4.00004665E-06	6.18727929E-10	-3.58083530E-14	2
4072	3.25861413E+04	-2.88794317E+01	2.31011292E+00	2.83747046E-02	-1.63836755E-05	3
4073	4.46251967E-09	-4.30510879E-13	3.55842945E+04	1.49105965E+01		4
4074	C4H4	H6W/94C	4H 4 0 0G	300.000	3000.00 1000.00	1
4075	0.66507092E+01	0.16129434E-01	-0.71938875E-05	0.14981787E-08	-0.11864110E-12	2
4076	0.31195992E+05	-0.97952118E+01	-0.19152479E+01	0.52750878E-01	-0.71655944E-04	3
4077	0.55072423E-07	-0.17286228E-10	0.32978504E+05	0.31419983E+02		4
4078	C4H3-I	AB1/93C	4H 3 0 0G	300.000	3000.00 1000.00	1
4079	0.90978165E+01	0.92207119E-02	-0.33878441E-05	0.49160498E-09	-0.14529780E-13	2
4080	0.56600574E+05	-0.19802597E+02	0.20830412E+01	0.40834274E-01	-0.62159685E-04	3
4081	0.51679358E-07	-0.17029184E-10	0.58005129E+05	0.13617462E+02		4
4082	C4H3-N	H6W/94C	4H 3 0 0G	300.000	3000.00 1000.00	1
4083	0.54328279E+01	0.16860981E-01	-0.94313109E-05	0.25703895E-08	-0.27456309E-12	2
4084	0.61600680E+05	-0.15673981E+01	-0.31684113E+00	0.46912100E-01	-0.68093810E-04	3
4085	0.53179921E-07	-0.16523005E-10	0.62476199E+05	0.24622559E+02		4
4086	C4H3	H6W/94C	4H 3 0 0G	300.000	3000.00 1000.00	1 !
	lumped C4H3-N					
4087	0.54328279E+01	0.16860981E-01	-0.94313109E-05	0.25703895E-08	-0.27456309E-12	2
4088	0.61600680E+05	-0.15673981E+01	-0.31684113E+00	0.46912100E-01	-0.68093810E-04	3
4089	0.53179921E-07	-0.16523005E-10	0.62476199E+05	0.24622559E+02		4
4090	C4H2	D11/99C	4H 2 0 0G	300.000	3000.000 1000.	1
4091	0.91576328E+01	0.55430518E-02	-0.13591604E-05	0.18780075E-10	0.23189536E-13	2
4092	0.52588039E+05	-0.23711460E+02	0.10543978E+01	0.41626960E-01	-0.65871784E-04	3
4093	0.53257075E-07	-0.16683162E-10	0.54185211E+05	0.14866591E+02		4
4094	C4H6O25	T 3/97C	4H 60 1 0G	200.000	5000.000 1000.0	1
4095	8.60658242E+00	2.08310051E-02	-8.42229481E-06	1.56717640E-09	-1.09391202E-13	2
4096	-1.76177415E+04	-2.32464750E+01	2.67053463E+00	4.92586420E-03	8.86967406E-05	3
4097	-1.26219194E-07	5.23991321E-11	-1.46572472E+04	1.45722395E+01	-1.30831522E+04	4
4098	C2H3CHOCH2	C 4H 60 1 0G	300.000	5000.000 1431.000		11
4099	1.26762790E+01	1.40819509E-02	-4.63473868E-06	7.01090838E-10	-3.99438277E-14	2
4100	-4.08065264E+03	-4.22515995E+01	-3.59388437E+00	5.79063450E-02	-4.97163294E-05	3
4101	2.15818682E-08	-3.69199072E-12	8.58852628E+02	4.28475443E+01		4
4102	FURAN	T03/97C	4H 40 1 0G	200.000	6000.0 1000.0	1
4103	9.38935003E+00	1.40291241E-02	-5.07755110E-06	8.24137332E-10	-4.95319963E-14	2
4104	-8.68241814E+03	-2.79162920E+01	8.47469463E-01	1.31773796E-02	5.99735901E-05	3
4105	-9.71562904E-08	4.22733796E-11	-5.36785445E+03	2.14945172E+01	-4.17166616E+03	4
4106	C4H6O23	T 3/97C	4H 60 1 0G	200.000	5000.000 1000.0	1
4107	8.60658242E+00	2.08310051E-02	-8.42229481E-06	1.56717640E-09	-1.09391202E-13	2
4108	-1.32392815E+04	-2.32464750E+01	2.67053463E+00	4.92586420E-03	8.86967406E-05	3
4109	-1.26219194E-07	5.23991321E-11	-1.02787872E+04	1.45722395E+01	-1.30831522E+04	4
4110	CH2CHCHCHO	C 4H 50 1 0G	300.000	5000.000 1385.000		11
4111	1.39299886E+01	1.13228814E-02	-3.87393567E-06	6.02378620E-10	-3.50120301E-14	2
4112	-2.39589898E+03	-4.79026849E+01	4.51553480E-01	4.37530418E-02	-3.37273602E-05	3
4113	1.31111496E-08	-2.04732021E-12	2.14943141E+03	2.40835867E+01		4
4114	H2C4O	120189H	2C 40 1 G	0300.00	4000.00 1000.00	1
4115	0.01026888E+03	0.04896164E-01	-0.04885081E-05	-0.02708566E-08	0.05107013E-12	2
4116	0.02346903E+06	-0.02815985E+03	0.04810971E+02	0.01313999E+00	0.09865073E-05	3
4117	-0.06120720E-07	0.01640003E-10	0.02545803E+06	0.02113424E+02		4

4118	NC3H7CHO	8/12/15	C	4H	80	1	OG	300.000	5000.000	1679.000	31
4119	1.19789345E+01	2.04894148E-02	-7.24831619E-06	1.15561709E-09	-6.84119824E-14						2
4120	-3.09272130E+04	-3.63929716E+01	1.24208539E+00	4.21277518E-02	-2.13832135E-05						3
4121	4.22614614E-09	-1.03710908E-13	-2.71049353E+04	2.21567167E+01							4
4122	NC3H7CO		C	4H	70	1	OG	300.000	5000.000	1496.000	31
4123	1.34870098E+01	1.58626861E-02	-5.41698905E-06	8.40508889E-10	-4.87570090E-14						2
4124	-1.30725285E+04	-4.38634081E+01	2.63537828E+00	3.40368642E-02	-1.24118988E-05						3
4125	-1.17886666E-09	1.16488136E-12	-8.65919992E+03	1.68407569E+01							4
4126	C3H6CHO-1		C	4H	70	1	OG	300.000	5000.000	1538.000	31
4127	1.33449137E+01	1.59347421E-02	-5.43143577E-06	8.41706117E-10	-4.87847084E-14						2
4128	-6.91281947E+03	-4.19662475E+01	2.21483383E+00	3.54113290E-02	-1.44082892E-05						3
4129	5.27605922E-11	8.95003230E-13	-2.46482792E+03	2.00076022E+01							4
4130	C3H6CHO-2		C	4H	70	1	OG	300.000	5000.000	1439.000	31
4131	1.27128605E+01	1.68632757E-02	-5.83779932E-06	9.14059755E-10	-5.33575736E-14						2
4132	-8.50165835E+03	-3.84620358E+01	4.01372834E+00	2.33173718E-02	5.72463585E-06						3
4133	-1.27182841E-08	3.69912722E-12	-4.16766399E+03	1.30545921E+01							4
4134	C3H6CHO-3		C	4H	70	1	OG	300.000	5000.000	1678.000	31
4135	1.21729663E+01	1.80056550E-02	-6.43783092E-06	1.03362049E-09	-6.14850407E-14						2
4136	-1.08642352E+04	-3.80322250E+01	5.29001237E-01	4.30707499E-02	-2.49474118E-05						3
4137	6.40934608E-09	-5.27769846E-13	-6.87667117E+03	2.48856420E+01							4
4138	SC3H5CHO		C	4H	60	1	OG	300.000	5000.000	1396.000	21
4139	1.33892118E+01	1.39115420E-02	-4.75820958E-06	7.38736618E-10	-4.28606559E-14						2
4140	-1.97917448E+04	-4.60146004E+01	1.09372823E+00	4.43315368E-02	-3.41918451E-05						3
4141	1.39369607E-08	-2.33791460E-12	-1.56745978E+04	1.94458467E+01							4
4142	SC3H5CO		C	4H	50	1	OG	300.000	5000.000	1396.000	11
4143	1.29925654E+01	1.22140721E-02	-4.19305277E-06	6.52697685E-10	-3.79407376E-14						2
4144	-2.74782380E+03	-4.51092470E+01	7.76401404E-01	4.26828436E-02	-3.37881191E-05						3
4145	1.39128174E-08	-2.33331638E-12	1.29903132E+03	1.98102013E+01							4
4146	C2H5COCH3	8/12/15	C	4H	80	1	OG	300.000	5000.000	1454.000	31
4147	1.28183044E+01	1.79874386E-02	-5.94194784E-06	9.01636365E-10	-5.14993729E-14						2
4148	-3.51711964E+04	-4.11609193E+01	2.57048052E+00	3.51446793E-02	-1.23849584E-05						3
4149	-1.21280927E-09	1.16163555E-12	-3.10194049E+04	1.61395232E+01							4
4150	C2H5COCH2		C	4H	70	1	OG	300.000	5000.000	1396.000	31
4151	1.35979480E+01	1.57187785E-02	-5.35200820E-06	8.28428039E-10	-4.79645862E-14						2
4152	-1.30111973E+04	-4.46215708E+01	1.96643032E+00	4.10271409E-02	-2.56193885E-05						3
4153	7.86244495E-09	-9.26825962E-13	-8.80149212E+03	1.84803948E+01							4
4154	CH2CH2COCH3		C	4H	70	1	OG	300.000	5000.000	1392.000	31
4155	1.17915603E+01	1.70296457E-02	-5.75444256E-06	8.86035114E-10	-5.11070778E-14						2
4156	-9.70683178E+03	-3.25532787E+01	2.36191763E+00	3.50400641E-02	-1.70487065E-05						3
4157	3.09070210E-09	2.80364847E-14	-6.02754073E+03	1.95184512E+01							4
4158	CH3CHCOCH3		C	4H	70	1	OG	300.000	5000.000	1438.000	31
4159	1.19651378E+01	1.63142163E-02	-5.39879520E-06	8.20454677E-10	-4.69197541E-14						2
4160	-1.51990676E+04	-3.30142593E+01	3.31082456E+00	2.83712402E-02	-5.64603859E-06						3
4161	-4.62626296E-09	1.82954207E-12	-1.14602301E+04	1.62217415E+01							4
4162	C2H3COCH3		C	4H	60	1	OG	300.000	5000.000	1390.000	21
4163	1.19989844E+01	1.52616304E-02	-5.26018882E-06	8.20774274E-10	-4.77834528E-14						2
4164	-2.12170620E+04	-3.71383523E+01	6.55910700E-01	4.19405303E-02	-3.00269693E-05						3
4165	1.16578089E-08	-1.92100897E-12	-1.72216627E+04	2.38412293E+01							4
4166	CH3CHOOCOCH3		C	4H	70	3	OG	300.000	5000.000	1411.000	41
4167	1.68056216E+01	1.70791389E-02	-5.69439450E-06	8.68878944E-10	-4.98008338E-14						2
4168	-3.06718613E+04	-5.51178960E+01	4.30171569E+00	4.62273591E-02	-3.12564494E-05						3
4169	1.08627824E-08	-1.51478379E-12	-2.63732146E+04	1.19724375E+01							4
4170	CH2CHOOHCOCH3		C	4H	70	3	OG	300.000	5000.000	1413.000	51
4171	1.78031394E+01	1.60286227E-02	-5.38152372E-06	8.25242310E-10	-4.74718968E-14						2
4172	-2.30767899E+04	-5.87370258E+01	4.45962223E+00	4.67200276E-02	-3.15878907E-05						3
4173	1.06245787E-08	-1.38857032E-12	-1.84720686E+04	1.29655977E+01							4
4174	C2H5CHCO		C	4H	60	1	OG	300.000	5000.000	1550.000	21
4175	-2.04040652E+02	2.93466880E-01	-1.15884523E-04	1.95253673E-08	-1.19030791E-12						2
4176	8.27380036E+04	1.21233386E+03	-2.28307043E+01	1.70978191E-01	-3.53394379E-04						3
4177	2.78221616E-07	-6.77325074E-11	-1.04125457E+04	1.31232921E+02							4
4178	IC4H6Q2-II	9/ 8/14	C	4H	80	4	OG	300.000	5000.000	1386.000	61
4179	2.50360805E+01	1.60230197E-02	-5.70704966E-06	9.10412038E-10	-5.38294659E-14						2
4180	-2.84196401E+04	-9.67186452E+01	2.16408482E-01	8.25572149E-02	-7.64540445E-05						3
4181	3.58211787E-08	-6.67718658E-12	-2.05694845E+04	3.36943223E+01							4
4182	C5H10-1		C	5H	10	0	OG	300.000	5000.000	1390.000	31
4183	1.43624894E+01	2.26076154E-02	-7.70500843E-06	1.19329968E-09	-6.91126022E-14						2
4184	-9.99915627E+03	-5.12512094E+01	-1.65023816E-01	5.30727359E-02	-3.10861587E-05						3
4185	8.92413402E-09	-9.81619602E-13	-4.57363143E+03	2.80570113E+01							4
4186	C5H81-3	9/ 8/14	C	5H	8	0	OG	300.000	5000.000	1385.000	21
4187	1.29945372E+01	1.92678312E-02	-6.58966712E-06	1.02295969E-09	-5.93441369E-14						2
4188	4.59040047E+03	-4.35689825E+01	1.54882436E+00	4.15042709E-02	-2.14359890E-05						3
4189	4.71145517E-09	-2.42142508E-13	9.05636062E+03	1.95665910E+01							4
4190	C5H9O1-3	9/ 8/14	C	5H	90	1	OG	300.000	5000.000	1379.000	31

4191	1.78860333E+01	2.04837367E-02	-7.16613461E-06	1.12948597E-09	-6.62221468E-14	2
4192	-4.33139568E+03	-6.72851315E+01	2.49666166E+00	5.20326105E-02	-3.09828268E-05	3
4193	9.02567482E-09	-1.04311127E-12	1.54758549E+03	1.70868328E+01		4
4194	BC5H10	9/ 8/14	C 5H 10 0 0G	300.000	5000.000 1389.000	31
4195	1.40426423E+01	2.27915348E-02	-7.74902598E-06	1.19814522E-09	-6.93127003E-14	2
4196	-1.32160483E+04	-5.14469569E+01	6.04882839E-01	4.96635256E-02	-2.66571142E-05	3
4197	6.47312078E-09	-4.84017883E-13	-8.06312207E+03	2.23818263E+01		4
4198	CC5H9-A		C 5H 9 0 0G	300.000	5000.000 1393.000	31
4199	1.38635892E+01	2.06362872E-02	-7.05717373E-06	1.09539676E-09	-6.35381849E-14	2
4200	1.36104251E+04	-4.72507189E+01	-6.78909715E-01	5.37496002E-02	-3.61116825E-05	3
4201	1.28563411E-08	-1.92155723E-12	1.87974429E+04	3.12403382E+01		4
4202	CC5H9-B	9/ 8/14	C 5H 9 0 0G	300.000	5000.000 1392.000	21
4203	1.35249511E+01	2.14363755E-02	-7.35304116E-06	1.14368637E-09	-6.64363518E-14	2
4204	5.41381916E+03	-5.00302394E+01	-6.91501860E-01	5.09804846E-02	-2.96448293E-05	3
4205	8.28273022E-09	-8.57575066E-13	1.07478467E+04	2.76711552E+01		4
4206	AC5H9O-C		C 5H 9O 1 0G	300.000	5000.000 1382.000	31
4207	1.76789601E+01	2.05915073E-02	-7.18764438E-06	1.13116483E-09	-6.62505034E-14	2
4208	-6.25146818E+03	-6.62131721E+01	2.04951318E+00	5.36584877E-02	-3.35086710E-05	3
4209	1.06174235E-08	-1.39224338E-12	-3.85112518E+02	1.91077262E+01		4
4210	CC5H9O-B	9/ 8/14	C 5H 9O 1 0G	300.000	5000.000 1377.000	31
4211	1.86974377E+01	1.84542537E-02	-6.18682537E-06	9.48850967E-10	-5.46203980E-14	2
4212	-7.15897769E+03	-7.26540429E+01	2.75614808E+00	5.20514036E-02	-3.10966938E-05	3
4213	8.25895065E-09	-6.59917121E-13	-1.35162741E+03	1.40990119E+01		4
4214	AC5H10		C 5H 10 0 0G	300.000	5000.000 1392.000	31
4215	1.41931279E+01	2.26551019E-02	-7.70008627E-06	1.19031326E-09	-6.88489604E-14	2
4216	-1.19491010E+04	-5.10688681E+01	-5.39429136E-01	5.44489715E-02	-3.32707895E-05	3
4217	1.03047694E-08	-1.28363329E-12	-6.53967251E+03	2.90349986E+01		4
4218	AC5H9-A2		C 5H 9 0 0G	300.000	5000.000 1385.000	21
4219	1.50019889E+01	1.95965428E-02	-6.60205927E-06	1.01535593E-09	-5.85454957E-14	2
4220	5.90081014E+03	-5.54528992E+01	-9.54047710E-01	5.50153471E-02	-3.58307910E-05	3
4221	1.16444141E-08	-1.49086833E-12	1.15959514E+04	3.08476806E+01		4
4222	AC5H9-C		C 5H 9 0 0G	300.000	5000.000 1392.000	21
4223	1.37918110E+01	2.09644966E-02	-7.13793293E-06	1.10480881E-09	-6.39628018E-14	2
4224	5.09555600E+03	-5.01391436E+01	-8.41372657E-01	5.27157283E-02	-3.27334707E-05	3
4225	1.01974035E-08	-1.26084730E-12	1.04321036E+04	2.93316754E+01		4
4226	AC5H9-D		C 5H 9 0 0G	300.000	5000.000 1393.000	31
4227	1.35607521E+01	2.07514878E-02	-7.06608626E-06	1.09362345E-09	-6.33083050E-14	2
4228	1.31896844E+04	-4.48718988E+01	-1.67398152E-01	5.09876974E-02	-3.22615638E-05	3
4229	1.05911843E-08	-1.43705463E-12	1.81792947E+04	2.95710715E+01		4
4230	TC4H8CHO	9/ 7/95	THERMC 5H 9O 1 0G	300.000	5000.000 1397.00	41
4231	1.79663933E+01	1.94207117E-02	-6.67409451E-06	1.03969221E-09	-6.04702651E-14	2
4232	-1.33368585E+04	-6.79819424E+01	-9.58078294E-01	6.42003258E-02	-4.70776827E-05	3
4233	1.75737698E-08	-2.64896151E-12	-6.86582501E+03	3.33781112E+01		4
4234	O2C4H8CHO	9/ 7/95	THERMC 5H 9O 3 0G	300.000	5000.000 1395.00	51
4235	2.12629904E+01	2.14072282E-02	-7.38342949E-06	1.15281523E-09	-6.71508438E-14	2
4236	-3.16854524E+04	-7.99828703E+01	1.91847699E+00	6.67245869E-02	-4.80871046E-05	3
4237	1.78588690E-08	-2.71163880E-12	-2.49837984E+04	2.38577867E+01		4
4238	O2HC4H8CO	9/ 7/95	THERMC 5H 9O 3 0G	300.000	5000.000 1394.00	61
4239	2.38219630E+01	1.91411448E-02	-6.67919154E-06	1.05127303E-09	-6.15876805E-14	2
4240	-3.23093973E+04	-9.42580755E+01	1.82607262E+00	6.93466111E-02	-4.93125140E-05	3
4241	1.69848340E-08	-2.26117657E-12	-2.46578311E+04	2.41167544E+01		4
4242	C6H101-5	4/12/13	THERMC 6H 10 0 0G	300.000	5000.000 1413.000	21
4243	1.60456030E+01	2.34774145E-02	-7.85797929E-06	1.20200542E-09	-6.90100029E-14	2
4244	2.11899382E+03	-5.88452460E+01	-1.01375402E+00	6.38242808E-02	-4.40653860E-05	3
4245	1.58295163E-08	-2.30830701E-12	7.94033696E+03	3.25056094E+01		4
4246	C6H9-A	12/ 5/12	THERMC 6H 9 0 0G	300.000	5000.000 1400.000	21
4247	1.70842767E+01	2.08842788E-02	-7.14529004E-06	1.10943563E-09	-6.43676989E-14	2
4248	2.01040204E+04	-6.39326012E+01	-2.66715213E+00	7.26196475E-02	-6.05323920E-05	3
4249	2.66000571E-08	-4.74613408E-12	2.64415017E+04	4.02220332E+01		4
4250	IC4H7CHO		C 5H 8O 1 0G	300.000	5000.000 1391.000	31
4251	1.59171638E+01	1.93357284E-02	-6.70857943E-06	1.05155191E-09	-6.14175906E-14	2
4252	-2.16140735E+04	-5.67616631E+01	-1.20982776E+00	5.92603375E-02	-4.26960089E-05	3
4253	1.60356164E-08	-2.49347521E-12	-1.56205327E+04	3.53137305E+01		4
4254	L-C6H4		H6W/94C 6H 4 0 0G	300.000	3000.00 1000.00	1
4255	0.12715182E+02	0.13839662E-01	-0.43765440E-05	0.31541636E-09	0.46619026E-13	2
4256	0.57031148E+05	-0.39464600E+02	0.29590225E+00	0.58053318E-01	-0.67766756E-04	3
4257	0.43376762E-07	-0.11418864E-10	0.60001371E+05	0.22318970E+02		4
4258	C-C6H4		H6W/94C 6H 4 0 0G	300.000	3000.00 1000.00	1
4259	0.13849209E+02	0.78807920E-02	0.18243836E-05	-0.21169166E-08	0.37459977E-12	2
4260	0.47446340E+05	-0.50404953E+02	-0.30991268E+01	0.54030564E-01	-0.40839004E-04	3
4261	0.10738837E-07	0.98078490E-12	0.52205711E+05	0.37415207E+02		4
4262	C6H3		H6W/94C 6H 3 0 0G	300.000	3000.00 1000.00	1
4263	0.58188343E+01	0.27933408E-01	-0.17825427E-04	0.53702536E-08	-0.61707627E-12	2

4264 0.85188250E+05-0.92147827E+00 0.11790619E+01 0.55547360E-01-0.73076168E-04 3
4265 0.52076736E-07-0.15046964E-10 0.85647312E+05 0.19179199E+02 4
4266 !C6H2 P 1/93C 6H 2 0 OG 300.000 3000.00 1000.00 1
!ARAMCO
4267 ! 0.13226281E+02 0.73904302E-02-0.22715381E-05 0.25875217E-09-0.55356741E-14 2
4268 ! 0.80565258E+05-0.41201176E+02-0.15932624E+01 0.80530145E-01-0.14800649E-03 3
4269 ! 0.13300031E-06-0.45332313E-10 0.83273227E+05 0.27980873E+02 4
4270 C6H6 G 6/01C 6H 6 0 OG 200.000 6000.000 1000.000 1
4271 1.10809576E+01 2.07176746E-02-7.52145991E-06 1.22320984E-09-7.36091279E-14 2
4272 4.30641035E+03-4.00413310E+01 5.04818632E-01 1.85020642E-02 7.38345881E-05 3
4273 -1.18135741E-07 5.07210429E-11 8.55247913E+03 2.16412893E+01 9.96811598E+03 4
4274 !FULVENE OC 6H 6 0 OG 200.000 5000.000 1000.00 0 1
!ARAMCO
4275 ! 0.11103525E+02 0.20600685E-01-0.75302224E-05 0.12388695E-08-0.75415976E-13 2
4276 ! 0.20361843E+05-0.36665197E+02-0.71813191E+00 0.37934312E-01 0.11398837E-04 3
4277 !-0.41333503E-07 0.18055927E-10 0.24223825E+05 0.27855714E+02 4
4278 FULVENE OC 6H 6 0 OG 200.000 5000.000 1000.00 0 1
!Burcat kik
4279 1.14345282E+01 1.99371432E-02-7.13567060E-06 1.14951842E-09-6.87263886E-14 2
4280 2.04411455E+04-3.86799524E+01 5.09714763E-01 2.58195980E-02 5.06504954E-05 3
4281 -9.32593825E-08 4.15963672E-11 2.44318827E+04 2.30638077E+01 2.60142888E+04 4
4282 !C6H5 T04/02C 6H 5 0 OG 200.000 6000.000 1000. 1 !
delete duplicate with above kik
4283 ! 1.08444762E+01 1.73212473E-02-6.29233249E-06 1.02369961E-09-6.16216828E-14 2
4284 ! 3.55598475E+04-3.53735134E+01 2.10306633E-01 2.04745507E-02 5.89743006E-05 3
4285 !-1.01534255E-07 4.47105660E-11 3.95468722E+04 2.52910455E+01 4.08610970E+04 4
4286 C6H5OO 3/26/ 9 THERMC 6H 50 2 OG 300.000 5000.000 1403.000 11
4287 1.67078262E+01 1.62326229E-02-5.47969630E-06 8.43510060E-10-4.86562431E-14 2
4288 8.14242915E+03-6.08346973E+01-2.99164672E+00 7.03857150E-02-6.34400574E-05 3
4289 2.91548920E-08-5.30706938E-12 1.41320240E+04 4.20142955E+01 4
4290 C6H5OOH 3/26/ 9 THERMC 6H 60 2 OG 300.000 5000.000 1404.000 21
4291 1.92317474E+01 1.63154699E-02-5.53448904E-06 8.55059974E-10-4.94583790E-14 2
4292 -1.01971012E+04-7.61674471E+01-4.03105975E+00 7.96101888E-02-7.21655013E-05 3
4293 3.27610696E-08-5.85584239E-12-3.10973017E+03 4.54324978E+01 4
4294 !C6H5OH L 4/84C 6H 60 1 OG 300.000 5000.000 1000. 1
!ARAMCO
4295 ! 0.14912073E+02 0.18378135E-01-0.61983128E-05 0.91983221E-09-0.49209565E-13 2
4296 !-0.18375199E+05-0.55924103E+02-0.16956539E+01 0.52271299E-01-0.72024050E-05 3
4297 !-0.35859603E-07 0.20449073E-10-0.13284121E+05 0.32542160E+02-0.11594207E+05 4
4298 C6H5OH phenol g 8/00C 6.H 6.O 1. 0.G 200.000 6000.000 1000. 1
!Burcat kik & same as POLIMI
4299 1.41552427E+01 1.99350340E-02-7.18219540E-06 1.16229002E-09-6.97147483E-14 2
4300 -1.81287441E+04-5.17984911E+01-2.90978575E-01 4.08562397E-02 2.42829425E-05 3
4301 -7.14477617E-08 3.46002146E-11-1.34129780E+04 2.68745637E+01-1.15940687E+04 4
4302 !C6H5O T05/02C 6H 50 1 OG 200.000 6000.000 1000. 1
!ARAMCO & POLIMI
4303 ! 1.37221720E+01 1.74688771E-02-6.35504520E-06 1.03492308E-09-6.23410504E-14 2
4304 ! 2.87274751E+02-4.88181680E+01-4.66204455E-01 4.13443975E-02 1.32412991E-05 3
4305 !-5.72872769E-08 2.89763707E-11 4.77858391E+03 2.76990274E+01 6.49467016E+03 4
4306 C6H5O phenyox ra T11/10C 6.H 5.O 1. 0.G 200.000 6000.000 1000. 1
!Burcat kik
4307 1.39194640E+01 1.82692821E-02-6.66348032E-06 1.08703146E-09-6.55586708E-14 2
4308 1.01826410E+03-5.03399303E+01-3.13089926E-01 3.91633523E-02 2.25817444E-05 3
4309 -6.76854803E-08 3.28002121E-11 5.67534849E+03 2.71661147E+01 7.40392398E+03 4
4310 C6H4OH 4/ 9/ 9 THERMC 6H 50 1 OG 300.000 5000.000 1402.000 11
4311 1.73187560E+01 1.36366984E-02-4.68316332E-06 7.29071204E-10-4.23805358E-14 2
4312 1.14990276E+04-6.89986593E+01-5.99875435E+00 8.59063379E-02-9.12525636E-05 3
4313 4.72275890E-08-9.35576749E-12 1.78621926E+04 4.99931427E+01 4
4314 OC6H4OH 4/ 9/ 9 THERMC 6H 50 2 OG 300.000 5000.000 1403.000 11
4315 2.22718210E+01 1.21038561E-02-4.18429526E-06 6.54475399E-10-3.81746504E-14 2
4316 -2.34827539E+04-9.61035467E+01-8.02205657E+00 1.09403210E-01-1.23489276E-04 3
4317 6.56286805E-08-1.31527870E-11-1.55949156E+04 5.72175202E+01 4
4318 C5H6 T 1/90C 5H 6 0 OG 200.000 6000.000 1000. 1
!ARAMCO
4319 0.99757848E+01 0.18905543E-01-0.68411461E-05 0.11099340E-08-0.66680236E-13 2
4320 0.11081693E+05-0.32209454E+02 0.86108957E+00 0.14804031E-01 0.72108895E-04 3
4321 -0.11338055E-06 0.48689972E-10 0.14801755E+05 0.21353453E+02 0.16152485E+05 4
4322 !C5H6 T 1/90C 5H 6 0 OG 200.000 6000.000 1000. 1
!Burcat kik
4323 ! 9.88465785E+00 1.89943852E-02-6.87485480E-06 1.11556894E-09-6.70255571E-14 2
4324 ! 7.14353103E+03-3.17238367E+01 9.77484017E-01 1.39109570E-02 7.36279225E-05 3
4325 !-1.14340239E-07 4.88766069E-11 1.08333853E+04 2.08861411E+01 1.21907364E+04 4
4326 C5H6 C 5H 6 G 200.00 3500.00 1000.00 1 !

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4327	1.27914695e+00	3.77288105e-02	-2.09426525e-05	5.50583680e-09	-5.53554405e-13	2
4328	1.40655989e+04	1.47486951e+01	-4.86268110e+00	6.22961227e-02	-5.77936208e-05	3
4329	3.00731490e-08	-6.69538246e-12	1.52939645e+04	4.43794652e+01		4
4330	C5H6-L	2/ 5/ 9	THERMC	5H 6 0	OG 300.000 5000.000 1372.000	21
4331	1.29600892E+01	1.48953758E-02	-5.23622902E-06	8.27916389E-10	-4.86464523E-14	2
4332	2.38180800E+04	-4.25312093E+01	3.58448213E+00	3.24459626E-02	-1.70150991E-05	3
4333	4.22715914E-09	-4.18452556E-13	2.76514681E+04	9.60644208E+00		4
4334	C5H7	1/22/ 9	WKM C	5H 7 0	OG 300.000 5000.000 1377.000	31
4335	1.36630213E+01	1.68061358E-02	-5.98746539E-06	9.55341072E-10	-5.64951981E-14	2
4336	1.27238941E+04	-5.46331286E+01	-6.75118368E+00	6.06461693E-02	-4.01260152E-05	3
4337	1.22051562E-08	-1.33459844E-12	2.01365277E+04	5.62694938E+01		4
4338	C5H5OH	5/ 2/91	THE.MC	5H 60 1	OG 300.000 5000.000 1398.000	11
4339	1.53433477E+01	1.50754059E-02	-5.13553582E-06	7.95807816E-10	-4.61311517E-14	2
4340	-1.19645453E+04	-5.85204430E+01	-4.26822012E+00	6.62446749E-02	-5.68494038E-05	3
4341	2.46858526E-08	-4.26820696E-12	-5.75581338E+03	4.47962850E+01		4
4342	C5H5O	5/16/90	THERMC	5H 50 1	OG 300.000 5000.000 1392.000	01
4343	1.48322894E+01	1.40483376E-02	-4.92302051E-06	7.77041219E-10	-4.56103939E-14	2
4344	1.45523665E+04	-5.73228191E+01	-2.83112840E+00	5.67277287E-02	-4.44757303E-05	3
4345	1.749224447E-08	-2.76004847E-12	2.04992154E+04	3.69634411E+01		4
4346	C5H4OH	T 8/99C	5H 50 1	OG 200.000 6000.000 1000.		1
4347	1.33741248E+01	1.51996469E-02	-5.45685046E-06	8.80944866E-10	-5.27493258E-14	2
4348	2.20358027E+03	-4.59569069E+01	-1.28398054E+00	4.90298511E-02	-1.35844414E-05	3
4349	-2.92983743E-08	1.90820619E-11	6.37364803E+03	3.08073591E+01	8.00114499E+03	4
4350	C5H4O	T 8/99C	5H 40 1	OG 200.000 6000.000 1000.		1
4351	1.00806824E+01	1.61143465E-02	-5.83314509E-06	9.46759320E-10	-5.68972206E-14	2
4352	1.94364771E+03	-2.94521623E+01	2.64576497E-01	3.34873827E-02	1.67738470E-06	3
4353	-2.96207455E-08	1.54431476E-11	5.11159287E+03	2.35409513E+01	6.64245999E+03	4
4354	C5H3O	TAK0905C	5H 30 1	OG 300.000 3500.000 1500.00		1
4355	1.19961781E+01	1.34287065E-02	-5.90045309E-06	1.22553862E-09	-9.86114716E-14	2
4356	2.89592010E+04	-4.07548249E+01	-3.03242604E+00	5.43937201E-02	-4.95018348E-05	3
4357	2.25523751E-08	-4.10727920E-12	3.35644081E+04	3.78374823E+01		4
4358	CVCCJCVC	3/1/95	Z&B C	5H 7 0	OG 300.000 5000.000 1388.000	21
4359	1.40879309E+01	1.62398907E-02	-5.64768950E-06	8.86857524E-10	-5.18698993E-14	2
4360	1.76798698E+04	-5.13735038E+01	-2.94595603E+00	5.68783623E-02	-4.31336497E-05	3
4361	1.68169537E-08	-2.67926433E-12	2.35156925E+04	3.98188778E+01		4
4362	CVCCVCCJ	Z&B C	5H 7 0	OG 300.000 5000.000 1386.000		21
4363	1.47302883E+01	1.59030900E-02	-5.57729508E-06	8.80604825E-10	-5.16963733E-14	2
4364	1.74050791E+04	-5.42670706E+01	-1.60087476E+00	5.38764703E-02	-3.96302225E-05	3
4365	1.49599474E-08	-2.31995284E-12	2.31199746E+04	3.35492960E+01		4
4366	CVCCJCVC	10/6/95	Z&B C	5H 70 1	OG 300.000 5000.000 1397.000	31
4367	1.67465815E+01	1.58357240E-02	-5.44954706E-06	8.49881387E-10	-4.94743246E-14	2
4368	-4.30972870E+03	-6.19378748E+01	-2.91175436E+00	6.69362484E-02	-5.71603047E-05	3
4369	2.48753749E-08	-4.33243894E-12	1.96441523E+03	4.17454344E+01		4
4370	HOCVCCVO	1/26/ 9	WKM C	3H 40 2	OG 300.000 5000.000 1413.000	21
4371	1.66505478E+01	6.11745137E-03	-2.09080785E-06	3.24985683E-10	-1.88875073E-14	2
4372	-3.82179939E+04	-6.36794754E+01	-2.01837189E+00	6.26539783E-02	-6.73359280E-05	3
4373	3.39430425E-08	-6.48917648E-12	-3.31367523E+04	3.18162860E+01		4
4374	CVCCVCCO	1/23/ 9	WKM C	5H 80 1	OG 300.000 5000.000 1396.000	31
4375	1.63079670E+01	1.79957763E-02	-6.03115896E-06	9.23992259E-10	-5.31254053E-14	2
4376	-1.58204603E+04	-5.84137244E+01	-5.31488384E-01	6.06983915E-02	-4.81499862E-05	3
4377	2.00308244E-08	-3.38987282E-12	-1.03301302E+04	3.07961436E+01		4
4378	OC5H7O	1/22/ 9	WKM C	5H 70 2	OG 300.000 5000.000 1375.000	31
4379	1.65416953E+01	1.86677673E-02	-6.44836048E-06	1.00787611E-09	-5.87521858E-14	2
4380	-2.82017168E+04	-5.47258181E+01	4.88394767E+00	4.03401300E-02	-1.97774150E-05	3
4381	3.68903501E-09	-3.40202384E-14	-2.35295942E+04	9.97070337E+00		4
4382	OC4H6O	1/23/ 9	WKM C	4H 60 2	OG 300.000 5000.000 1382.000	31
4383	1.41894774E+01	1.53345510E-02	-5.24594862E-06	8.14655154E-10	-4.72759368E-14	2
4384	-4.10001835E+04	-4.43771751E+01	4.21628848E+00	3.57422725E-02	-2.04226185E-05	3
4385	5.63821367E-09	-5.88888993E-13	-3.72055911E+04	1.02814620E+01		4
4386	OC4H5O	1/23/ 9	WKM C	4H 50 2	OG 300.000 5000.000 1388.000	21
4387	1.32138775E+01	1.37339051E-02	-4.62639517E-06	7.10941370E-10	-4.09538499E-14	2
4388	-2.16535271E+04	-3.64185255E+01	4.60550978E+00	3.30498712E-02	-2.13102363E-05	3
4389	7.37021089E-09	-1.08289438E-12	-1.85460831E+04	1.01599453E+01		4
4390	O2CCHOOJ	Z&B C	2H 10 4	OG 300.000 5000.000 1682.000		01
4391	1.09910849E+01	7.46985861E-03	-2.75568271E-06	4.51353051E-10	-2.72108652E-14	2
4392	-3.51335323E+04	-2.11652231E+01	8.91497688E+00	8.60571847E-03	5.24416766E-07	3
4393	-2.79301331E-09	7.62963051E-13	-3.40867754E+04	-8.72978273E+00		4
4394	HOCVCCJVO	1/26/ 9	WKM C	3H 30 2	OG 300.000 5000.000 1414.000	11
4395	1.52720985E+01	5.02586331E-03	-1.68408578E-06	2.58390706E-10	-1.48849424E-14	2
4396	-1.98506828E+04	-5.54641734E+01	6.07270082E-01	4.96011303E-02	-5.32300885E-05	3
4397	2.68392951E-08	-5.13094510E-12	-1.58814562E+04	1.94817133E+01		4
4398	CJVCVCCVO	2/ 5/ 9	THERMC	5H 50 1	OG 300.000 5000.000 1396.000	21

4399	1.62360823E+01	1.18297101E-02-4.11454219E-06	6.46026823E-10-3.77767639E-14	2
4400	1.93499885E+04-5.83498817E+01-5.06628841E-01	6.04671965E-02-5.97396749E-05	3	
4401	2.96804228E-08-5.76240010E-12	2.42765544E+04	2.82994148E+01	4
4402	CVCCVCCJVO 2/ 5/ 9 THERMC 5H 50 1 OG	300.000 5000.000 1399.000	11	
4403	1.53178248E+01	1.27352911E-02-4.35882964E-06	6.76912763E-10-3.92771371E-14	2
4404	7.60582726E+03-5.43599625E+01-2.18492198E-01	5.92100223E-02-5.89241174E-05	3	
4405	2.97411920E-08-5.85244770E-12	1.20600764E+04	2.55968530E+01	4
4406	CJVCCVO 4/ 8/94 THERMC 3H 30 1 OG	300.000 5000.000 1402.000	11	
4407	1.07482537E+01	6.19822688E-03-2.06130981E-06	3.14418872E-10-1.80309517E-14	2
4408	1.51410162E+04-3.01266033E+01	1.46654466E+00	3.23390476E-02-3.05588208E-05	3
4409	1.44081861E-08-2.65600505E-12	1.78850058E+04	1.80850321E+01	4
4410	C#CCVCCJ GLAR C 5H 5 0 OG	300.000 5000.000 1396.000	11	
4411	1.41230912E+01	1.14233190E-02-3.95851276E-06	6.20128961E-10-3.62097887E-14	2
4412	4.25158384E+04-5.02942871E+01-6.16143558E-01	5.06466579E-02-4.48561743E-05	3	
4413	2.02459419E-08-3.64542145E-12	4.71532377E+04	2.71623299E+01	4
4414	O-C6H4O2 AK0405C 6H 40 2 OG	270.000 3000.000 1370.00	1	
4415	1.23614349E+01	2.40491397E-02-1.16529057E-05	2.71332785E-09-2.47593219E-13	2
4416	-1.67079717E+04-4.00310857E+01-2.36179712E+00	6.86058343E-02-6.39129516E-05	3	
4417	3.06903009E-08-5.97357785E-12-1.26704431E+04	3.53724482E+01	4	
4418	P-C6H4O2 AK0405C 6H 40 2 OG	270.000 3000.000 1370.00	1	
4419	1.23423732E+01	2.40612690E-02-1.16565184E-05	2.71393504E-09-2.47643065E-13	2
4420	-2.06185312E+04-4.08244024E+01-2.43170113E+00	6.87937608E-02-6.41382837E-05	3	
4421	3.08126855E-08-5.99832072E-12-1.65696994E+04	3.48309430E+01	4	
4422	O-OC6H5OJ WKM C 60 2H 5 OG	300.000 5000.000 1400.000	01	
4423	1.84625733E+01	1.57607263E-02-5.44671499E-06	8.51765760E-10-4.96759541E-14	2
4424	-1.72770226E+02-7.28742484E+01-2.65459198E+00	7.17179095E-02-6.31552372E-05	3	
4425	2.81132946E-08-4.97463333E-12	6.45283150E+03	3.81123139E+01	4
4426	P-OC6H5OJ WKM C 60 2H 5 OG	300.000 5000.000 1400.000	01	
4427	1.82799770E+01	1.59280974E-02-5.50765220E-06	8.61649836E-10-5.02677539E-14	2
4428	-6.25907994E+01-7.25809444E+01-3.29683290E+00	7.27365977E-02-6.36158220E-05	3	
4429	2.80683553E-08-4.92279426E-12	6.73402222E+03	4.09349895E+01	4
4430	P-C6H3O2 AK0505C 6H 30 2 OG	270.000 3000.000 1290.00	1	
4431	1.22963699E+01	2.15055142E-02-1.07516136E-05	2.57528163E-09-2.41023652E-13	2
4432	1.15428998E+04-3.72584002E+01-1.57852347E+00	6.55376473E-02-6.50308721E-05	3	
4433	3.32026554E-08-6.86665555E-12	1.51750093E+04	3.31518638E+01	4
4434	H15DE25DM C 8H 14 0 OG	300.000 5000.000 1395.000	51	
4435	2.25355644E+01	3.23955734E-02-1.10270814E-05	1.70640907E-09-9.87758061E-14	2
4436	-1.04808866E+04-9.19784905E+01-1.71853441E+00	8.82613783E-02-6.03140500E-05	3	
4437	2.15862289E-08-3.19690882E-12-1.95255748E+03	3.86048681E+01	4	
4438	H15DE25DM-S C 8H 13 0 OG	300.000 5000.000 1395.000	41	
4439	2.21422958E+01	3.06966055E-02-1.04617380E-05	1.62037747E-09-9.38578511E-14	2
4440	6.56045671E+03-9.04059585E+01-2.04235551E+00	8.66261688E-02-5.99110976E-05	3	
4441	2.15551630E-08-3.18976697E-12	1.50224279E+04	3.96917763E+01	4
4442	H15DE25DM-A C 8H 13 0 OG	300.000 5000.000 1391.000	41	
4443	2.33282646E+01	2.93694154E-02-9.94258906E-06	1.53368063E-09-8.86030202E-14	2
4444	7.37319036E+03-9.55902415E+01-2.21863377E+00	8.91652629E-02-6.33360636E-05	3	
4445	2.32007379E-08-3.46329567E-12	1.61971179E+04	4.15116620E+01	4
4446	H15DE25DM-AO C 8H 130 1 OG	300.000 5000.000 1378.000	51	
4447	2.50985951E+01	3.15085628E-02-1.10076915E-05	1.73332426E-09-1.01557468E-13	2
4448	-2.49465338E+03-1.01097942E+02	3.03691957E+00	7.50640438E-02-4.17779534E-05	3
4449	1.07915725E-08-9.97734397E-13	6.11649780E+03	2.04746031E+01	4
4450	H15DE25DM-SO C 8H 130 1 OG	300.000 5000.000 1388.000	51	
4451	2.60152179E+01	3.04295766E-02-1.05676513E-05	1.65746547E-09-9.68470091E-14	2
4452	-4.79568520E+03-1.06442472E+02	9.30464015E-01	8.71669873E-02-5.99582593E-05	3
4453	2.15026041E-08-3.21687573E-12	4.19310073E+03	2.90924508E+01	4
4454	H15DE2M-T C 7H 11 0 OG	300.000 5000.000 1389.000	41	
4455	1.90144729E+01	2.61932198E-02-9.01183878E-06	1.40455988E-09-8.17075251E-14	2
4456	2.35551101E+04-7.15568628E+01	3.88856066E-01	6.70215700E-02-4.29671268E-05	3
4457	1.42489875E-08-1.96105571E-12	3.03627273E+04	2.95444186E+01	4
4458	B2E2M1OJ C 5H 90 1 OG	300.000 5000.000 2003.000	31	
4459	1.35666458E+01	2.56547934E-02-9.37226256E-06	1.52518398E-09-9.15378763E-14	2
4460	-3.58767067E+03-4.27272791E+01	5.64762692E+00	3.43609862E-02-5.60649548E-06	3
4461	-5.19111402E-09	1.73155461E-12-6.65737793E+00	3.13825267E+00	4
4462	B13DE2M C 5H 8 0 OG	300.000 5000.000 1397.000	21	
4463	1.40757545E+01	1.82375566E-02-6.20747687E-06	9.60350919E-10-5.55741525E-14	2
4464	2.40033881E+03-5.12988284E+01-4.72170009E-01	5.59413257E-02-4.50458826E-05	3	
4465	1.96181377E-08-3.52009647E-12	7.14960489E+03	2.56276807E+01	4
4466	B13DE2MJ C 5H 7 0 OG	300.000 5000.000 1393.000	11	
4467	1.48413344E+01	1.52425753E-02-5.13559858E-06	7.89787260E-10-4.55353492E-14	2
4468	2.02661570E+04-5.54474955E+01-8.98037227E-01	5.65174321E-02-4.76107829E-05	3	
4469	2.09672106E-08-3.73076319E-12	2.52881763E+04	2.74966602E+01	4
4470	B12DE3M 11/12/12 THERMC 5H 8 0 OG	300.000 5000.000 1388.000	21	
4471	1.37093177E+01	1.85726726E-02-6.33115904E-06	9.80719059E-10-5.68099894E-14	2

4472	8.59518752E+03-4.88749621E+01	1.27860173E+00	4.54917474E-02-2.82334169E-05	3
4473	8.98449372E-09-1.17220042E-12	1.31637341E+04	1.87039373E+01	4
4474	B2E3M1OJ	C 5H 90 1 0G	300.000 5000.000 2003.000	31
4475	1.35666458E+01 2.56547934E-02-9.37226256E-06	1.52518398E-09-9.15378763E-14		2
4476	-3.58767067E+03-4.27272791E+01 5.64762692E+00	3.43609862E-02-5.60649548E-06		3
4477	-5.19111402E-09 1.73155461E-12-6.65737793E+00	3.13825267E+00		4
4478	C8H141-5,3-4	C 8H 14 0 0G	300.000 5000.000 1396.000	51
4479	2.30690680E+01 3.23154042E-02-1.10795683E-05	1.72276354E-09-1.00052582E-13		2
4480	-8.91240214E+03-9.49655754E+01-2.52713194E+00	9.28837673E-02-6.67176819E-05		3
4481	2.53683579E-08-4.01212661E-12-4.55965940E+01	4.23180878E+01		4
4482	C8H141-5,3 8/25/15	C 8H 14 0 0G	300.000 5000.000 1392.000	51
4483	2.25173982E+01 3.26748629E-02-1.11807923E-05	1.73629966E-09-1.00752481E-13		2
4484	-8.96062790E+03-9.10857551E+01-1.02072126E+00	8.47808555E-02-5.47568199E-05		3
4485	1.81792070E-08-2.47335881E-12-4.53248586E+02	3.64247438E+01		4
4486	C8H142-6 8/25/15	C 8H 14 0 0G	300.000 5000.000 1386.000	51
4487	2.20960852E+01 3.27887472E-02-1.11700037E-05	1.72970378E-09-1.00179059E-13		2
4488	-9.04951881E+03-8.92942652E+01 3.43524821E-01	7.72359120E-02-4.34861460E-05		3
4489	1.12949093E-08-9.77995416E-13-8.37798357E+02	2.98241439E+01		4
4490	C8H131-5,3-4,TA	C 8H 13 0 0G	300.000 5000.000 1394.000	41
4491	2.22822575E+01 3.10651867E-02-1.06940907E-05	1.66739777E-09-9.70243450E-14		2
4492	7.57680613E+03-9.19858764E+01-3.23996819E+00	9.13494930E-02-6.60037456E-05		3
4493	2.51706078E-08-3.99030974E-12 1.64345368E+04	4.49498860E+01		4
4494	C8H131-5,3,TA	C 8H 13 0 0G	300.000 5000.000 1389.000	41
4495	2.16161787E+01 3.14326704E-02-1.07786324E-05	1.67632587E-09-9.73755313E-14		2
4496	7.60897211E+03-8.80384104E+01-5.03201172E-01	7.78854227E-02-4.63156182E-05		3
4497	1.32834166E-08-1.42623050E-12 1.58388712E+04	3.26514434E+01		4
4498	C8H131-5,3,SA	C 8H 13 0 0G	300.000 5000.000 1392.000	41
4499	2.21141889E+01 3.09871348E-02-1.06198459E-05	1.65100088E-09-9.58788408E-14		2
4500	8.08509780E+03-9.01448021E+01-1.32185914E+00	8.30473789E-02-5.42213233E-05		3
4501	1.80737386E-08-2.45105483E-12 1.65183103E+04	3.67169651E+01		4
4502	C8H131-5,3,PA	C 8H 13 0 0G	300.000 5000.000 1389.000	41
4503	2.32085707E+01 2.97529224E-02-1.01333635E-05	1.56925634E-09-9.09001242E-14		2
4504	8.95338901E+03-9.40777602E+01-1.57063382E+00	8.60080913E-02-5.83884368E-05		3
4505	2.02048105E-08-2.83115953E-12 1.77015232E+04	3.95476224E+01		4
4506	C8H132-6,SA	C 8H 13 0 0G	300.000 5000.000 1387.000	41
4507	2.16167233E+01 3.12260643E-02-1.06640216E-05	1.65409816E-09-9.59112187E-14		2
4508	8.03384556E+03-8.72194430E+01 2.20017932E-01	7.48621425E-02-4.21239973E-05		3
4509	1.07414215E-08-8.66560315E-13 1.61027987E+04	2.99517204E+01		4
4510	C8H132-6,PA	C 8H 13 0 0G	300.000 5000.000 1378.000	41
4511	2.29293875E+01 2.97187394E-02-1.00712335E-05	1.55505094E-09-8.99129602E-14		2
4512	8.77975921E+03-9.24517461E+01 1.05119796E-01	7.70150350E-02-4.48890925E-05		3
4513	1.19516688E-08-1.04377517E-12 1.72713386E+04	3.22058738E+01		4
4514	C6H101-3,3	C 6H 10 0 0G	300.000 5000.000 1395.000	31
4515	1.69678361E+01 2.28868236E-02-7.78758381E-06	1.20465198E-09-6.97080856E-14		2
4516	-2.97276905E+03-6.58632941E+01-3.01310455E-02	6.43105079E-02-4.75083462E-05		3
4517	1.89877768E-08-3.17681035E-12 2.82367411E+03	2.49254708E+01		4
4518	C8H131-5,3-4,TAO	C 8H 130 1 0G	300.000 5000.000 1394.000	51
4519	2.70579050E+01 2.84726632E-02-9.66434779E-06	1.49337149E-09-8.63788413E-14		2
4520	-4.43111126E+03-1.12228392E+02 1.00679908E+00	8.90191278E-02-6.27963646E-05		3
4521	2.24161585E-08-3.20587060E-12 4.56422741E+03	2.76546640E+01		4
4522	C8H131-5,3,TAO	C 8H 130 1 0G	300.000 5000.000 1396.000	51
4523	2.16638860E+01 2.77253448E-02-9.69375951E-06	1.67582120E-09-1.08059396E-13		2
4524	-5.70300683E+03-9.33237797E+01 1.46771925E+00	7.67800622E-02-5.63189881E-05		3
4525	2.22689786E-08-3.64813515E-12 1.17475936E+03	1.45619856E+01		4
4526	C8H131-5,3,SAO	C 8H 130 1 0G	300.000 5000.000 1385.000	51
4527	2.61023602E+01 3.05036647E-02-1.06268215E-05	1.67026867E-09-9.77389024E-14		2
4528	-3.64744193E+03-1.06781316E+02 1.60953926E+00	8.39738786E-02-5.49469234E-05		3
4529	1.84255257E-08-2.56040058E-12 5.33713436E+03	2.62653941E+01		4
4530	C8H131-5,3,PAO	C 8H 130 1 0G	300.000 5000.000 1374.000	51
4531	2.51902631E+01 3.15630048E-02-1.10568300E-05	1.74424175E-09-1.02327221E-13		2
4532	-1.34401684E+03-1.01448477E+02 3.91532442E+00	7.10319966E-02-3.55623644E-05		3
4533	6.98595095E-09-1.83465840E-13 7.22911524E+03	1.67145758E+01		4
4534	C8H132-6,SAO	C 8H 130 1 0G	300.000 5000.000 1381.000	51
4535	2.54267504E+01 3.10421548E-02-1.08045689E-05	1.69716523E-09-9.92701997E-14		2
4536	-3.28641768E+03-1.02872762E+02 3.34168622E+00	7.49917518E-02-4.18382842E-05		3
4537	1.06108028E-08-8.96488454E-13 5.24458399E+03	1.86128166E+01		4
4538	C8H132-6,PAO	C 8H 130 1 0G	300.000 5000.000 2014.000	51
4539	1.99391776E+01 3.79081645E-02-1.37893231E-05	2.23770591E-09-1.34044177E-13		2
4540	1.42981257E+03-7.07923233E+01 6.30807632E+00	5.80374259E-02-1.75637726E-05		3
4541	-2.70887760E-09 1.61702129E-12 7.07839485E+03	6.29344560E+00		4
4542	C7H111-5,3,6P	C 7H 11 0 0G	300.000 5000.000 1396.000	41
4543	1.95787047E+01 2.54213538E-02-8.68127275E-06	1.34629701E-09-7.80464853E-14		2
4544	2.58537943E+04-7.44112330E+01-6.76848821E-01	7.38082653E-02-5.35945220E-05		3

4545	2.06293915E-08-3.29701110E-12	3.28160434E+04	3.40518079E+01	4
4546	C7H111-5,1P	C 7H 11 0 OG	300.000 5000.000 1388.000	41
4547	1.91915682E+01 2.55013021E-02-8.65881522E-06	1.33796943E-09-7.73784878E-14	2	
4548	2.60946287E+04-7.21387547E+01 8.16831855E-01	6.56745024E-02-4.14490949E-05	3	
4549	1.32234876E-08-1.69289568E-12	3.27646149E+04	2.75442934E+01	4
4550	C4H64,2-1OH	C 4H 70 1 OG	300.000 5000.000 1366.000	21
4551	1.36259446E+01 1.70233137E-02-6.00460246E-06	9.51603754E-10-5.60055773E-14	2	
4552	-7.81498890E+03-4.44948073E+01 2.50804582E+00	3.53393033E-02-1.41418095E-05	3	
4553	5.65501810E-10 5.94838384E-13-3.08574102E+03	1.81061546E+01	4	
4554	C4H63,1-1OH	C 4H 70 1 OG	300.000 5000.000 1401.000	21
4555	1.38675222E+01 1.54795810E-02-5.17720236E-06	7.91828077E-10-4.54656891E-14	2	
4556	-1.07655481E+04-4.87820652E+01-5.96640682E-01	5.31885124E-02-4.34791765E-05	3	
4557	1.86514084E-08-3.23780972E-12-6.15543596E+03	2.74734171E+01	4	
4558	C4H63,1-3OH	C 4H 70 1 OG	300.000 5000.000 1380.000	21
4559	1.33633351E+01 1.70222596E-02-5.95245190E-06	9.37896168E-10-5.49767305E-14	2	
4560	-9.90113178E+03-4.54753472E+01 5.96155469E-01	4.35893351E-02-2.65985265E-05	3	
4561	8.14250262E-09-1.02316366E-12-5.05630797E+03	2.43923636E+01	4	
4562	C4H63,1-2OH	C 4H 70 1 OG	300.000 5000.000 1404.000	21
4563	1.46899596E+01 1.48008021E-02-4.94483770E-06	7.55542892E-10-4.33461574E-14	2	
4564	-1.29448240E+04-5.45653093E+01-1.58903600E+00	6.17722944E-02-5.78263835E-05	3	
4565	2.78090017E-08-5.26779799E-12-8.17977186E+03	2.96999338E+01	4	
4566	C4H5OH-13 9/24/15	C 4H 60 1 OG	300.000 5000.000 1405.000	21
4567	1.40975061E+01 1.29826578E-02-4.36356696E-06	6.69260196E-10-3.84920001E-14	2	
4568	-1.41099189E+04-4.94340793E+01-1.60022758E+00	6.12386329E-02-6.18933585E-05	3	
4569	3.14927455E-08-6.20396658E-12-9.77435172E+03	3.08328186E+01	4	
4570	SQC4H7OHP-4	C 4H 90 3 OG	300.000 5000.000 1410.000	61
4571	1.99207495E+01 1.89422879E-02-6.39488327E-06	9.84231371E-10-5.67606301E-14	2	
4572	-2.89250584E+04-7.01061222E+01 1.44518283E+00	6.52944119E-02-5.10380130E-05	3	
4573	2.05238910E-08-3.32050656E-12-2.29059890E+04	2.78546218E+01	4	
4574	CY(CCCO)COH	C 4H 80 2 OG	300.000 5000.000 1396.000	21
4575	1.34636332E+01 2.28745777E-02-9.93619553E-06	1.89605197E-09-1.26466856E-13	2	
4576	-3.96396606E+04-4.51064489E+01-6.97589766E+00	7.98392838E-02-7.11131714E-05	3	
4577	3.16611877E-08-5.61324136E-12-3.35777839E+04	6.12093340E+01	4	
4578	SQC4H7OHP-4O2	C 4H 90 5 OG	300.000 5000.000 1402.000	71
4579	2.35936348E+01 2.08588461E-02-7.13602285E-06	1.10820581E-09-6.43133049E-14	2	
4580	-4.78452356E+04-8.49505816E+01 2.62618431E+00	7.26812595E-02-5.64956508E-05	3	
4581	2.25892409E-08-3.65246549E-12-4.08999596E+04	2.65615323E+01	4	
4582	PQC4H7OHS-3O2	C 4H 90 5 OG	300.000 5000.000 1414.000	71
4583	2.46607662E+01 1.92947770E-02-6.45433722E-06	9.87246207E-10-5.66889630E-14	2	
4584	-4.98467067E+04-9.10424907E+01 2.90986916E+00	7.76596028E-02-6.68513896E-05	3	
4585	2.93627835E-08-5.12008013E-12-4.31551961E+04	2.29130715E+01	4	
4586	SQC4H7OHS-4O2	C 4H 90 5 OG	300.000 5000.000 1414.000	71
4587	2.46607662E+01 1.92947770E-02-6.45433722E-06	9.87246207E-10-5.66889630E-14	2	
4588	-4.98467067E+04-9.10424907E+01 2.90986916E+00	7.76596028E-02-6.68513896E-05	3	
4589	2.93627835E-08-5.12008013E-12-4.31551961E+04	2.29130715E+01	4	
4590	C4H7O2-1,3OOH	C 4H 90 5 OG	300.000 5000.000 1425.000	71
4591	2.54691227E+01 1.86441036E-02-6.23825706E-06	9.54422873E-10-5.48154425E-14	2	
4592	-4.01531561E+04-9.60389710E+01 4.88339443E+00	7.18219147E-02-5.86792171E-05	3	
4593	2.42823866E-08-3.98538527E-12-3.36575518E+04	1.24696185E+01	4	
4594	SC4H8OH-3O2	C 4H 90 3 OG	300.000 5000.000 1417.000	51
4595	1.93082953E+01 1.92156764E-02-6.34250732E-06	9.60912935E-10-5.47939937E-14	2	
4596	-3.84370805E+04-6.88887622E+01 1.78918281E+00	6.62988026E-02-5.52280656E-05	3	
4597	2.40247962E-08-4.18762027E-12-3.30428157E+04	2.28885942E+01	4	
4598	CCY(COCC)OH	C 4H 80 2 OG	300.000 5000.000 1328.000	21
4599	1.03816782E+01 2.53052690E-02-1.00511826E-05	1.68204740E-09-9.58092966E-14	2	
4600	-3.94348914E+04-2.73522595E+01-6.13260697E+00	7.75376285E-02-6.73066149E-05	3	
4601	2.82841623E-08-4.65470382E-12-3.57825027E+04	5.53089299E+01	4	
4602	COHQCYC(COC)	C 4H 80 4 OG	300.000 5000.000 1319.000	51
4603	2.44599226E+01 1.64187782E-02-5.74024372E-06	9.05710407E-10-5.31829152E-14	2	
4604	-6.01811228E+04-1.02049722E+02 2.40687943E+00	5.95180442E-02-3.16913659E-05	3	
4605	4.23694824E-09 8.42033474E-13-5.19694864E+04	1.88941416E+01	4	
4606	QCYC(CCOC)OH	C 4H 80 4 OG	300.000 5000.000 1411.000	41
4607	2.20860197E+01 1.83743733E-02-6.29478769E-06	9.78787994E-10-5.68621317E-14	2	
4608	-5.89652037E+04-8.64964494E+01-2.0909972E+00	8.02656739E-02-6.69756245E-05	3	
4609	2.79282034E-08-4.60981823E-12-5.12529252E+04	4.11897260E+01	4	
4610	HOCOCQ(CH3)2	C 4H 80 4 OG	300.000 5000.000 1380.000	61
4611	2.28935401E+01 1.78627606E-02-6.34627520E-06	1.01068546E-09-5.96885712E-14	2	
4612	-8.05400680E+04-9.08953779E+01 1.56326363E+00	6.77165643E-02-5.14600149E-05	3	
4613	1.99184629E-08-3.16007445E-12-7.30943302E+04	2.37255421E+01	4	
4614	IQC4H7OHTO2	C 4H 90 5 OG	300.000 5000.000 1389.000	71
4615	2.41720261E+01 2.09397176E-02-7.29061406E-06	1.14554056E-09-6.70217517E-14	2	
4616	-5.04772118E+04-8.95996685E+01 3.83287364E+00	6.90926177E-02-5.15031144E-05	3	
4617	1.99235553E-08-3.17456897E-12-4.34442789E+04	1.94648622E+01	4	

4618	IQC4H8OTQ-I	C	4H	90	5	OG	300.000	5000.000	1386.000	71
4619	2.53249383E+01	2.00634820E-02	-7.01249558E-06	1.10475030E-09	-6.47561724E-14					2
4620	-4.09610593E+04	-9.73592779E+01	5.90219800E+00	6.26952142E-02	-4.17351838E-05					3
4621	1.35422162E-08	-1.71169663E-12	-3.39620020E+04	7.89290087E+00						4
4622	IQC4H7OHTQ-P	C	4H	90	5	OG	300.000	5000.000	1391.000	81
4623	2.45769593E+01	2.01889393E-02	-7.03584537E-06	1.10623327E-09	-6.47523225E-14					2
4624	-4.25783112E+04	-9.05052742E+01	3.45242802E+00	7.14541224E-02	-5.54616790E-05					3
4625	2.22754676E-08	-3.66067450E-12	-3.54133076E+04	2.23024492E+01						4
4626	CHOC(CH3)OHCH2Q	C	4H	80	4	OG	300.000	5000.000	1383.000	61
4627	2.24480753E+01	1.78753902E-02	-6.26904597E-06	9.90084046E-10	-5.81417382E-14					2
4628	-6.55093075E+04	-8.56747327E+01	2.40933530E+00	6.13326038E-02	-4.03874986E-05					3
4629	1.22738404E-08	-1.32997480E-12	-5.83049516E+04	2.29870742E+01						4
4630	CO(CH2OOH)2	C	3H	60	5	OG	300.000	5000.000	1393.000	61
4631	2.43376341E+01	1.14074110E-02	-4.08931881E-06	6.55183244E-10	-3.88570518E-14					2
4632	-5.16862647E+04	-9.01518175E+01	-2.47626577E+00	8.93736793E-02	-9.25891121E-05					3
4633	4.63168490E-08	-8.93300309E-12	-4.38924057E+04	4.84479477E+01						4
4634	AR	G	5/97AR	1	0	OG	200.000	6000.00	1000.00	1
4635	2.50000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00					2
4636	-7.45375000E+02	4.37967491E+00	2.50000000E+00	0.00000000E+00	0.00000000E+00					3
4637	0.00000000E+00	0.00000000E+00	-7.45375000E+02	4.37967491E+00	0.00000000E+00					4
4638	N2	G	8/02N	2	0	OG	200.000	6000.00	1000.00	1
4639	2.95257637E+00	1.39690040E-03	-4.92631603E-07	7.86010195E-11	-4.60755204E-15					2
4640	-9.23948688E+02	5.87188762E+00	3.53100528E+00	-1.23660988E-04	-5.02999433E-07					3
4641	2.43530612E-09	-1.40881235E-12	-1.04697628E+03	2.96747038E+00	0.00000000E+00					4
4642	HE	G	5/97HE	1	0	OG	200.000	6000.00	1000.00	1
4643	2.50000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00					2
4644	-7.45375000E+02	9.28723974E-01	2.50000000E+00	0.00000000E+00	0.00000000E+00					3
4645	0.00000000E+00	0.00000000E+00	-7.45375000E+02	9.28723974E-01	0.00000000E+00					4
4646	IC3H7	8/12/15	C	3H	7	OG	298.000	5000.000	1000.000	21
4647	6.70775549E+00	1.74048076E-02	-6.07615926E-06	9.60084351E-10	-5.65656490E-14					2
4648	7.55377821E+03	-1.03686516E+01	-8.97467137E-01	4.15744022E-02	-4.94778349E-05					3
4649	4.56493655E-08	-1.79085437E-11	9.93950407E+03	2.92641758E+01						4
4650	NC3H7	8/12/15	C	3H	7	OG	298.000	5000.000	1000.000	21
4651	7.48614243E+00	1.65769478E-02	-5.74876481E-06	9.04103694E-10	-5.30867231E-14					2
4652	8.93710008E+03	-1.42595379E+01	-2.20120865E+00	5.29641653E-02	-7.23640506E-05					3
4653	6.36996940E-08	-2.29332581E-11	1.15130744E+04	3.43669174E+01						4
4654	BIN1C	C	20H	4	G	300.00	5000.00	1000.00		1
4655	-.689260191e+01	.129240060e+00	-.835430297e-04	.291897333e-07	-.322093608e-11					2
4656	.186873844e+05	.352242700e+02	-.689260191e+01	.129240060e+00	-.835430297e-04					3
4657	.291897333e-07	-.322093608e-11	.186873844e+05	.352242700e+02						4
4658	BIN2A	C	40H	31	G	300.00	5000.00	1000.00		1
4659	.290747022E+02	.412337670E-01	-.126077060E-04	.127453580E-08	.000000000E+00					2
4660	.141687238E+05	-.136431347E+03	-.106811200E+02	.146535400E+00	-.103943520E-03					3
4661	.270645390E-07	.000000000E+00	.252715000E+05	.699617500E+02						4
4662	BIN2B	C	40H	16	G	300.00	5000.00	1000.00		1
4663	-.121984902e+02	.277403120e+00	-.173125315e-03	.563663815e-07	-.684448918e-11					2
4664	.492041936e+05	.814417312e+02	-.121984902e+02	.277403120e+00	-.173125315e-03					3
4665	.563663815e-07	-.684448918e-11	.492041936e+05	.814417312e+02						4
4666	BIN2C	C	40H	8	G	300.00	5000.00	1000.00		1
4667	-.137852038e+02	.258480121e+00	-.167086059e-03	.583794665e-07	-.644187217e-11					2
4668	.368211705e+05	.704485401e+02	-.137852038e+02	.258480121e+00	-.167086059e-03					3
4669	.583794665e-07	-.644187217e-11	.368211705e+05	.704485401e+02						4
4670	BIN3A	C	80H	60	G	300.00	5000.00	1000.00		1
4671	.290747022E+02	.412337670E-01	-.126077060E-04	.127453580E-08	.000000000E+00					2
4672	.141687238E+05	-.136431347E+03	-.106811200E+02	.146535400E+00	-.103943520E-03					3
4673	.270645390E-07	.000000000E+00	.252715000E+05	.699617500E+02						4
4674	BIN3B	C	80H	24	G	300.00	5000.00	1000.00		1
4675	-.259836940e+02	.535883241e+00	-.340211374e-03	.114745848e-06	-.132863613e-10					2
4676	.860253641e+05	.151890271e+03	-.259836940e+02	.535883241e+00	-.340211374e-03					3
4677	.114745848e-06	-.132863613e-10	.860253641e+05	.151890271e+03						4
4678	BIN3C	C	80H	8	G	300.00	5000.00	1000.00		1
4679	-.291571213e+02	.498037242e+00	-.328132864e-03	.118772018e-06	-.124811273e-10					2
4680	.612593178e+05	.129903889e+03	-.291571213e+02	.498037242e+00	-.328132864e-03					3
4681	.118772018e-06	-.124811273e-10	.612593178e+05	.129903889e+03						4
4682	BIN4A	C	160H	116	G	300.00	5000.00	1000.00		1
4683	.290747022E+02	.412337670E-01	-.126077060E-04	.127453580E-08	.000000000E+00					2
4684	.141687238E+05	-.136431347E+03	-.106811200E+02	.146535400E+00	-.103943520E-03					3
4685	.270645390E-07	.000000000E+00	.252715000E+05	.699617500E+02						4
4686	BIN4B	C	160H	32	G	300.00	5000.00	1000.00		1
4687	-.551408153e+02	.103392048e+01	-.668344238e-03	.233517866e-06	-.257674887e-10					2
4688	.147284682e+06	.281794160e+03	-.551408153e+02	.103392048e+01	-.668344238e-03					3
4689	.233517866e-06	-.257674887e-10	.147284682e+06	.281794160e+03						4
4690	BIN4C	C	160H	8	G	300.00	5000.00	1000.00		1

4691	-.599009562e+02	.977151485e+00	-.650226472e-03	.239557121e-06	-.245596376e-10	2
4692	.110135613e+06	.248814587e+03	-.599009562e+02	.977151485e+00	-.650226472e-03	3
4693	.239557121e-06	-.245596376e-10	.110135613e+06	.248814587e+03		4
4694	BIN5A	C 320H 224	G	300.00	5000.00 1000.00	1
4695	.290747022E+02	.412337670E-01	-.126077060E-04	.127453580E-08	.000000000E+00	2
4696	.141687238E+05	-.136431347E+03	-.106811200E+02	.146535400E+00	-.103943520E-03	3
4697	.270645390E-07	.000000000E+00	.252715000E+05	.699617500E+02		4
4698	BIN5B	C 320H 64	G	300.00	5000.00 1000.00	1
4699	-.110281631e+03	.206784097e+01	-.133668848e-02	.467035732e-06	-.515349774e-10	2
4700	.295122962e+06	.563588320e+03	-.110281631e+03	.206784097e+01	-.133668848e-02	3
4701	.467035732e-06	-.515349774e-10	.295122962e+06	.563588320e+03		4
4702	BIN5C	C 320H 16	G	300.00	5000.00 1000.00	1
4703	-.119801912e+03	.195430297e+01	-.130045294e-02	.479114243e-06	-.491192753e-10	2
4704	.220271225e+06	.497629173e+03	-.119801912e+03	.195430297e+01	-.130045294e-02	3
4705	.479114243e-06	-.491192753e-10	.220271225e+06	.497629173e+03		4
4706	BIN6A	C 640H 432	G	300.00	5000.00 1000.00	1
4707	.290747022E+02	.412337670E-01	-.126077060E-04	.127453580E-08	.000000000E+00	2
4708	.141687238E+05	-.136431347E+03	-.106811200E+02	.146535400E+00	-.103943520E-03	3
4709	.270645390E-07	.000000000E+00	.252715000E+05	.699617500E+02		4
4710	BIN6B	C 640H 128	G	300.00	5000.00 1000.00	1
4711	-.220563261e+03	.413568193e+01	-.267337695e-02	.934071465e-06	-.103069955e-09	2
4712	.590245924e+06	.112717664e+04	-.220563261e+03	.413568193e+01	-.267337695e-02	3
4713	.934071465e-06	-.103069955e-09	.590245924e+06	.112717664e+04		4
4714	BIN6C	C 640H 32	G	300.00	5000.00 1000.00	1
4715	-.239603825e+03	.390860594e+01	-.260090589e-02	.958228485e-06	-.982385506e-10	2
4716	.440542450e+06	.995258347e+03	-.239603825e+03	.390860594e+01	-.260090589e-02	3
4717	.958228485e-06	-.982385506e-10	.440542450e+06	.995258347e+03		4
4718	BIN7A	C 0H 0	G	300.00	5000.00 1000.00	1&
4719	C	1250 H 813				
4720	.290747022E+02	.412337670E-01	-.126077060E-04	.127453580E-08	.000000000E+00	2
4721	.141687238E+05	-.136431347E+03	-.106811200E+02	.146535400E+00	-.103943520E-03	3
4722	.270645390E-07	.000000000E+00	.252715000E+05	.699617500E+02		4
4723	BIN7B	C 0H 0	G	300.00	5000.00 1000.00	1&
4724	C	1250 H 250				
4725	-.430050931e+03	.807639658e+01	-.522093608e-02	.182385506e-05	-.201308505e-09	2
4726	.115397291e+07	.219420763e+04	-.430050931e+03	.807639658e+01	-.522093608e-02	3
4727	.182385506e-05	-.201308505e-09	.115397291e+07	.219420763e+04		4
4728	BIN7C	C 0H 0	G	300.00	5000.00 1000.00	1&
4729	C	1250 H 63				
4730	-.467508707e+03	.763462506e+01	-.508002013e-02	.187116256e-05	-.191897333e-09	2
4731	.862448881e+06	.194089641e+04	-.467508707e+03	.763462506e+01	-.508002013e-02	3
4732	.187116256e-05	-.191897333e-09	.862448881e+06	.194089641e+04		4
4733	BIN8A	C 0H 0	G	300.00	5000.00 1000.00	1&
4734	C	2500 H 1563				
4735	.290747022E+02	.412337670E-01	-.126077060E-04	.127453580E-08	.000000000E+00	2
4736	.141687238E+05	-.136431347E+03	-.106811200E+02	.146535400E+00	-.103943520E-03	3
4737	.270645390E-07	.000000000E+00	.252715000E+05	.699617500E+02		4
4738	BIN8B	C 0H 0	G	300.00	5000.00 1000.00	1&
4739	C	2500 H 500				
4740	-.861575239e+03	.161550075e+02	-.104428787e-01	.364871666e-05	-.402617011e-09	2
4741	.230547514e+07	.440303375e+04	-.861575239e+03	.161550075e+02	-.104428787e-01	3
4742	.364871666e-05	-.402617011e-09	.230547514e+07	.440303375e+04		4
4743	BIN8C	C 0H 0	G	300.00	5000.00 1000.00	1&
4744	C	2500 H 125				
4745	-.935584097e+03	.152674383e+02	-.101595370e-01	.374282838e-05	-.383744338e-09	2
4746	.172252461e+07	.388407330e+04	-.935584097e+03	.152674383e+02	-.101595370e-01	3
4747	.374282838e-05	-.383744338e-09	.172252461e+07	.388407330e+04		4
4748	BIN9A	C 0H 0	G	300.00	5000.00 1000.00	1&
4749	C	5000 H 3000				
4750	-.132647207e+04	.370407650e+02	-.223955712e-01	.679416205e-05	-.905888274e-09	2
4751	.772331402e+07	.115543653e+05	-.132647207e+04	.370407650e+02	-.223955712e-01	3
4752	.679416205e-05	-.905888274e-09	.772331402e+07	.115543653e+05		4
4753	BIN9B	C 0H 0	G	300.00	5000.00 1000.00	1&
4754	C	5000 H 1000				
4755	-.172315048e+04	.323100151e+02	-.208857574e-01	.729743332e-05	-.805234021e-09	2
4756	.461095029e+07	.880606751e+04	-.172315048e+04	.323100151e+02	-.208857574e-01	3
4757	.729743332e-05	-.805234021e-09	.461095029e+07	.880606751e+04		4
4758	BIN9C	C 0H 0	G	300.00	5000.00 1000.00	1&
4759	C	5000 H 250				
4760	-.187116819e+04	.305348767e+02	-.203190740e-01	.748565677e-05	-.767488676e-09	2
4761	.344504923e+07	.776814659e+04	-.187116819e+04	.305348767e+02	-.203190740e-01	3
4762	.748565677e-05	-.767488676e-09	.344504923e+07	.776814659e+04		4
4763	BIN10A	C 0H 0	G	300.00	5000.00 1000.00	1&

4764	C	10000	H	5750							
4765		-.270179225e+04		.734890790e+02-	.446019124e-01	.136507297e-04-	.179919477e-08				2
4766		.150588179e+08		.227578841e+05-	.270179225e+04	.734890790e+02-	.446019124e-01				3
4767		.136507297e-04-		.179919477e-08		.150588179e+08		.227578841e+05			4
4768	BIN10B		C	0H	0	G	300.00	5000.00	1000.00		1&
4769	C	10000	H	2000							
4770		-.344630096e+04		.646200302e+02-	.417715148e-01	.145948666e-04-	.161046804e-08				2
4771		.922190057e+07		.176121350e+05-	.344630096e+04	.646200302e+02-	.417715148e-01				3
4772		.145948666e-04-		.161046804e-08		.922190057e+07		.176121350e+05			4
4773	BIN10C		C	0H	0	G	300.00	5000.00	1000.00		1&
4774	C	10000	H	500							
4775		-.374380976e+04		.610719678e+02-	.406391545e-01	.149723201e-04-	.153497735e-08				2
4776		.688762777e+07		.155509117e+05-	.374380976e+04	.610719678e+02-	.406391545e-01				3
4777		.149723201e-04-		.153497735e-08		.688762777e+07		.155509117e+05			4
4778	BIN11A		C	0H	0	G	300.00	5000.00	1000.00		1&
4779	C	20000	H	11000							
4780		-.550422748e+04		.145797685e+03-	.888273780e-01	.274282838e-04-	.357322597e-08				2
4781		.293370742e+08		.448433123e+05-	.550422748e+04	.145797685e+03-	.888273780e-01				3
4782		.274282838e-04-		.357322597e-08		.293370742e+08		.448433123e+05			4
4783	BIN11B		C	0H	0	G	300.00	5000.00	1000.00		1&
4784	C	20000	H	4000							
4785		-.689260191e+04		.129240060e+03-	.835430297e-01	.291897333e-04-	.322093608e-08				2
4786		.184438011e+08		.352242700e+05-	.689260191e+04	.129240060e+03-	.835430297e-01				3
4787		.291897333e-04-		.322093608e-08		.184438011e+08		.352242700e+05			4
4788	BIN11C		C	0H	0	G	300.00	5000.00	1000.00		1&
4789	C	20000	H	1000							
4790		-.748761953e+04		.122143936e+03-	.812783090e-01	.299446402e-04-	.306995471e-08				2
4791		.137752555e+08		.311018233e+05-	.748761953e+04	.122143936e+03-	.812783090e-01				3
4792		.299446402e-04-		.306995471e-08		.137752555e+08		.311018233e+05			4
4793	BIN12A		C	0H	0	G	300.00	5000.00	1000.00		1&
4794	C	40000	H	21000							
4795		-.112067942e+05		.289229995e+03-	.176899849e+00	.551082033e-04-	.709612481e-08				2
4796		.571179665e+08		.883124757e+05-	.112067942e+05	.289229995e+03-	.176899849e+00				3
4797		.551082033e-04-		.709612481e-08		.571179665e+08		.883124757e+05			4
4798	BIN12B		C	0H	0	G	300.00	5000.00	1000.00		1&
4799	C	40000	H	8000							
4800		-.137852038e+05		.258480121e+03-	.167086059e+00	.583794665e-04-	.644187217e-08				2
4801		.368876023e+08		.704485401e+05-	.137852038e+05	.258480121e+03-	.167086059e+00				3
4802		.583794665e-04-		.644187217e-08		.368876023e+08		.704485401e+05			4
4803	BIN12C		C	0H	0	G	300.00	5000.00	1000.00		1&
4804	C	40000	H	2000							
4805		-.149752391e+05		.244287871e+03-	.162556618e+00	.598892803e-04-	.613990941e-08				2
4806		.275505111e+08		.622036467e+05-	.149752391e+05	.244287871e+03-	.162556618e+00				3
4807		.598892803e-04-		.613990941e-08		.275505111e+08		.622036467e+05			4
4808	BIN13A		C	0H	0	G	300.00	5000.00	1000.00		1&
4809	C	80000	H	40000							
4810		-.228102667e+05		.573729240e+03-	.352289884e+00	.110719678e-03-	.140915954e-07				2
4811		.111123569e+09		.173876654e+06-	.228102667e+05	.573729240e+03-	.352289884e+00				3
4812		.110719678e-03-		.140915954e-07		.111123569e+09		.173876654e+06			4
4813	BIN13B		C	0H	0	G	300.00	5000.00	1000.00		1&
4814	C	80000	H	16000							
4815		-.275704076e+05		.516960242e+03-	.334172119e+00	.116758933e-03-	.128837443e-07				2
4816		.737752046e+08		.140897080e+06-	.275704076e+05	.516960242e+03-	.334172119e+00				3
4817		.116758933e-03-		.128837443e-07		.737752046e+08		.140897080e+06			4
4818	BIN13C		C	0H	0	G	300.00	5000.00	1000.00		1&
4819	C	80000	H	4000							
4820		-.299504781e+05		.488575742e+03-	.325113236e+00	.119778561e-03-	.122798188e-07				2
4821		.551010222e+08		.124407293e+06-	.299504781e+05	.488575742e+03-	.325113236e+00				3
4822		.119778561e-03-		.122798188e-07		.551010222e+08		.124407293e+06			4
4823	BIN14A		C	0H	0	G	300.00	5000.00	1000.00		1&
4824	C	160000	H	76000							
4825		-.464138903e+05		.113799698e+04-	.701560141e+00	.222445898e-03-	.279818822e-07				2
4826		.216022411e+09		.342256712e+06-	.464138903e+05	.113799698e+04-	.701560141e+00				3
4827		.222445898e-03-		.279818822e-07		.216022411e+09		.342256712e+06			4
4828	BIN14B		C	0H	0	G	300.00	5000.00	1000.00		1&
4829	C	160000	H	32000							
4830		-.551408153e+05		.103392048e+04-	.668344238e+00	.233517866e-03-	.257674887e-07				2
4831		.147550409e+09		.281794160e+06-	.551408153e+05	.103392048e+04-	.668344238e+00				3
4832		.233517866e-03-		.257674887e-07		.147550409e+09		.281794160e+06			4
4833	BIN14C		C	0H	0	G	300.00	5000.00	1000.00		1&
4834	C	160000	H	8000							
4835		-.599009562e+05		.977151485e+03-	.650226472e+00	.239557121e-03-	.245596376e-07				2
4836		.110202044e+09		.248814587e+06-	.599009562e+05	.977151485e+03-	.650226472e+00				3

4837	.239557121e-03-.245596376e-07	.110202044e+09	.248814587e+06	4
4838	BIN15A	C OH 0	G 300.00 5000.00 1000.00	1&
4839	C	320000 H 144000		
4840	-.944144942e+05 .225707096e+04-	.139708103e+01	.446904882e-03-.555611475e-07	2
4841	.419595367e+09 .673520232e+06-	.944144942e+05	.225707096e+04-.139708103e+01	3
4842	.446904882e-03-.555611475e-07	.419595367e+09	.673520232e+06	4
4843	BIN15B	C OH 0	G 300.00 5000.00 1000.00	1&
4844	C	320000 H 64000		
4845	-.110281631e+06 .206784097e+04-	.133668848e+01	.467035732e-03-.515349774e-07	2
4846	.295100818e+09 .563588320e+06-	.110281631e+06	.206784097e+04-.133668848e+01	3
4847	.467035732e-03-.515349774e-07	.295100818e+09	.563588320e+06	4
4848	BIN15C	C OH 0	G 300.00 5000.00 1000.00	1&
4849	C	320000 H 16000		
4850	-.119801912e+06 .195430297e+04-	.130045294e+01	.479114243e-03-.491192753e-07	2
4851	.220404089e+09 .497629173e+06-	.119801912e+06	.195430297e+04-.130045294e+01	3
4852	.479114243e-03-.491192753e-07	.220404089e+09	.497629173e+06	4
4853	BIN16A	C OH 0	G 300.00 5000.00 1000.00	1&
4854	C	640000 H 272000		
4855	-.192002416e+06 .447629592e+04-	.278208354e+01	.897835934e-03-.110317061e-06	2
4856	.814291825e+09 .132505408e+07-	.192002416e+06	.447629592e+04-.278208354e+01	3
4857	.897835934e-03-.110317061e-06	.814291825e+09	.132505408e+07	4
4858	BIN16B	C OH 0	G 300.00 5000.00 1000.00	1&
4859	C	640000 H 128000		
4860	-.220563261e+06 .413568193e+04-	.267337695e+01	.934071465e-03-.103069955e-06	2
4861	.590201637e+09 .112717664e+07-	.220563261e+06	.413568193e+04-.267337695e+01	3
4862	.934071465e-03-.103069955e-06	.590201637e+09	.112717664e+07	4
4863	BIN16C	C OH 0	G 300.00 5000.00 1000.00	1&
4864	C	640000 H 32000		
4865	-.239603825e+06 .390860594e+04-	.260090589e+01	.958228485e-03-.982385506e-07	2
4866	.440808177e+09 .995258347e+06-	.239603825e+06	.390860594e+04-.260090589e+01	3
4867	.958228485e-03-.982385506e-07	.440808177e+09	.995258347e+06	4
4868	BIN17A	C OH 0	G 300.00 5000.00 1000.00	1&
4869	C	1250000 H 500000		
4870	-.381202818e+06 .866884751e+04-	.541016608e+01	.176144942e-02-.213890287e-06	2
4871	.154178304e+10 .254505410e+07-	.381202818e+06	.866884751e+04-.541016608e+01	3
4872	.176144942e-02-.213890287e-06	.154178304e+10	.254505410e+07	4
4873	BIN17B	C OH 0	G 300.00 5000.00 1000.00	1&
4874	C	1250000 H 250000		
4875	-.430787620e+06 .807750377e+04-	.522143936e+01	.182435833e-02-.201308505e-06	2
4876	.115273757e+10 .220151688e+07-	.430787620e+06	.807750377e+04-.522143936e+01	3
4877	.182435833e-02-.201308505e-06	.115273757e+10	.220151688e+07	4
4878	BIN17C	C OH 0	G 300.00 5000.00 1000.00	1&
4879	C	1250000 H 62500		
4880	-.467976220e+06 .763399597e+04-	.507989431e+01	.187154001e-02-.191872169e-06	2
4881	.860953472e+09 .194386396e+07-	.467976220e+06	.763399597e+04-.507989431e+01	3
4882	.187154001e-02-.191872169e-06	.860953472e+09	.194386396e+07	4
4883	BIN18A	C OH 0	G 300.00 5000.00 1000.00	1&
4884	C	2500000 H 937500		
4885	-.774801837e+06 .171898591e+05-	.107731505e+02	.353862607e-02-.424635128e-06	2
4886	.298630471e+10 .500422390e+07-	.774801837e+06	.171898591e+05-.107731505e+02	3
4887	.353862607e-02-.424635128e-06	.298630471e+10	.500422390e+07	4
4888	BIN18B	C OH 0	G 300.00 5000.00 1000.00	1&
4889	C	2500000 H 500000		
4890	-.861575239e+06 .161550075e+05-	.104428787e+02	.364871666e-02-.402617011e-06	2
4891	.230547514e+10 .440303375e+07-	.861575239e+06	.161550075e+05-.104428787e+02	3
4892	.364871666e-02-.402617011e-06	.230547514e+10	.440303375e+07	4
4893	BIN18C	C OH 0	G 300.00 5000.00 1000.00	1&
4894	C	2500000 H 125000		
4895	-.935952441e+06 .152679919e+05-	.101597886e+02	.374308002e-02-.383744338e-06	2
4896	.172190694e+10 .388772792e+07-	.935952441e+06	.152679919e+05-.101597886e+02	3
4897	.374308002e-02-.383744338e-06	.172190694e+10	.388772792e+07	4
4898	BIN19A	C OH 0	G 300.00 5000.00 1000.00	1&
4899	C	5000000 H 1750000		
4900	-.157439607e+07 .340840463e+05-	.214519376e+02	.710870659e-02-.842979366e-06	2
4901	.577808668e+10 .983667918e+07-	.157439607e+07	.340840463e+05-.214519376e+02	3
4902	.710870659e-02-.842979366e-06	.577808668e+10	.983667918e+07	4
4903	BIN19B	C OH 0	G 300.00 5000.00 1000.00	1&
4904	C	5000000 H 1000000		
4905	-.172315048e+07 .323100151e+05-	.208857574e+02	.729743332e-02-.805234021e-06	2
4906	.461095029e+10 .880606751e+07-	.172315048e+07	.323100151e+05-.208857574e+02	3
4907	.729743332e-02-.805234021e-06	.461095029e+10	.880606751e+07	4
4908	BIN19C	C OH 0	G 300.00 5000.00 1000.00	1&
4909	C	5000000 H 250000		

4910	-.187190488e+07	.305359839e+05	-.203195773e+02	.748616004e-02	-.767488676e-06	2
4911	.344381389e+10	.777545583e+07	-.187190488e+07	.305359839e+05	-.203195773e+02	3
4912	.748616004e-02	-.767488676e-06	.344381389e+10	.777545583e+07		4
4913	BIN20A	C	OH	0	G	300.00 5000.00 1000.00 1&
4914	C	10000000	H	3250000		
4915	-.319837695e+07	.675767489e+05	-.427151485e+02	.142803221e-01	-.167337695e-05	2
4916	.111671279e+11	.193298211e+08	-.319837695e+07	.675767489e+05	-.427151485e+02	3
4917	.142803221e-01	-.167337695e-05	.111671279e+11	.193298211e+08		4
4918	BIN20B	C	OH	0	G	300.00 5000.00 1000.00 1&
4919	C	10000000	H	2000000		
4920	-.344630096e+07	.646200302e+05	-.417715148e+02	.145948666e-01	-.161046804e-05	2
4921	.922190057e+10	.176121350e+08	-.344630096e+07	.646200302e+05	-.417715148e+02	3
4922	.145948666e-01	-.161046804e-05	.922190057e+10	.176121350e+08		4
4923	BIN20C	C	OH	0	G	300.00 5000.00 1000.00 1&
4924	C	10000000	H	500000		
4925	-.374380976e+07	.610719678e+05	-.406391545e+02	.149723201e-01	-.153497735e-05	2
4926	.688762777e+10	.155509117e+08	-.374380976e+07	.610719678e+05	-.406391545e+02	3
4927	.149723201e-01	-.153497735e-05	.688762777e+10	.155509117e+08		4
4928	BIN21A	C	OH	0	G	300.00 5000.00 1000.00 1&
4929	C	20000000	H	6000000		
4930	-.649592350e+07	.133970810e+06	-.850528435e+02	.286864620e-01	-.332159034e-05	2
4931	.215561649e+11	.379725678e+08	-.649592350e+07	.133970810e+06	-.850528435e+02	3
4932	.286864620e-01	-.332159034e-05	.215561649e+11	.379725678e+08		4
4933	BIN21B	C	OH	0	G	300.00 5000.00 1000.00 1&
4934	C	20000000	H	4000000		
4935	-.689260191e+07	.129240060e+06	-.835430297e+02	.291897333e-01	-.322093608e-05	2
4936	.184438011e+11	.352242700e+08	-.689260191e+07	.129240060e+06	-.835430297e+02	3
4937	.291897333e-01	-.322093608e-05	.184438011e+11	.352242700e+08		4
4938	BIN21C	C	OH	0	G	300.00 5000.00 1000.00 1&
4939	C	20000000	H	1000000		
4940	-.748761953e+07	.122143936e+06	-.812783090e+02	.299446402e-01	-.306995471e-05	2
4941	.137752555e+11	.311018233e+08	-.748761953e+07	.122143936e+06	-.812783090e+02	3
4942	.299446402e-01	-.306995471e-05	.137752555e+11	.311018233e+08		4
4943	BIN22A	C	OH	0	G	300.00 5000.00 1000.00 1&
4944	C	40000000	H	12000000		
4945	-.129918470e+08	.267941621e+06	-.170105687e+03	.573729240e-01	-.664318067e-05	2
4946	.431123297e+11	.759451356e+08	-.129918470e+08	.267941621e+06	-.170105687e+03	3
4947	.573729240e-01	-.664318067e-05	.431123297e+11	.759451356e+08		4
4948	BIN22B	C	OH	0	G	300.00 5000.00 1000.00 1&
4949	C	40000000	H	8000000		
4950	-.137852038e+08	.258480121e+06	-.167086059e+03	.583794665e-01	-.644187217e-05	2
4951	.368876023e+11	.704485401e+08	-.137852038e+08	.258480121e+06	-.167086059e+03	3
4952	.583794665e-01	-.644187217e-05	.368876023e+11	.704485401e+08		4
4953	BIN22C	C	OH	0	G	300.00 5000.00 1000.00 1&
4954	C	40000000	H	2000000		
4955	-.149752391e+08	.244287871e+06	-.162556618e+03	.598892803e-01	-.613990941e-05	2
4956	.275505111e+11	.622036467e+08	-.149752391e+08	.244287871e+06	-.162556618e+03	3
4957	.598892803e-01	-.613990941e-05	.275505111e+11	.622036467e+08		4
4958	BIN23A	C	OH	0	G	300.00 5000.00 1000.00 1&
4959	C	80000000	H	24000000		
4960	-.259836940e+08	.535883241e+06	-.340211374e+03	.114745848e+00	-.132863613e-04	2
4961	.862246595e+11	.151890271e+09	-.259836940e+08	.535883241e+06	-.340211374e+03	3
4962	.114745848e+00	-.132863613e-04	.862246595e+11	.151890271e+09		4
4963	BIN23B	C	OH	0	G	300.00 5000.00 1000.00 1&
4964	C	80000000	H	16000000		
4965	-.275704076e+08	.516960242e+06	-.334172119e+03	.116758933e+00	-.128837443e-04	2
4966	.737752046e+11	.140897080e+09	-.275704076e+08	.516960242e+06	-.334172119e+03	3
4967	.116758933e+00	-.128837443e-04	.737752046e+11	.140897080e+09		4
4968	BIN23C	C	OH	0	G	300.00 5000.00 1000.00 1&
4969	C	80000000	H	4000000		
4970	-.299504781e+08	.488575742e+06	-.325113236e+03	.119778561e+00	-.122798188e-04	2
4971	.551010222e+11	.124407293e+09	-.299504781e+08	.488575742e+06	-.325113236e+03	3
4972	.119778561e+00	-.122798188e-04	.551010222e+11	.124407293e+09		4
4973	BIN24A	C	OH	0	G	300.00 5000.00 1000.00 1&
4974	C	160000000	H	48000000		
4975	-.519673880e+08	.107176648e+07	-.680422748e+03	.229491696e+00	-.265727227e-04	2
4976	.172449319e+12	.303780543e+09	-.519673880e+08	.107176648e+07	-.680422748e+03	3
4977	.229491696e+00	-.265727227e-04	.172449319e+12	.303780543e+09		4
4978	BIN24B	C	OH	0	G	300.00 5000.00 1000.00 1&
4979	C	160000000	H	32000000		
4980	-.551408153e+08	.103392048e+07	-.668344238e+03	.233517866e+00	-.257674887e-04	2
4981	.147550409e+12	.281794160e+09	-.551408153e+08	.103392048e+07	-.668344238e+03	3
4982	.233517866e+00	-.257674887e-04	.147550409e+12	.281794160e+09		4

4983	BIN24C	C	0H	0	G	300.00	5000.00	1000.00	1&
4984	C	160000000	H	8000000					
4985	-.599009562e+08	.977151485e+06-	.650226472e+03	.239557121e+00-	.245596376e-04				2
4986	.110202044e+12	.248814587e+09-	.599009562e+08	.977151485e+06-	.650226472e+03				3
4987	.239557121e+00-	.245596376e-04	.110202044e+12	.248814587e+09					4
4988	BIN25A	C	0H	0	G	300.00	5000.00	1000.00	1&
4989	C	320000000	H	96000000					
4990	-.103934776e+09	.214353296e+07-	.136084550e+04	.458983392e+00-	.531454454e-04				2
4991	.344898638e+12	.607561085e+09-	.103934776e+09	.214353296e+07-	.136084550e+04				3
4992	.458983392e+00-	.531454454e-04	.344898638e+12	.607561085e+09					4
4993	BIN25B	C	0H	0	G	300.00	5000.00	1000.00	1&
4994	C	320000000	H	64000000					
4995	-.110281631e+09	.206784097e+07-	.133668848e+04	.467035732e+00-	.515349774e-04				2
4996	.295100818e+12	.563588320e+09-	.110281631e+09	.206784097e+07-	.133668848e+04				3
4997	.467035732e+00-	.515349774e-04	.295100818e+12	.563588320e+09					4
4998	BIN25C	C	0H	0	G	300.00	5000.00	1000.00	1&
4999	C	320000000	H	16000000					
5000	-.119801912e+09	.195430297e+07-	.130045294e+04	.479114243e+00-	.491192753e-04				2
5001	.2204404089e+12	.497629173e+09-	.119801912e+09	.195430297e+07-	.130045294e+04				3
5002	.479114243e+00-	.491192753e-04	.2204404089e+12	.497629173e+09					4
5003	BIN1AJ	C	20H	15	G	300.00	5000.00	1000.00	1
5004	-.313739305e+01	.151585304e+00-	.885757423e-04	.251635632e-07-	.326119779e-11				2
5005	.804153368e+05	.422944709e+02-	.313739305e+01	.151585304e+00-	.885757423e-04				3
5006	.251635632e-07-	.326119779e-11	.804153368e+05	.422944709e+02					4
5007	BIN1BJ	C	20H	9	G	300.00	5000.00	1000.00	1
5008	-.570256668e+01	.143432310e+00-	.880724711e-04	.276799195e-07-	.352289884e-11				2
5009	.878362522e+05	.434691634e+02-	.570256668e+01	.143432310e+00-	.880724711e-04				3
5010	.276799195e-07-	.352289884e-11	.878362522e+05	.434691634e+02					4
5011	BIN1CJ	C	20H	3	G	300.00	5000.00	1000.00	1
5012	-.689260191e+01	.129240060e+00-	.835430297e-04	.291897333e-07-	.322093608e-11				2
5013	.786873844e+05	.352242700e+02-	.689260191e+01	.129240060e+00-	.835430297e-04				3
5014	.291897333e-07-	.322093608e-11	.786873844e+05	.352242700e+02					4
5015	BIN2AJ	C	40H	30	G	300.00	5000.00	1000.00	1
5016	.161628784E+02	.696969850E-01-	.371786410E-04	.946306230E-08-	.935417110E-12				2
5017	.461067047E+05-	.652717249E+02-	.114972670E+02	.151166960E+00-	.116351410E-03				3
5018	.317097570E-07	.218082760E-11	.532378630E+05	.757195740E+02					4
5019	BIN2BJ	C	40H	15	G	300.00	5000.00	1000.00	1
5020	-.121984902e+02	.277403120e+00-	.173125315e-03	.563663815e-07-	.684448918e-11				2
5021	.109204194e+06	.814417312e+02-	.121984902e+02	.277403120e+00-	.173125315e-03				3
5022	.563663815e-07-	.684448918e-11	.109204194e+06	.814417312e+02					4
5023	BIN2CJ	C	40H	7	G	300.00	5000.00	1000.00	1
5024	-.137852038e+02	.258480121e+00-	.167086059e-03	.583794665e-07-	.644187217e-11				2
5025	.968211705e+05	.704485401e+02-	.137852038e+02	.258480121e+00-	.167086059e-03				3
5026	.583794665e-07-	.644187217e-11	.968211705e+05	.704485401e+02					4
5027	BIN3AJ	C	80H	59	G	300.00	5000.00	1000.00	1
5028	.161628784E+02	.696969850E-01-	.371786410E-04	.946306230E-08-	.935417110E-12				2
5029	.461067047E+05-	.652717249E+02-	.114972670E+02	.151166960E+00-	.116351410E-03				3
5030	.317097570E-07	.218082760E-11	.532378630E+05	.757195740E+02					4
5031	BIN3BJ	C	80H	23	G	300.00	5000.00	1000.00	1
5032	-.259836940e+02	.535883241e+00-	.340211374e-03	.114745848e-06-	.132863613e-10				2
5033	.146025364e+06	.151890271e+03-	.259836940e+02	.535883241e+00-	.340211374e-03				3
5034	.114745848e-06-	.132863613e-10	.146025364e+06	.151890271e+03					4
5035	BIN3CJ	C	80H	7	G	300.00	5000.00	1000.00	1
5036	-.291571213e+02	.498037242e+00-	.328132864e-03	.118772018e-06-	.124811273e-10				2
5037	.121259318e+06	.129903889e+03-	.291571213e+02	.498037242e+00-	.328132864e-03				3
5038	.118772018e-06-	.124811273e-10	.121259318e+06	.129903889e+03					4
5039	BIN4AJ	C	160H	115	G	300.00	5000.00	1000.00	1
5040	.161628784E+02	.696969850E-01-	.371786410E-04	.946306230E-08-	.935417110E-12				2
5041	.461067047E+05-	.652717249E+02-	.114972670E+02	.151166960E+00-	.116351410E-03				3
5042	.317097570E-07	.218082760E-11	.532378630E+05	.757195740E+02					4
5043	BIN4BJ	C	160H	31	G	300.00	5000.00	1000.00	1
5044	-.551408153e+02	.103392048e+01-	.668344238e-03	.233517866e-06-	.257674887e-10				2
5045	.207284682e+06	.281794160e+03-	.551408153e+02	.103392048e+01-	.668344238e-03				3
5046	.233517866e-06-	.257674887e-10	.207284682e+06	.281794160e+03					4
5047	BIN4CJ	C	160H	7	G	300.00	5000.00	1000.00	1
5048	-.599009562e+02	.977151485e+00-	.650226472e-03	.239557121e-06-	.245596376e-10				2
5049	.170135613e+06	.248814587e+03-	.599009562e+02	.977151485e+00-	.650226472e-03				3
5050	.239557121e-06-	.245596376e-10	.170135613e+06	.248814587e+03					4
5051	BIN5AJ	C	320H	223	G	300.00	5000.00	1000.00	1
5052	-.587716155e+02	.226602919e+01-	.142073478e-02	.429793659e-06-	.567186714e-10				2
5053	.512777220e+06	.371112636e+03-	.587716155e+02	.226602919e+01-	.142073478e-02				3
5054	.429793659e-06-	.567186714e-10	.512777220e+06	.371112636e+03					4
5055	BIN5BJ	C	320H	63	G	300.00	5000.00	1000.00	1

5056	-.110281631e+03	.206784097e+01-	.133668848e-02	.467035732e-06-	.515349774e-10	2
5057	.355122962e+06	.563588320e+03-	.110281631e+03	.206784097e+01-	.133668848e-02	3
5058	.467035732e-06-	.515349774e-10	.355122962e+06	.563588320e+03		4
5059	BIN5CJ	C 320H 15	G	300.00	5000.00 1000.00	1
5060	-.119801912e+03	.195430297e+01-	.130045294e-02	.479114243e-06-	.491192753e-10	2
5061	.280271225e+06	.497629173e+03-	.119801912e+03	.195430297e+01-	.130045294e-02	3
5062	.479114243e-06-	.491192753e-10	.280271225e+06	.497629173e+03		4
5063	BIN6AJ	C 640H 431	G	300.00	5000.00 1000.00	1
5064	.161628784E+02	.696969850E-01-	.371786410E-04	.946306230E-08-	.935417110E-12	2
5065	.461067047E+05-	.652717249E+02-	.114972670E+02	.151166960E+00-	.116351410E-03	3
5066	.317097570E-07	.218082760E-11	.532378630E+05	.757195740E+02		4
5067	BIN6BJ	C 640H 127	G	300.00	5000.00 1000.00	1
5068	-.220563261e+03	.413568193e+01-	.267337695e-02	.934071465e-06-	.103069955e-09	2
5069	.650245924e+06	.112717664e+04-	.220563261e+03	.413568193e+01-	.267337695e-02	3
5070	.934071465e-06-	.103069955e-09	.650245924e+06	.112717664e+04		4
5071	BIN6CJ	C 640H 31	G	300.00	5000.00 1000.00	1
5072	-.239603825e+03	.390860594e+01-	.260090589e-02	.958228485e-06-	.982385506e-10	2
5073	.500542450e+06	.995258347e+03-	.239603825e+03	.390860594e+01-	.260090589e-02	3
5074	.958228485e-06-	.982385506e-10	.500542450e+06	.995258347e+03		4
5075	BIN7AJ	C 0H 0	G	300.00	5000.00 1000.00	1&
5076	C	1250 H 812				
5077	.161628784E+02	.696969850E-01-	.371786410E-04	.946306230E-08-	.935417110E-12	2
5078	.461067047E+05-	.652717249E+02-	.114972670E+02	.151166960E+00-	.116351410E-03	3
5079	.317097570E-07	.218082760E-11	.532378630E+05	.757195740E+02		4
5080	BIN7BJ	C 0H 0	G	300.00	5000.00 1000.00	1&
5081	C	1250 H 249				
5082	-.430050931e+03	.807639658e+01-	.522093608e-02	.182385506e-05-	.201308505e-09	2
5083	.121397291e+07	.219420763e+04-	.430050931e+03	.807639658e+01-	.522093608e-02	3
5084	.182385506e-05-	.201308505e-09	.121397291e+07	.219420763e+04		4
5085	BIN7CJ	C 0H 0	G	300.00	5000.00 1000.00	1&
5086	C	1250 H 62				
5087	-.467508707e+03	.763462506e+01-	.508002013e-02	.187116256e-05-	.191897333e-09	2
5088	.922448881e+06	.194089641e+04-	.467508707e+03	.763462506e+01-	.508002013e-02	3
5089	.187116256e-05-	.191897333e-09	.922448881e+06	.194089641e+04		4
5090	BIN8AJ	C 0H 0	G	300.00	5000.00 1000.00	1&
5091	C	2500 H 1562				
5092	.161628784E+02	.696969850E-01-	.371786410E-04	.946306230E-08-	.935417110E-12	2
5093	.461067047E+05-	.652717249E+02-	.114972670E+02	.151166960E+00-	.116351410E-03	3
5094	.317097570E-07	.218082760E-11	.532378630E+05	.757195740E+02		4
5095	BIN8BJ	C 0H 0	G	300.00	5000.00 1000.00	1&
5096	C	2500 H 499				
5097	-.861575239e+03	.161550075e+02-	.104428787e-01	.364871666e-05-	.402617011e-09	2
5098	.236547514e+07	.440303375e+04-	.861575239e+03	.161550075e+02-	.104428787e-01	3
5099	.364871666e-05-	.402617011e-09	.236547514e+07	.440303375e+04		4
5100	BIN8CJ	C 0H 0	G	300.00	5000.00 1000.00	1&
5101	C	2500 H 124				
5102	-.935584097e+03	.152674383e+02-	.101595370e-01	.374282838e-05-	.383744338e-09	2
5103	.178252461e+07	.388407330e+04-	.935584097e+03	.152674383e+02-	.101595370e-01	3
5104	.374282838e-05-	.383744338e-09	.178252461e+07	.388407330e+04		4
5105	BIN9AJ	C 0H 0	G	300.00	5000.00 1000.00	1&
5106	C	5000 H 2999				
5107	-.132647207e+04	.370407650e+02-	.223955712e-01	.679416205e-05-	.905888274e-09	2
5108	.778331402e+07	.115543653e+05-	.132647207e+04	.370407650e+02-	.223955712e-01	3
5109	.679416205e-05-	.905888274e-09	.778331402e+07	.115543653e+05		4
5110	BIN9BJ	C 0H 0	G	300.00	5000.00 1000.00	1&
5111	C	5000 H 999				
5112	-.172315048e+04	.323100151e+02-	.208857574e-01	.729743332e-05-	.805234021e-09	2
5113	.467095029e+07	.880606751e+04-	.172315048e+04	.323100151e+02-	.208857574e-01	3
5114	.729743332e-05-	.805234021e-09	.467095029e+07	.880606751e+04		4
5115	BIN9CJ	C 0H 0	G	300.00	5000.00 1000.00	1&
5116	C	5000 H 249				
5117	-.187116819e+04	.305348767e+02-	.203190740e-01	.748565677e-05-	.767488676e-09	2
5118	.350504923e+07	.776814659e+04-	.187116819e+04	.305348767e+02-	.203190740e-01	3
5119	.748565677e-05-	.767488676e-09	.350504923e+07	.776814659e+04		4
5120	BIN10AJ	C 0H 0	G	300.00	5000.00 1000.00	1&
5121	C	10000 H 5749				
5122	-.270179225e+04	.734890790e+02-	.446019124e-01	.136507297e-04-	.179919477e-08	2
5123	.151188179e+08	.227578841e+05-	.270179225e+04	.734890790e+02-	.446019124e-01	3
5124	.136507297e-04-	.179919477e-08	.151188179e+08	.227578841e+05		4
5125	BIN10BJ	C 0H 0	G	300.00	5000.00 1000.00	1&
5126	C	10000 H 1999				
5127	-.344630096e+04	.646200302e+02-	.417715148e-01	.145948666e-04-	.161046804e-08	2
5128	.928190057e+07	.176121350e+05-	.344630096e+04	.646200302e+02-	.417715148e-01	3

5129	.145948666e-04-.161046804e-08	.928190057e+07	.176121350e+05	4
5130	BIN10CJ	C OH 0	G 300.00 5000.00 1000.00	1&
5131	C	10000 H 499		
5132	-.374380976e+04 .610719678e+02-	.406391545e-01	.149723201e-04-.153497735e-08	2
5133	.694762777e+07 .155509117e+05-	.374380976e+04	.610719678e+02-.406391545e-01	3
5134	.149723201e-04-.153497735e-08	.694762777e+07	.155509117e+05	4
5135	BIN11AJ	C OH 0	G 300.00 5000.00 1000.00	1&
5136	C	20000 H 10999		
5137	-.550422748e+04 .145797685e+03-	.888273780e-01	.274282838e-04-.357322597e-08	2
5138	.293970742e+08 .448433123e+05-	.550422748e+04	.145797685e+03-.888273780e-01	3
5139	.274282838e-04-.357322597e-08	.293970742e+08	.448433123e+05	4
5140	BIN11BJ	C OH 0	G 300.00 5000.00 1000.00	1&
5141	C	20000 H 3999		
5142	-.689260191e+04 .129240060e+03-	.835430297e-01	.291897333e-04-.322093608e-08	2
5143	.185038011e+08 .352242700e+05-	.689260191e+04	.129240060e+03-.835430297e-01	3
5144	.291897333e-04-.322093608e-08	.185038011e+08	.352242700e+05	4
5145	BIN11CJ	C OH 0	G 300.00 5000.00 1000.00	1&
5146	C	20000 H 999		
5147	-.748761953e+04 .122143936e+03-	.812783090e-01	.299446402e-04-.306995471e-08	2
5148	.138352555e+08 .311018233e+05-	.748761953e+04	.122143936e+03-.812783090e-01	3
5149	.299446402e-04-.306995471e-08	.138352555e+08	.311018233e+05	4
5150	BIN12AJ	C OH 0	G 300.00 5000.00 1000.00	1&
5151	C	40000 H 20999		
5152	-.112067942e+05 .289229995e+03-	.176899849e+00	.551082033e-04-.709612481e-08	2
5153	.571779665e+08 .883124757e+05-	.112067942e+05	.289229995e+03-.176899849e+00	3
5154	.551082033e-04-.709612481e-08	.571779665e+08	.883124757e+05	4
5155	BIN12BJ	C OH 0	G 300.00 5000.00 1000.00	1&
5156	C	40000 H 7999		
5157	-.137852038e+05 .258480121e+03-	.167086059e+00	.583794665e-04-.644187217e-08	2
5158	.369476023e+08 .704485401e+05-	.137852038e+05	.258480121e+03-.167086059e+00	3
5159	.583794665e-04-.644187217e-08	.369476023e+08	.704485401e+05	4
5160	BIN12CJ	C OH 0	G 300.00 5000.00 1000.00	1&
5161	C	40000 H 1999		
5162	-.149752391e+05 .244287871e+03-	.162556618e+00	.598892803e-04-.613990941e-08	2
5163	.276105111e+08 .622036467e+05-	.149752391e+05	.244287871e+03-.162556618e+00	3
5164	.598892803e-04-.613990941e-08	.276105111e+08	.622036467e+05	4
5165	BIN13AJ	C OH 0	G 300.00 5000.00 1000.00	1&
5166	C	80000 H 39999		
5167	-.228102667e+05 .573729240e+03-	.352289884e+00	.110719678e-03-.140915954e-07	2
5168	.111183569e+09 .173876654e+06-	.228102667e+05	.573729240e+03-.352289884e+00	3
5169	.110719678e-03-.140915954e-07	.111183569e+09	.173876654e+06	4
5170	BIN13BJ	C OH 0	G 300.00 5000.00 1000.00	1&
5171	C	80000 H 15999		
5172	-.275704076e+05 .516960242e+03-	.334172119e+00	.116758933e-03-.128837443e-07	2
5173	.738352046e+08 .140897080e+06-	.275704076e+05	.516960242e+03-.334172119e+00	3
5174	.116758933e-03-.128837443e-07	.738352046e+08	.140897080e+06	4
5175	BIN13CJ	C OH 0	G 300.00 5000.00 1000.00	1&
5176	C	80000 H 3999		
5177	-.299504781e+05 .488575742e+03-	.325113236e+00	.119778561e-03-.122798188e-07	2
5178	.551610222e+08 .124407293e+06-	.299504781e+05	.488575742e+03-.325113236e+00	3
5179	.119778561e-03-.122798188e-07	.551610222e+08	.124407293e+06	4
5180	BIN14AJ	C OH 0	G 300.00 5000.00 1000.00	1&
5181	C	160000 H 75999		
5182	-.464138903e+05 .113799698e+04-	.701560141e+00	.222445898e-03-.279818822e-07	2
5183	.216082411e+09 .342256712e+06-	.464138903e+05	.113799698e+04-.701560141e+00	3
5184	.222445898e-03-.279818822e-07	.216082411e+09	.342256712e+06	4
5185	BIN14BJ	C OH 0	G 300.00 5000.00 1000.00	1&
5186	C	160000 H 31999		
5187	-.551408153e+05 .103392048e+04-	.668344238e+00	.233517866e-03-.257674887e-07	2
5188	.147610409e+09 .281794160e+06-	.551408153e+05	.103392048e+04-.668344238e+00	3
5189	.233517866e-03-.257674887e-07	.147610409e+09	.281794160e+06	4
5190	BIN14CJ	C OH 0	G 300.00 5000.00 1000.00	1&
5191	C	160000 H 7999		
5192	-.599009562e+05 .977151485e+03-	.650226472e+00	.239557121e-03-.245596376e-07	2
5193	.110262044e+09 .248814587e+06-	.599009562e+05	.977151485e+03-.650226472e+00	3
5194	.239557121e-03-.245596376e-07	.110262044e+09	.248814587e+06	4
5195	BIN15AJ	C OH 0	G 300.00 5000.00 1000.00	1&
5196	C	320000 H 143999		
5197	-.944144942e+05 .225707096e+04-	.139708103e+01	.446904882e-03-.555611475e-07	2
5198	.419655367e+09 .673520232e+06-	.944144942e+05	.225707096e+04-.139708103e+01	3
5199	.446904882e-03-.555611475e-07	.419655367e+09	.673520232e+06	4
5200	BIN15BJ	C OH 0	G 300.00 5000.00 1000.00	1&
5201	C	320000 H 63999		

5202	-.110281631e+06	.206784097e+04	-.133668848e+01	.467035732e-03	-.515349774e-07	2
5203	.295160818e+09	.563588320e+06	-.110281631e+06	.206784097e+04	-.133668848e+01	3
5204	.467035732e-03	-.515349774e-07	.295160818e+09	.563588320e+06		4
5205	BIN15CJ	C	OH	0	G	300.00 5000.00 1000.00 1&
5206	C	320000	H	15999		
5207	-.119801912e+06	.195430297e+04	-.130045294e+01	.479114243e-03	-.491192753e-07	2
5208	.220464089e+09	.497629173e+06	-.119801912e+06	.195430297e+04	-.130045294e+01	3
5209	.479114243e-03	-.491192753e-07	.220464089e+09	.497629173e+06		4
5210	BIN16AJ	C	OH	0	G	300.00 5000.00 1000.00 1&
5211	C	640000	H	271999		
5212	-.192002416e+06	.447629592e+04	-.278208354e+01	.897835934e-03	-.110317061e-06	2
5213	.814351825e+09	.132505408e+07	-.192002416e+06	.447629592e+04	-.278208354e+01	3
5214	.897835934e-03	-.110317061e-06	.814351825e+09	.132505408e+07		4
5215	BIN16BJ	C	OH	0	G	300.00 5000.00 1000.00 1&
5216	C	640000	H	127999		
5217	-.220563261e+06	.413568193e+04	-.267337695e+01	.934071465e-03	-.103069955e-06	2
5218	.590261637e+09	.112717664e+07	-.220563261e+06	.413568193e+04	-.267337695e+01	3
5219	.934071465e-03	-.103069955e-06	.590261637e+09	.112717664e+07		4
5220	BIN16CJ	C	OH	0	G	300.00 5000.00 1000.00 1&
5221	C	640000	H	31999		
5222	-.239603825e+06	.390860594e+04	-.260090589e+01	.958228485e-03	-.982385506e-07	2
5223	.440868177e+09	.995258347e+06	-.239603825e+06	.390860594e+04	-.260090589e+01	3
5224	.958228485e-03	-.982385506e-07	.440868177e+09	.995258347e+06		4
5225	BIN17AJ	C	OH	0	G	300.00 5000.00 1000.00 1&
5226	C	1250000	H	499999		
5227	-.381202818e+06	.866884751e+04	-.541016608e+01	.176144942e-02	-.213890287e-06	2
5228	.154184304e+10	.254505410e+07	-.381202818e+06	.866884751e+04	-.541016608e+01	3
5229	.176144942e-02	-.213890287e-06	.154184304e+10	.254505410e+07		4
5230	BIN17BJ	C	OH	0	G	300.00 5000.00 1000.00 1&
5231	C	1250000	H	249999		
5232	-.430787620e+06	.807750377e+04	-.522143936e+01	.182435833e-02	-.201308505e-06	2
5233	.115279757e+10	.220151688e+07	-.430787620e+06	.807750377e+04	-.522143936e+01	3
5234	.182435833e-02	-.201308505e-06	.115279757e+10	.220151688e+07		4
5235	BIN17CJ	C	OH	0	G	300.00 5000.00 1000.00 1&
5236	C	1250000	H	62499		
5237	-.467976220e+06	.763399597e+04	-.507989431e+01	.187154001e-02	-.191872169e-06	2
5238	.861013472e+09	.194386396e+07	-.467976220e+06	.763399597e+04	-.507989431e+01	3
5239	.187154001e-02	-.191872169e-06	.861013472e+09	.194386396e+07		4
5240	BIN18AJ	C	OH	0	G	300.00 5000.00 1000.00 1&
5241	C	2500000	H	937499		
5242	-.774801837e+06	.171898591e+05	-.107731505e+02	.353862607e-02	-.424635128e-06	2
5243	.298636471e+10	.500422390e+07	-.774801837e+06	.171898591e+05	-.107731505e+02	3
5244	.353862607e-02	-.424635128e-06	.298636471e+10	.500422390e+07		4
5245	BIN18BJ	C	OH	0	G	300.00 5000.00 1000.00 1&
5246	C	2500000	H	499999		
5247	-.861575239e+06	.161550075e+05	-.104428787e+02	.364871666e-02	-.402617011e-06	2
5248	.230553514e+10	.440303375e+07	-.861575239e+06	.161550075e+05	-.104428787e+02	3
5249	.364871666e-02	-.402617011e-06	.230553514e+10	.440303375e+07		4
5250	BIN18CJ	C	OH	0	G	300.00 5000.00 1000.00 1&
5251	C	2500000	H	124999		
5252	-.935952441e+06	.152679919e+05	-.101597886e+02	.374308002e-02	-.383744338e-06	2
5253	.172196694e+10	.388772792e+07	-.935952441e+06	.152679919e+05	-.101597886e+02	3
5254	.374308002e-02	-.383744338e-06	.172196694e+10	.388772792e+07		4
5255	BIN19AJ	C	OH	0	G	300.00 5000.00 1000.00 1&
5256	C	5000000	H	1749999		
5257	-.157439607e+07	.340840463e+05	-.214519376e+02	.710870659e-02	-.842979366e-06	2
5258	.577814668e+10	.983667918e+07	-.157439607e+07	.340840463e+05	-.214519376e+02	3
5259	.710870659e-02	-.842979366e-06	.577814668e+10	.983667918e+07		4
5260	BIN19BJ	C	OH	0	G	300.00 5000.00 1000.00 1&
5261	C	5000000	H	999999		
5262	-.172315048e+07	.323100151e+05	-.208857574e+02	.729743332e-02	-.805234021e-06	2
5263	.461101029e+10	.880606751e+07	-.172315048e+07	.323100151e+05	-.208857574e+02	3
5264	.729743332e-02	-.805234021e-06	.461101029e+10	.880606751e+07		4
5265	BIN19CJ	C	OH	0	G	300.00 5000.00 1000.00 1&
5266	C	5000000	H	249999		
5267	-.187190488e+07	.305359839e+05	-.203195773e+02	.748616004e-02	-.767488676e-06	2
5268	.344387389e+10	.777545583e+07	-.187190488e+07	.305359839e+05	-.203195773e+02	3
5269	.748616004e-02	-.767488676e-06	.344387389e+10	.777545583e+07		4
5270	BIN20AJ	C	OH	0	G	300.00 5000.00 1000.00 1&
5271	C	10000000	H	3249999		
5272	-.319837695e+07	.675767489e+05	-.427151485e+02	.142803221e-01	-.167337695e-05	2
5273	.111671879e+11	.193298211e+08	-.319837695e+07	.675767489e+05	-.427151485e+02	3
5274	.142803221e-01	-.167337695e-05	.111671879e+11	.193298211e+08		4

5275	BIN20BJ	C	OH	0	G	300.00	5000.00	1000.00	1&
5276	C	10000000	H	1999999					
5277		-.344630096e+07	.646200302e+05-	.417715148e+02	.145948666e-01-	.161046804e-05			2
5278		.922196057e+10	.176121350e+08-	.344630096e+07	.646200302e+05-	.417715148e+02			3
5279		.145948666e-01-	.161046804e-05	.922196057e+10	.176121350e+08				4
5280	BIN20CJ	C	OH	0	G	300.00	5000.00	1000.00	1&
5281	C	10000000	H	4999999					
5282		-.374380976e+07	.610719678e+05-	.406391545e+02	.149723201e-01-	.153497735e-05			2
5283		.688768777e+10	.155509117e+08-	.374380976e+07	.610719678e+05-	.406391545e+02			3
5284		.149723201e-01-	.153497735e-05	.688768777e+10	.155509117e+08				4
5285	BIN21AJ	C	OH	0	G	300.00	5000.00	1000.00	1&
5286	C	20000000	H	5999999					
5287		-.649592350e+07	.133970810e+06-	.850528435e+02	.286864620e-01-	.332159034e-05			2
5288		.215562249e+11	.379725678e+08-	.649592350e+07	.133970810e+06-	.850528435e+02			3
5289		.286864620e-01-	.332159034e-05	.215562249e+11	.379725678e+08				4
5290	BIN21BJ	C	OH	0	G	300.00	5000.00	1000.00	1&
5291	C	20000000	H	3999999					
5292		-.689260191e+07	.129240060e+06-	.835430297e+02	.291897333e-01-	.322093608e-05			2
5293		.184438611e+11	.352242700e+08-	.689260191e+07	.129240060e+06-	.835430297e+02			3
5294		.291897333e-01-	.322093608e-05	.184438611e+11	.352242700e+08				4
5295	BIN21CJ	C	OH	0	G	300.00	5000.00	1000.00	1&
5296	C	20000000	H	9999999					
5297		-.748761953e+07	.122143936e+06-	.812783090e+02	.299446402e-01-	.306995471e-05			2
5298		.137753155e+11	.311018233e+08-	.748761953e+07	.122143936e+06-	.812783090e+02			3
5299		.299446402e-01-	.306995471e-05	.137753155e+11	.311018233e+08				4
5300	BIN22AJ	C	OH	0	G	300.00	5000.00	1000.00	1&
5301	C	40000000	H	11999999					
5302		-.129918470e+08	.267941621e+06-	.170105687e+03	.573729240e-01-	.664318067e-05			2
5303		.431123897e+11	.759451356e+08-	.129918470e+08	.267941621e+06-	.170105687e+03			3
5304		.573729240e-01-	.664318067e-05	.431123897e+11	.759451356e+08				4
5305	BIN22BJ	C	OH	0	G	300.00	5000.00	1000.00	1&
5306	C	40000000	H	7999999					
5307		-.137852038e+08	.258480121e+06-	.167086059e+03	.583794665e-01-	.644187217e-05			2
5308		.368876623e+11	.704485401e+08-	.137852038e+08	.258480121e+06-	.167086059e+03			3
5309		.583794665e-01-	.644187217e-05	.368876623e+11	.704485401e+08				4
5310	BIN22CJ	C	OH	0	G	300.00	5000.00	1000.00	1&
5311	C	40000000	H	1999999					
5312		-.149752391e+08	.244287871e+06-	.162556618e+03	.598892803e-01-	.613990941e-05			2
5313		.275505711e+11	.622036467e+08-	.149752391e+08	.244287871e+06-	.162556618e+03			3
5314		.598892803e-01-	.613990941e-05	.275505711e+11	.622036467e+08				4
5315	BIN23AJ	C	OH	0	G	300.00	5000.00	1000.00	1&
5316	C	80000000	H	23999999					
5317		-.259836940e+08	.535883241e+06-	.340211374e+03	.114745848e+00-	.132863613e-04			2
5318		.862247195e+11	.151890271e+09-	.259836940e+08	.535883241e+06-	.340211374e+03			3
5319		.114745848e+00-	.132863613e-04	.862247195e+11	.151890271e+09				4
5320	BIN23BJ	C	OH	0	G	300.00	5000.00	1000.00	1&
5321	C	80000000	H	15999999					
5322		-.275704076e+08	.516960242e+06-	.334172119e+03	.116758933e+00-	.128837443e-04			2
5323		.737752646e+11	.140897080e+09-	.275704076e+08	.516960242e+06-	.334172119e+03			3
5324		.116758933e+00-	.128837443e-04	.737752646e+11	.140897080e+09				4
5325	BIN23CJ	C	OH	0	G	300.00	5000.00	1000.00	1&
5326	C	80000000	H	3999999					
5327		-.299504781e+08	.488575742e+06-	.325113236e+03	.119778561e+00-	.122798188e-04			2
5328		.551010822e+11	.124407293e+09-	.299504781e+08	.488575742e+06-	.325113236e+03			3
5329		.119778561e+00-	.122798188e-04	.551010822e+11	.124407293e+09				4
5330	BIN24AJ	C	OH	0	G	300.00	5000.00	1000.00	1&
5331	C	160000000	H	47999999					
5332		-.519673880e+08	.107176648e+07-	.680422748e+03	.229491696e+00-	.265727227e-04			2
5333		.172449379e+12	.303780543e+09-	.519673880e+08	.107176648e+07-	.680422748e+03			3
5334		.229491696e+00-	.265727227e-04	.172449379e+12	.303780543e+09				4
5335	BIN24BJ	C	OH	0	G	300.00	5000.00	1000.00	1&
5336	C	160000000	H	31999999					
5337		-.551408153e+08	.103392048e+07-	.668344238e+03	.233517866e+00-	.257674887e-04			2
5338		.147550469e+12	.281794160e+09-	.551408153e+08	.103392048e+07-	.668344238e+03			3
5339		.233517866e+00-	.257674887e-04	.147550469e+12	.281794160e+09				4
5340	BIN24CJ	C	OH	0	G	300.00	5000.00	1000.00	1&
5341	C	160000000	H	79999999					
5342		-.599009562e+08	.977151485e+06-	.650226472e+03	.239557121e+00-	.245596376e-04			2
5343		.110202104e+12	.248814587e+09-	.599009562e+08	.977151485e+06-	.650226472e+03			3
5344		.239557121e+00-	.245596376e-04	.110202104e+12	.248814587e+09				4
5345	BIN25AJ	C	OH	0	G	300.00	5000.00	1000.00	1&
5346	C	320000000	H	95999999					
5347		-.103934776e+09	.214353296e+07-	.136084550e+04	.458983392e+00-	.531454454e-04			2

5348 .344898698e+12 .607561085e+09-.103934776e+09 .214353296e+07-.136084550e+04 3
5349 .458983392e+00-.531454454e-04 .344898698e+12 .607561085e+09 4
5350 BIN25BJ C OH 0 G 300.00 5000.00 1000.00 1&
5351 C 320000000 H 63999999
5352 -.110281631e+09 .206784097e+07-.133668848e+04 .467035732e+00-.515349774e-04 2
5353 .295100878e+12 .563588320e+09-.110281631e+09 .206784097e+07-.133668848e+04 3
5354 .467035732e+00-.515349774e-04 .295100878e+12 .563588320e+09 4
5355 BIN25CJ C OH 0 G 300.00 5000.00 1000.00 1&
5356 C 320000000 H 15999999
5357 -.119801912e+09 .195430297e+07-.130045294e+04 .479114243e+00-.491192753e-04 2
5358 .220404149e+12 .497629173e+09-.119801912e+09 .195430297e+07-.130045294e+04 3
5359 .479114243e+00-.491192753e-04 .220404149e+12 .497629173e+09 4
5360 ! Kik add C6H4C2H3 radical from Burcat AlC2H3*
5361 C6H4C2H3 T12/07C 8.H 7. 0. 0.G 200.000 6000.000 1000.00 1
5362 1.57334515E+01 2.38965492E-02-8.60829763E-06 1.39223384E-09-8.35065775E-14 2
5363 4.08827573E+04-5.82476667E+01 1.17830774E+00 3.40765502E-02 5.85065530E-05 3
5364 -1.10953244E-07 4.95222636E-11 4.61414992E+04 2.36053284E+01 4.83284254E+04 4
5365 !Blanq AlC2H3Y
5366 !C6H4C2H3 000000N OH 7O 0C 8G 300 3000 1000 1
5367 ! 3.90114779E+00 5.15894020E-02-3.05080522E-05 8.55910896E-09-9.23046757E-13 2
5368 ! 4.59935428E+04 5.96930655E+00-5.36214520E+00 8.67033297E-02-7.54297960E-05 3
5369 ! 3.01139854E-08-3.40681418E-12 4.77818209E+04 5.07407949E+01 4
5370 !KAUST
5371 !AlC2H3* 000000N OH 7O 0C 8G 300 3000 1000 1
5372 ! 3.90114779E+00 5.15894020E-02-3.05080522E-05 8.55910896E-09-9.23046757E-13 2
5373 ! 4.59935428E+04 5.96930655E+00-5.36214520E+00 8.67033297E-02-7.54297960E-05 3
5374 ! 3.01139854E-08-3.40681418E-12 4.77818209E+04 5.07407949E+01 4
5375 !
5376 ! Add all intermediates from burcat
5377 !1-naphthyl-W2 C 10H 7 G 300.00 4000.00 1000.00 1
5378 ! .146529084E+02 .356159360E-01-.121796480E-04 .138747960E-08 .000000000E+00 2
5379 ! .405898415E+05-.575649187E+02-.631700500E+01 .913910790E-01-.608201990E-04 3
5380 ! .152228010E-07 .000000000E+00 .464268700E+05 .512234700E+02 4
5381 !2-naphthyl-W4 C 10H 7 G 300.00 4000.00 1000.00 1
5382 ! .146529084E+02 .356159360E-01-.121796480E-04 .138747960E-08 .000000000E+00 2
5383 ! .405898415E+05-.575649187E+02-.631700500E+01 .913910790E-01-.608201990E-04 3
5384 ! .152228010E-07 .000000000E+00 .464268700E+05 .512234700E+02 4
5385 !RA1R5CH3
5386 !
5387 !
5388 !
5389 naphthylne12 T 7/98C 10.H 6. 0. 0.G 200.000 6000.000 3000.0 1
5390 1.87728941E+01 2.48768793E-02-9.09940935E-06 1.48730676E-09-8.98228135E-14 2
5391 5.15727443E+04-7.68608875E+01-1.50617131E+00 6.03325879E-02 1.09063952E-05 3
5392 -6.91994009E-08 3.54144371E-11 5.80261788E+04 3.24494940E+01 6.02350349E+04 4
5393 naphthylne23 T 7/98C 10.H 6. 0. 0.G 200.000 6000.000 3000.0 1
5394 1.87728941E+01 2.48768793E-02-9.09940935E-06 1.48730676E-09-8.98228135E-14 2
5395 5.15727443E+04-7.68608875E+01-1.50617131E+00 6.03325879E-02 1.09063952E-05 3
5396 -6.91994009E-08 3.54144371E-11 5.80261788E+04 3.24494940E+01 6.02350349E+04 4
5397 !
5398 !126738-27-0 or 182180-84-3
5399 !C10H9 phenyl-butadienyl radical C6H5-CH=CH-CH=CH* SIGMA=1 STATWT=2 IA=17.2514
5400 !IB=140.1877 IC=157.4391 Ir(-CH=CH-CH=CH*)=7.03118 ROSYM=1 V(3)=1224. cm-1
5401 !est. Ir(-CH=CH*)=2.59427 ROSYM=1 V(3)524. cm-1 as in butadiene. Nu=3268,
5402 !3212,3204,3195,3186,3183,3176,3144,3040,1693,1661,1645,1631,1546,1497,1380,1372,
5403 !1343,1321,1253,1249,1218,1193,1162,1112,1060,1015,1013,991,964,927,889,859,852,
5404 !832(2),768,705,639,635,621,513,510,414,343,313,297,174.8,124.54 HF298=106.24
5405 !kcal REF=Thergas c(#1)&ch&ch&ch&ch&1,1/ch//ch//ch//ch(.) {HF298=106.5
5406 !kcal REF=NIST 94} Max Lst Sq Error Cp @ 200 K 0.66%
5407 C6H5CHCHCHCH /06C 10.H 9. 0. 0.G 200.000 6000.000 3000.0 1
5408 1.97227364E+01 3.05121625E-02-1.10537483E-05 1.79050874E-09-1.07387763E-13 2
5409 4.42281159E+04-7.53736816E+01 2.29508183E+00 4.52323197E-02 5.98076375E-05 3
5410 -1.21133405E-07 5.46626377E-11 5.04522033E+04 2.21435730E+01 5.34617386E+04 4
5411 !1785-61-1
5412 !C10H6 1,3-diethynylBenzene 1,3-C6H4(CCH)2 SIGMA=2 STATWT=1 IA=31.252
5413 !IB=92.9373 IC=124.1894 Nu=115,126,162,186,368,388,465,469,500,505,561,572,576,
5414 !629.5(2),646,702,718,812,916,921,925,983,1014,1122,1175,1205,1273,1313.5,1355,
5415 !1446,1525,1623,1649,2227.6(2),3197,3216,3223,3228,3494.3(2) HF298=131.96+/-2.
5416 !kcal REF=Elke Goos G3B3 Max Lst Sq Error Cp @ 1300 K 0.47%.
5417 C6H4(C2H)2 T10/15C 10.H 6. 0. 0.G 200.000 6000.000 3000.0 1
5418 1.94890277E+01 2.35101034E-02-8.43787249E-06 1.36207463E-09-8.15578305E-14 2
5419 5.80245053E+04-7.66298995E+01-1.92263481E+00 8.57578670E-02-7.03095425E-05 3
5420 2.10427011E-08 1.27338464E-12 6.37450309E+04 3.30657524E+01 6.64044712E+04 4

5421 ! Fei Qi
5422 ! Benzofulvene
5423 !C9H6CH2 MATSUGI2013 C 10H 8 0 OG 300.000 5000.000 1401.00 1
5424 Benzofulvene C 10H 8 0 OG 300.000 5000.000 1401.00 1
5425 2.37888939E+01 2.39146033E-02-8.24877665E-06 1.28829948E-09-7.50678039E-14 2
5426 1.43968777E+04-1.07094280E+02-8.01337918E+00 1.08401947E-01-9.55671696E-05 3
5427 4.25996671E-08-7.54462202E-12 2.43488603E+04 5.99659944E+01 4
5428 !benzofulvenyl radical
5429 !C9H7CH2 MATSUGI2013 C 10H 9 0 OG 300.000 5000.000 1400.00 1
5430 ! 2.48973930E+01 2.55147986E-02-8.79922194E-06 1.37404921E-09-8.00535169E-14 2
5431 ! 1.83072953E+04-1.12654689E+02-8.02975915E+00 1.12889393E-01-9.91274443E-05 3
5432 ! 4.41732177E-08-7.83596047E-12 2.86367245E+04 6.03761192E+01 4
5433 !536738-49-5
5434 !C10H9 1-methyl-1-indenyl Radical SIGMA=1 STATWT=2 IA=32.0588 IB=66.8991
5435 !Ic=98.4347 Ir=0.549 ROSYM=3 V(3)=~760. cm-1 Nu=3227,3209,3198,3185,3173,
5436 !3168,3116,3055,3008,1633,1628,1504,1488,1476,1443,1438,1433,1387,1376,1312,1287,
5437 !1211,1186,1168,1102,1081,1036,1033,1019,987,952.950,895,876,863,794,765,756,733,
5438 !692,602,560,557,524,459,421,312,228,209,144 HF298=62.7 kcal REF=Lifshitz
5439 !Dubnikova JPC A 108,(2004),3430 DFT QCISD(T)//B3LYP/(cc-pVDZ) calc
5440 !{HF298=60.264 kcal REF=MOPAC 2000 PM3} Max Lst Sq Error Cp @ 200 K 0.73%.
5441 !C10H9 1-methyl A03/05C 10.H 9. 0. 0.G 200.000 6000.000 B 129.17846 1
5442 ! 1.90083931E+01 3.18459404E-02-1.15126596E-05 1.86706540E-09-1.12145139E-13 2
5443 ! 2.23250010E+04-7.80332683E+01 4.07035729E-01 4.80530672E-02 6.13610491E-05 3
5444 !-1.25042167E-07 5.63176095E-11 2.89729160E+04 2.60120139E+01 3.15516849E+04 4
5445 !862559-83-9
5446 !C10H9 2-Hydro-Naphthalene Radical STATWT = 2 Ia = 27.990458 Ib = 71.911452
5447 !Ic = 99.39347 NU= 3126,3110,3106,3095,3093,3090,3082,2851,2843,1636,1575,1528,
5448 !1473,1430,1416,1397,1375,1353,1319,1260,1218,1185,1150,1137,1135,1112,1029,1016,
5449 !949,928,900,899,891,886,831,764,761,734(2),678,667,594,525,491,484,445,390,344,
5450 !256,169,125. REF =Curran et al, JPCRD 29,(2000),463 Hf(298)= 54.86 kcal/mole
5451 !REF = Marinov et al, Comb. Sci. Technol. 116-117,(1996), 211. Max Lst Sq Error
5452 !Cp @ 200 K 0.87%
5453 naphthyl2H Rad T 7/98C 10.H 9. 0. 0.G 200.000 6000.000 3000.0 1
5454 1.96879334E+01 3.20520257E-02-1.16715110E-05 1.90182471E-09-1.14603906E-13 2
5455 1.80099777E+04-8.29833882E+01-1.21356342E+00 5.48913745E-02 5.55281159E-05 3
5456 -1.24860759E-07 5.75105005E-11 2.52575495E+04 3.28077928E+01 2.76064663E+04 4
5457 ! copy from C10H8
5458 C6H4C2HC2H3 C 10H 8 G 300.00 4000.00 1401.00 1
5459 .234023214E+02 .242434427E-01-.836282016E-05 .130620111E-08-.761153748E-13 2
5460 .651941329E+04-.107433208E+03-.883645988E+01 .109300567E+00-.955200914E-04 3
5461 .421647669E-07-.739851710E-11 .166533366E+05 .621064766E+02 4
5462 !benzofulvenyl c10h7 assume naphthyl
5463 Benzofulvenyl C 10H 7 G 300.00 4000.00 1000.00 1
5464 .146529084E+02 .356159360E-01-.121796480E-04 .138747960E-08 .000000000E+00 2
5465 .405898415E+05-.575649187E+02-.631700500E+01 .913910790E-01-.608201990E-04 3
5466 .152228010E-07 .000000000E+00 .464268700E+05 .512234700E+02 4
5467 ! copy from C10H8
5468 C6H5CHCHCCH C 10H 8 G 300.00 4000.00 1401.00 1
5469 .234023214E+02 .242434427E-01-.836282016E-05 .130620111E-08-.761153748E-13 2
5470 .651941329E+04-.107433208E+03-.883645988E+01 .109300567E+00-.955200914E-04 3
5471 .421647669E-07-.739851710E-11 .166533366E+05 .621064766E+02 4
5472 ! to connect
5473 C6H4CH3 RadT10/13C 7.H 7. 0. 0.G 200.000 6000.000 3000.00 1
5474 1.28543060E+01 2.42712778E-02-8.75277064E-06 1.41703290E-09-8.50082345E-14 2
5475 3.10872386E+04-4.29177096E+01 2.43474215E+00 2.10368651E-02 7.20305506E-05 3
5476 -1.14038924E-07 4.82416036E-11 3.53949018E+04 1.83045052E+01 3.74896416E+04 4
5477 C7H6 G3SX B3LYPTC 7H 6 0 OG 300.000 5000.000 1401.00 1
5478 1.70564548E+01 1.67766601E-02-5.75637904E-06 8.95748927E-10-5.20574674E-14 2
5479 3.43929834E+04-6.83510071E+01-3.96406850E+00 7.40750426E-02-6.68009279E-05 3
5480 3.06821623E-08-5.59258820E-12 4.08575050E+04 4.16088550E+01 4
5481 C7H5 G3SX ref819C 7H 5 0 OG 300.000 5000.000 1404.00 1
5482 1.65644050E+01 1.44569152E-02-4.91369020E-06 7.59739947E-10-4.39556749E-14 2
5483 4.96364603E+04-6.29487260E+01-2.77567748E+00 6.97210344E-02-6.63891369E-05 3
5484 3.18329494E-08-5.98040634E-12 5.53261073E+04 3.73111448E+01 4
5485 CYC5H4 T 3/94C 5H 4 0 OG 200.000 6000.000 1000.000 1
Corrected Matteo
5486 9.60146855E+00 1.27845927E-02-4.64192639E-06 7.54921528E-10-4.54306065E-14 2
5487 5.86289983E+04-2.86475654E+01 9.04714034E-01 1.97150903E-02 3.07188653E-05 3
5488 -6.15860687E-08 2.81182783E-11 5.97127601E+04 1.90281769E+01 6.10217434E+04 4
5489 C5H3 20387C 5H 3 G 0300.00 5000.00 1000.00 1
5490 0.01078762E+03 0.09539619E-01-0.03206745E-04 0.04733323E-08-0.02512135E-12 2
5491 0.06392904E+06-0.03005444E+03 0.04328720E+02 0.02352480E+00-0.05856723E-04 3
5492 -0.01215449E-06 0.07726478E-10 0.06588531E+06 0.04173259E+02 4

5493	C5H2	20587C	5H	2	G	0300.00	5000.00	1000.00	1		
5494	0.01132917E+03	0.07424057E-01	-0.02628189E-04	0.04082541E-08	-0.02301333E-12				2		
5495	0.07878706E+06	-0.03617117E+03	0.03062322E+02	0.02709998E+00	-0.01009170E-03				3		
5496	-0.01272745E-06	0.09167219E-10	0.08114969E+06	0.07071078E+02					4		
5497	C5H5CH3	C	6H	8	G	300.00	5000.00	1399.00	1		
5498	.154352848E+02	.199801707E-01	-.680270423E-05	.105349633E-08	-.610336727E-13				2		
5499	.447456576E+04	-.636393642E+02	-.665320026E+01	.744640477E-01	-.582864186E-04				3		
5500	.231603543E-07	-.369017129E-11	.117669311E+05	.538162769E+02					4		
5501	C7H7O2	QB3-MF11	OC	7H	7O	2	OG	300.00	5000.00	1000.00	1
5502	1.71115179E+01	2.68198282E-02	-1.06205723E-05	1.91920856E-09	-1.30061244E-13				2		
5503	6.71623207E+03	-6.12436900E+01	-2.24622429E+00	7.26022303E-02	-3.67327921E-05				3		
5504	-8.74034681E-09	1.01564683E-11	1.24729027E+04	4.07042530E+01					4		
5505	O2C6H4CH3	9/21/15	C	7H	7O	2	OG	300.000	5000.000	1408.000	21
5506	2.12862164E+01	1.93020680E-02	-6.48485440E-06	9.95146950E-10	-5.72828260E-14				2		
5507	3.19865442E+03	-8.60791351E+01	-5.17635366E+00	9.32722534E-02	-8.64517889E-05				3		
5508	4.02042133E-08	-7.33445923E-12	1.10698763E+04	5.15568699E+01					4		
5509	OC6H4CH2	012508C	7H	6O	1	G	300.000	5000.000	1000.00	1	
5510	1.24204756E+01	2.70171830E-02	-1.09476851E-05	2.02705529E-09	-1.40757462E-13				2		
5511	4.49159466E+02	-4.10236260E+01	-6.21979546E-01	5.14918065E-02	-6.11682462E-06				3		
5512	-2.88887155E-08	1.45119845E-11	4.44241036E+03	2.88224802E+01					4		
5513	C6H5CH2O	4/14/94	THE.MC	7H	7O	1	OG	300.000	5000.000	1392.000	1
5514	1.78843033E+01	2.09011735E-02	-7.21832713E-06	1.12839851E-09	-6.57955260E-14				2		
5515	4.93182818E+03	-7.01304667E+01	-4.77736690E+00	7.51049308E-02	-5.68532831E-05				3		
5516	2.18290029E-08	-3.38134298E-12	1.26234438E+04	5.10429366E+01					4		
5517	BZCOOH	C	7H	8O	2	OG	300.000	5000.000	1388.000	31	
5518	2.32849942E+01	2.11249905E-02	-7.42176803E-06	1.17341778E-09	-6.89572814E-14				2		
5519	-1.39352842E+04	-9.56328725E+01	-3.90619768E+00	8.82323518E-02	-7.17190897E-05				3		
5520	2.95644635E-08	-4.91898930E-12	-4.87198921E+03	4.90970451E+01					4		
5521	C6H5O2	C	6H	5O	2	G	300.00	5000.00	1400.00	1	
5522	1.67078262E+01	1.62326229E-02	-5.47969630E-06	8.43510060E-10	-4.86562431E-14				2		
5523	8.14242915E+03	-6.08346973E+01	-2.99164672E+00	7.03857150E-02	-6.34400574E-05				3		
5524	2.915448920E-08	-5.30706938E-12	1.41320240E+04	4.20142955E+01					4		
5525	C6H5CO	C	7H	5O	1	OG	300.000	5000.000	1396.000	11	
5526	1.79587471E+01	1.58218495E-02	-5.48154854E-06	8.58709339E-10	-5.01435299E-14				2		
5527	3.78486787E+03	-7.06341032E+01	-1.71526142E+00	6.53320500E-02	-5.36914036E-05				3		
5528	2.23697440E-08	-3.73946626E-12	1.02136508E+04	3.36880709E+01					4		
5529	RBBENZOOH	3/19/ 9	THERMC	14H	14O	2	OG	300.000	5000.000	1395.000	51
5530	4.01427062E+01	3.93395367E-02	-1.37664348E-05	2.17056135E-09	-1.27304368E-13				2		
5531	-1.39277882E+04	-1.84904308E+02	-1.04261530E+01	1.68709899E-01	-1.42892982E-04				3		
5532	6.15601039E-08	-1.06485940E-11	2.47291567E+03	8.26365480E+01					4		
5533	RBBENZOO	3/19/ 9	THERMC	14H	13O	2	OG	300.000	5000.000	1394.000	41
5534	3.76701265E+01	3.91886728E-02	-1.36838688E-05	2.15430957E-09	-1.26216113E-13				2		
5535	4.38748283E+03	-1.69872607E+02	-9.53800906E+00	1.60095043E-01	-1.34982895E-04				3		
5536	5.84090458E-08	-1.01919995E-11	1.97390228E+04	7.99308597E+01					4		
5537	QBENZOOH	3/19/ 9	THERMC	14H	13O	2	OG	300.000	5000.000	1394.000	41
5538	4.02968908E+01	3.71210431E-02	-1.30088643E-05	2.05309245E-09	-1.20495552E-13				2		
5539	3.67900543E+03	-1.86479334E+02	-8.32529422E+00	1.61762848E-01	-1.37724101E-04				3		
5540	5.95672829E-08	-1.03363053E-11	1.94259748E+04	7.06782085E+01					4		
5541	ZBBENZ	9/ 9	THERMC	14H	13O	4	OG	300.000	5000.000	1391.000	71
5542	4.48785960E+01	3.75685709E-02	-1.32824040E-05	2.10858085E-09	-1.24255944E-13				2		
5543	-9.97231472E+03	-2.04041648E+02	-9.40646930E+00	1.77878119E-01	-1.55260847E-04				3		
5544	6.84418245E-08	-1.20655066E-11	7.52457116E+03	8.27128410E+01					4		
5545	KHYBBENZ	19/ 9	THERMC	14H	12O	3	OG	300.000	5000.000	1393.000	41
5546	4.03057402E+01	3.72594407E-02	-1.30902950E-05	2.06942373E-09	-1.21596482E-13				2		
5547	-2.78034193E+04	-1.82398868E+02	-7.77794671E+00	1.57347464E-01	-1.29564931E-04				3		
5548	5.40605490E-08	-9.07699935E-12	-1.19364337E+04	7.29984559E+01					4		
5549	C14H13O	3/19/ 9	THERMC	14H	13O	1	OG	300.000	5000.000	1397.000	31
5550	3.62205336E+01	3.75634484E-02	-1.29678295E-05	2.02688785E-09	-1.18180078E-13				2		
5551	5.74597621E+03	-1.65590808E+02	-1.19190739E+01	1.59861239E-01	-1.33105430E-04				3		
5552	5.60228564E-08	-9.42896323E-12	2.13328544E+04	8.92151705E+01					4		
5553	BZCOOH	C	7H	8O	2	OG	300.000	5000.000	1388.000	31	
5554	2.32849942E+01	2.11249905E-02	-7.42176803E-06	1.17341778E-09	-6.89572814E-14				2		
5555	-1.39352842E+04	-9.56328725E+01	-3.90619768E+00	8.82323518E-02	-7.17190897E-05				3		
5556	2.95644635E-08	-4.91898930E-12	-4.87198921E+03	4.90970451E+01					4		
5557	RBBENZ	C	14H	13	G	300.00	4000.00	1000.00	1		
5558	.299291000E+02	.383042200E-01	-.118663300E-04	.177305900E-08	-.104476700E-12				2		
5559	.197099600E+05	-.131713300E+03	-.766215500E+01	.133505200E+00	-.973103200E-04				3		
5560	.342829900E-07	-.478937100E-11	.309915700E+05	.658134800E+02					4		
5561	STILB	C	14H	12	G	300.00	4000.00	1000.00	1		
5562	.268497500E+02	.428429300E-01	-.150785000E-04	.246643600E-08	-.154717900E-12				2		
5563	.164217700E+05	-.117418300E+03	-.792701200E+01	.132075300E+00	-.881173300E-04				3		
5564	.190952300E-07	.176879600E-11	.263867200E+05	.640743300E+02					4		
5565	C14H12O	10/19/15	C	14H	12O	1	OG	300.000	5000.000	1394.000	31

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5566 3.48141204E+01 3.67953648E-02-1.28282619E-05 2.01783856E-09-1.18158524E-13 2
5567 -1.68668837E+04-1.61938007E+02-9.56374055E+00 1.44801295E-01-1.13794706E-04 3
5568 4.50882665E-08-7.17648586E-12-2.00559523E+03 7.46678724E+01 4
5569 !+++++
5570 !NOx MODULE (from Burcat http://garfield.chem.elte.hu/Burcat/THERM.DAT)
5571 !+++++
5572 NO RUS 89N 10 1 0 OG 200.000 6000.000 1000. 1
5573 3.26071234E+00 1.19101135E-03-4.29122646E-07 6.94481463E-11-4.03295681E-15 2
5574 9.92143132E+03 6.36900518E+00 4.21859896E+00-4.63988124E-03 1.10443049E-05 3
5575 -9.34055507E-09 2.80554874E-12 9.84509964E+03 2.28061001E+00 1.09770882E+04 4
5576 N2O L 7/88N 20 1 0 OG 200.000 6000.000 1000. 1
5577 0.48230729E+01 0.26270251E-02-0.95850872E-06 0.16000712E-09-0.97752302E-14 2
5578 0.80734047E+04-0.22017208E+01 0.22571502E+01 0.11304728E-01-0.13671319E-04 3
5579 0.96819803E-08-0.29307182E-11 0.87417746E+04 0.10757992E+02 0.98141682E+04 4
5580 NO2 L 7/88N 10 2 0 OG 200.000 6000.000 1000. 1
5581 0.48847540E+01 0.21723955E-02-0.82806909E-06 0.15747510E-09-0.10510895E-13 2
5582 0.23164982E+04-0.11741695E+00 0.39440312E+01-0.15854290E-02 0.16657812E-04 3
5583 -0.20475426E-07 0.78350564E-11 0.28966180E+04 0.63119919E+01 0.41124701E+04 4
5584 HNO ATcT/AH 1.N 1.O 1. 0.G 200.000 6000.000 1000. 1
5585 3.16598124E+00 2.99958892E-03-3.94376786E-07-3.85344089E-11 7.07602668E-15 2
5586 1.17726311E+04 7.64511172E+00 4.53525574E+00-5.68543377E-03 1.85198540E-05 3
5587 -1.71881225E-08 5.55818157E-12 1.16183003E+04 1.74315886E+00 1.28500657E+04 4
5588 HNNO H 10 1N 2 G 300.00 4000.00 1500.00 1 !
Not present in Burcat. Old Thermochemistry data were kept
5589 .699121930E+01 .187597000E-02-.212458400E-06-.671047200E-10 .123050800E-13 2
5590 .249756641E+05-.112352384E+02 .223829800E+01 .135920000E-01-.117987300E-04 3
5591 .539297100E-08-.101085900E-11 .266025900E+05 .141367900E+02 4
5592 !HNO2 equil ATcT T 9/11H 1.N 1.O 2. 0.G 200.000 6000.000 1000. 1
5593 ! 5.79182717E+00 3.65162554E-03-1.29293390E-06 2.06892796E-10-1.23154749E-14 2
5594 !-1.15953895E+04-4.05538852E+00 3.21415915E+00 8.12778066E-03 1.65998916E-06 3
5595 !-9.52814708E-09 4.87131424E-12-1.07830727E+04 9.82200056E+00-9.46538040E+03 4
5596 HNO2 ATcT3EH 1N 10 2 OG 200.00 6000.00 1000.00 1 !
Glarborg PECS 2018
5597 4.66358504E+00 4.89854351E-03-1.79694193E-06 2.94420361E-10-1.78235577E-14 2
5598 -7.25216334E+03-3.06053640E-02 4.03779347E+00-4.46123109E-03 3.19440815E-05 3
5599 -3.79359490E-08 1.44570885E-11-6.53088236E+03 5.90620097E+00-5.31122753E+03 4
5600 HONO ATcT3EH 1N 10 2 OG 200.00 6000.00 1000.00 1 !
Glarborg PECS 2018
5601 5.79144641E+00 3.64630732E-03-1.29112765E-06 2.06498233E-10-1.22138679E-14 2
5602 -1.15974343E+04-4.07145349E+00 3.16416438E+00 8.50517773E-03 5.48561573E-07 3
5603 -8.27656474E-09 4.39957151E-12-1.07744086E+04 1.00231941E+01-9.46242812E+03 4
5604 HONO2 T 8/03H 1.N 1.O 3. 0.G 200.000 6000.000 1000. 1 !
Is HNO3 in Burcat database
5605 8.03098942E+00 4.46958589E-03-1.72459491E-06 2.91556153E-10-1.80102702E-14 2
5606 -1.93138183E+04-1.62616537E+01 1.69329154E+00 1.90167702E-02-8.25176697E-06 3
5607 -6.06113827E-09 4.65236978E-12-1.74198909E+04 1.71839838E+01-1.61524852E+04 4
5608 N2H2 equil & transT 9/11N 2.H 2. 0. 0.G 200.000 6000.000 1000. 1
5609 1.31115117E+00 9.00187208E-03-3.14911824E-06 4.81449581E-10-2.71897891E-14 2
5610 2.33863341E+04 1.64091067E+01 4.91066031E+00-1.07791880E-02 3.86516489E-05 3
5611 -3.86501698E-08 1.34852134E-11 2.28241901E+04 9.10273396E-02 2.40806734E+04 4
5612 H2NN Isodiazene T 9/11N 2.H 2. 0. 0.G 200.000 6000.000 1000. 1 !
Is 'N2H2 Isodiazene' in Burcat database
5613 3.05903670E+00 6.18382347E-03-2.22171165E-06 3.58539206E-10-2.14532905E-14 2
5614 3.48530149E+04 6.69893515E+00 4.53204001E+00-7.32418578E-03 3.00803713E-05 3
5615 -3.04000551E-08 1.04700639E-11 3.49580003E+04 1.51074195E+00 3.61943157E+04 4
5616 HNNO 5/30/18 THERM N 2.H 1.O 1 0.G 300.000 5000.000 1790.000 61 !
Dean AM Bozzelli JW (Gardiner WC) Gas Phase Combustion Chemistry, Springer 2000.
5617 2.15594002E+06-4.13111192E+03 2.65627771E+00-6.70395293E-04 5.57827338E-08 2
5618 -8.03468100E+08-1.18702032E+07-8.96779017E-01 3.69714359E-02-4.80099825E-05 3
5619 2.62274393E-08-5.11382966E-12 2.68675048E+04 2.64521806E+01 4
5620 NH2NO 5/30/18 THERM N 2.H 2.O 1 0.G 300.000 5000.000 1371.000 61 !
Dean AM Bozzelli JW (Gardiner WC) Gas Phase Combustion Chemistry, Springer 2000.
5621 7.93898100E+00 5.21842622E-03-2.12493130E-06 3.53331059E-10-2.12447889E-14 2
5622 5.42322972E+03-1.84299492E+01 1.85914077E+00 1.68525394E-02-9.37240888E-06 3
5623 1.71380329E-09 4.84625807E-14 7.78108234E+03 1.51172833E+01 4
5624 HNOH trans & Equ T11/11H 2.N 1.O 1. 0.G 200.000 6000.000 1000. 1
5625 3.98321933E+00 4.88846374E-03-1.65086637E-06 2.55371446E-10-1.48308561E-14 2
5626 1.05780106E+04 3.62582838E+00 3.95608248E+00-3.02611020E-03 2.56874396E-05 3
5627 -3.15645120E-08 1.24084574E-11 1.09199790E+04 5.55950983E+00 1.21354115E+04 4
5628 NH2OH ATcT/AH 1.H 3.O 1. 0.G 200.000 6000.000 1000. 1
5629 3.88112502E+00 8.15708448E-03-2.82615576E-06 4.37930933E-10-2.52724604E-14 2
5630 -6.86018419E+03 3.79156136E+00 3.21016092E+00 6.19671676E-03 1.10594948E-05 3
5631 -1.96668262E-08 8.82516590E-12-6.58148481E+03 7.93293571E+00-5.28593988E+03 4

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5632	NH3	ATcT3EH	3N	1	0	0G	200.00	4000.00	1000.00	1 !
	Glarborg PECS 2018									
5633	2.36074311E+00	6.31850146E-03	-2.28966806E-06	4.11767411E-10	-2.90836787E-14					2
5634	-6.41596473E+03	8.02154329E+00	4.14027871E+00	-3.58489142E-03	1.89475904E-05					3
5635	-1.98833970E-08	7.15267961E-12	-6.68545158E+03	-1.66754883E-02	-5.47888720E+03					4
5636	N2H4	HYDRAZINE	L 5/90N	2H	4	0	0G	200.000	6000.000	1000.
5637	4.93957357E+00	8.75017187E-03	-2.99399058E-06	4.67278418E-10	-2.73068599E-14					2
5638	9.28265548E+03	-2.69439772E+00	3.83472149E+00	-6.49129555E-04	3.76848463E-05					3
5639	-5.00709182E-08	2.03362064E-11	1.000893925E+04	5.75272030E+00	1.14474575E+04					4
5640	HCN	ATcT/AH	1.C	1.N	1.	0.G	200.000	6000.000	1000.	1
5641	3.80231648E+00	3.14630087E-03	-1.06315727E-06	1.66185438E-10	-9.79891962E-15					2
5642	1.42849502E+04	1.57501632E+00	2.25901199E+00	1.00510475E-02	-1.33514567E-05					3
5643	1.00920479E-08	-3.00880408E-12	1.45903166E+04	8.91631960E+00	1.56111424E+04					4
5644	HNC	ATcT/AH	1.N	1.C	1.	0.G	200.000	6000.000	1000.	1
5645	4.22248262E+00	2.59458082E-03	-8.58480324E-07	1.30744940E-10	-7.50339813E-15					2
5646	2.17156730E+04	-7.79706410E-02	2.30186822E+00	1.54157449E-02	-3.13261898E-05					3
5647	3.08816218E-08	-1.11912204E-11	2.19306327E+04	8.14749128E+00	2.30810956E+04					4
5648	HNCO	Isocyanic Acid	A 5/05H	1.N	1.C	1.O	1.G	200.000	6000.000	1000.
5649	5.30045051E+00	4.02250821E-03	-1.40962280E-06	2.23855342E-10	-1.32499966E-14					2
5650	-1.61995274E+04	-3.11770684E+00	2.24009031E+00	1.45600497E-02	-1.54352330E-05					3
5651	8.55535028E-09	-1.79631611E-12	-1.54589951E+04	1.21663775E+01	-1.42642740E+04					4
5652	HCNO	Fulminic Acid	A 5/05H	1.N	1.C	1.O	1.G	200.000	6000.000	1000.
5653	5.91979744E+00	4.00114600E-03	-1.42063343E-06	2.27569621E-10	-1.35504870E-14					2
5654	1.80385534E+04	-8.26935223E+00	6.07949401E-01	2.82182431E-02	-4.60451618E-05					3
5655	3.82559486E-08	-1.23226501E-11	1.90714209E+04	1.69199098E+01	2.01698706E+04					4
5656	HOCN	Cyanic Acid	A 5/05H	1.N	1.C	1.O	1.G	200.000	6000.000	1000.
5657	5.28767714E+00	4.01746511E-03	-1.40407465E-06	2.22562614E-10	-1.31562375E-14					2
5658	-3.77409807E+03	-2.64470976E+00	2.88943546E+00	1.16487242E-02	-1.08005006E-05					3
5659	5.44138776E-09	-1.06857286E-12	-3.15296691E+03	9.51295652E+00	-1.85890558E+03					4
5660	CH3NO	Nitrosomethyl	T12/09C	1.H	3.N	1.O	1.G	200.000	6000.000	1000.
5661	5.04711802E+00	9.21544305E-03	-3.29034831E-06	5.28940397E-10	-3.15689858E-14					2
5662	6.23718102E+03	-7.74395570E-01	5.18534727E+00	-6.34085575E-03	4.57171139E-05					3
5663	-5.30421813E-08	1.99501601E-11	6.93771506E+03	2.18492659E+00	8.51040025E+03					4
5664	CH3NO2	T01/00C	1H	3N	1O	2G	200.000	6000.000	1000.	1
5665	6.73034758E+00	1.09601272E-02	-4.05357875E-06	6.67102246E-10	-4.04686823E-14					2
5666	-1.29143475E+04	-1.01800883E+01	3.54053638E+00	1.86559899E-03	4.44946580E-05					3
5667	-5.87057133E-08	2.30684496E-11	-1.11385976E+04	1.06884657E+01	-9.71208165E+03					4
5668	CH3ONO	A 5/05C	1.H	3.O	2.N	1.G	200.000	6000.000	1000.	1
5669	6.93605239E+00	9.97319424E-03	-3.60642537E-06	5.83462161E-10	-3.50058729E-14					2
5670	-1.08381899E+04	-6.98144573E+00	6.15261387E+00	-2.91937431E-03	4.14526828E-05					3
5671	-4.93954776E-08	1.85608328E-11	-9.85260262E+03	8.04057190E-01	-7.87057806E+03					4
5672	CH3ONO2	T05/98C	1H	3N	1O	3G	200.000	6000.000	1000.	1
5673	9.77845489E+00	1.10069541E-02	-4.25928645E-06	7.18198185E-10	-4.42041793E-14					2
5674	-1.88804487E+04	-2.39163197E+01	3.91363583E+00	1.52137945E-02	-1.73479131E-05					3
5675	-3.37074473E-08	1.44322204E-11	-1.66103232E+04	9.44208392E+00	-1.46737980E+04					4
5676	CH3CN	Methyl-Cya	T01/03C	2.H	3.N	1.	0.G	200.000	6000.000	1000.
5677	5.09921882E+00	9.69585649E-03	-3.48051966E-06	5.61420173E-10	-3.35835856E-14					2
5678	6.60967324E+03	-3.36087178E+00	3.82392803E+00	4.08201943E-03	2.16209537E-05					3
5679	-2.89807789E-08	1.12962700E-11	7.44430382E+03	5.52656156E+00	8.90492212E+03					4
5680	N	L 6/88N	1	0	0	0G	200.000	6000.000	1000.	1
5681	0.24159429E+01	0.17489065E-03	-0.11902369E-06	0.30226244E-10	-0.20360983E-14					2
5682	0.56133775E+05	0.46496095E+01	0.25000000E+01	0.00000000E+00	0.00000000E+00					3
5683	0.00000000E+00	0.00000000E+00	0.56104638E+05	0.41939088E+01	0.56850013E+05					4
5684	NO3	ATcT/AN	1.O	3.	0.	0.G	200.000	6000.000	1000.	1
5685	7.48347702E+00	2.57772064E-03	-1.00945831E-06	1.72314063E-10	-1.07154008E-14					2
5686	6.12990474E+03	-1.41618136E+01	2.17359330E+00	1.04902685E-02	1.10472669E-05					3
5687	-2.81561867E-08	1.36583960E-11	7.81290905E+03	1.46022090E+01	8.97563416E+03					4
5688	NH	ATcT/AN	1.H	1.	0.	0.G	200.000	6000.000	1000.	1
5689	2.78372644E+00	1.32985888E-03	-4.24785573E-07	7.83494442E-11	-5.50451310E-15					2
5690	4.23461945E+04	5.74084863E+00	3.49295037E+00	3.11795720E-04	-1.48906628E-06					3
5691	2.48167402E-09	-1.03570916E-12	4.21059722E+04	1.84834973E+00	4.31525130E+04					4
5692	NNH	T 8/11N	2.H	1.	0.	0.G	200.000	6000.000	1000.	1 !
	Is N2H in Burcat database									
5693	3.42744423E+00	3.23295234E-03	-1.17296299E-06	1.90508356E-10	-1.14491506E-14					2
5694	2.87676026E+04	6.39209233E+00	4.25474632E+00	-3.45098298E-03	1.37788699E-05					3
5695	-1.33263744E-08	4.41023397E-12	2.87932080E+04	3.28551762E+00	3.00058572E+04					4
5696	NH2	AMIDOGEN	RAD IU3/03N	1.H	2.	0.	0.G	200.000	3000.000	1000.
5697	2.59263049E+00	3.47683597E-03	-1.08271624E-06	1.49342558E-10	-5.75241187E-15					2
5698	2.15737320E+04	7.90565351E+00	4.19198016E+00	-2.04602827E-03	6.67756134E-06					3
5699	-5.24907235E-09	1.55589948E-12	2.11863286E+04	-9.04785244E-02	2.23945849E+04					4
5700	H2NO	RADICAL	T09/09N	1.H	2.O	1.	0.G	200.000	6000.000	1000.
	From Glarborg thermo database (cannot find in Burcat)									
5701	3.75555914E+00	5.16219354E-03	-1.76387387E-06	2.75052692E-10	-1.60643143E-14					2

5702	6.51826177E+03	4.30933053E+00	3.93201139E+00	-1.64028165E-04	1.39161409E-05	3
5703	-1.62747853E-08	6.00352834E-12	6.71178975E+03	4.58837038E+00	7.97044877E+03	4
5704	N2H3 Rad.	T 7/11N	2.H 3.	0.	0.G 200.000 6000.000 1000.	1
5705	4.04483566E+00	7.31130186E-03	-2.47625799E-06	3.83733021E-10	-2.23107573E-14	2
5706	2.53241420E+04	2.88423392E+00	3.42125505E+00	1.34901590E-03	2.23459071E-05	3
5707	-2.99727732E-08	1.20978970E-11	2.58198956E+04	7.83176309E+00	2.70438066E+04	4
5708	CN	IU8/03C	1.N 1.	0.	0.G 200.000 6000.000 1000.	1
5709	3.39912850E+00	7.46548662E-04	-1.41493852E-07	1.86747736E-11	-1.26032540E-15	2
5710	5.16569715E+04	4.67148681E+00	3.61256069E+00	-9.53015737E-04	2.13757271E-06	3
5711	-3.05001808E-10	-4.70518097E-13	5.17084034E+04	3.98238722E+00	5.27611901E+04	4
5712	NCN MethaneTetr	T 5/14C	1.N 2.	0.	0.G 200.000 6000.000 1000.	1
5713	5.68744173E+00	1.82662756E-03	-7.07546249E-07	1.19515592E-10	-7.31827071E-15	2
5714	5.15901177E+04	-6.31954433E+00	2.79807977E+00	1.00008683E-02	-9.59229469E-06	3
5715	4.75546842E-09	-1.04340146E-12	5.24021705E+04	8.62129767E+00	5.36050832E+04	4
5716	NCO (NCO)	A 5/05N	1.C 1.O 1.	0.G 200.000 6000.000 1000.	1 !	
	Is CNO (NCO) in Burcat database					
5717	5.08064474E+00	2.37443587E-03	-9.07098904E-07	1.52286713E-10	-9.31009234E-15	2
5718	1.35781204E+04	-2.15734434E+00	2.77405177E+00	9.24523481E-03	-9.91773586E-06	3
5719	6.68461303E-09	-2.09520542E-12	1.42369570E+04	9.75458670E+00	1.53995606E+04	4
5720	HNCN Cyanamide	T03/10C	1.H 1.N 2.	0.G 200.000 6000.000 1000.	1	
5721	5.53846448E+00	3.89054126E-03	-1.38104752E-06	2.21294765E-10	-1.31827325E-14	2
5722	3.59635337E+04	-3.39587098E+00	3.06754311E+00	1.06789939E-02	-7.96224305E-06	3
5723	2.59883390E-09	-1.27057612E-13	3.66623508E+04	9.41074995E+00	3.79863165E+04	4
5724	H2CN H2C=N*	T 1/11C	1.H 2.N 1.	0.G 200.000 6000.000 1000.	1 !	
	Is CH2N in Burcat database					
5725	3.80315578E+00	5.47197362E-03	-1.95314875E-06	3.13362403E-10	-1.86249384E-14	2
5726	2.71302747E+04	3.31759436E+00	3.97799555E+00	-3.43275801E-03	2.59134260E-05	3
5727	-3.04692171E-08	1.16272717E-11	2.74854081E+04	4.43067396E+00	2.86930920E+04	4
5728	C2N2 Dicyanogen	ATcT/AC	2.N 2.	0.	0.G 200.000 6000.000 1000.	1
5729	6.70549520E+00	3.64271185E-03	-1.30939702E-06	2.16421413E-10	-1.31193815E-14	2
5730	3.48824335E+04	-1.04803146E+01	2.32928126E+00	2.61540993E-02	-4.90009889E-05	3
5731	4.61923035E-08	-1.64325831E-11	3.56900732E+04	9.86348075E+00	3.71976220E+04	4
5732	CH2CN	1/16/17	THERMC	2.H 2.N 1.	0.G 300.000 5000.000 1414.000	61 ! K
	Sendt E Ikeda GB Bacskay JC Mackie JPCA 103 (1999) 1054-1072					
5733	6.36314975E+00	6.36391885E-03	-2.75175653E-06	5.78264246E-10	-4.21050412E-14	2
5734	2.90725105E+04	-8.80921516E+00	3.13213813E+00	1.42275608E-02	-1.03390720E-05	3
5735	4.00717364E-09	-6.45501720E-13	3.01853547E+04	8.46664206E+00		4
5736	HCNH H*C=NH Trans	T11/11C	1.H 2.N 1.	0.G 200.000 6000.000 1000.	1	
5737	4.04014700E+00	5.16591694E-03	-1.82276828E-06	2.90299053E-10	-1.71614589E-14	2
5738	3.11540211E+04	2.58894095E+00	3.97114555E+00	-3.88875724E-03	2.92918950E-05	3
5739	-3.57482411E-08	1.40303911E-11	3.15789298E+04	5.06388721E+00	3.27848544E+04	4
5740	C3HN Cyano-Acety	A 2/05C	3.H 1.N 1.	0.G 200.000 6000.000 1000.	1	
5741	7.44515032E+00	5.27107604E-03	-1.86735278E-06	2.98683734E-10	-1.77665376E-14	2
5742	4.16450237E+04	-1.46187448E+01	5.87779106E-01	3.84323486E-02	-6.61566501E-05	3
5743	5.72555769E-08	-1.89892637E-11	4.29066005E+04	1.74909167E+01	4.43097371E+04	4
5744	CH3NH2	T04/14C	1.H 5.N 1.	0.G 200.000 6000.000 1000.	1 !	
	Burcat database (CH5N)					
5745	4.46959661E+00	1.21969427E-02	-4.31573211E-06	6.89638406E-10	-4.09907834E-14	2
5746	-4.86166208E+03	-1.73983318E+00	4.93595327E+00	-1.06687240E-02	6.66595644E-05	3
5747	-7.68165338E-08	2.88891949E-11	-3.96311166E+03	1.01955189E+00	-2.51488061E+03	4
5748	CH2NH	T 8/11C	1.H 3.N 1.	0.G 200.000 6000.000 1000.	1 !	
	Burcat database (CH3N)					
5749	3.44258358E+00	8.37600036E-03	-2.97819078E-06	4.77352867E-10	-2.84295062E-14	2
5750	8.97134621E+03	3.95595397E+00	4.79302577E+00	-1.26841692E-02	5.69766521E-05	3
5751	-6.34985251E-08	2.37023330E-11	9.41385818E+03	1.10277996E+00	1.06682174E+04	4
5752	CH2NH2	T 8/11C	1.H 4.N 1.	0.G 200.000 6000.000 1000.	1 !	
	Burcat database (*CH2NH2)					
5753	4.55329728E+00	9.42002581E-03	-3.20781399E-06	4.98961894E-10	-2.90872284E-14	2
5754	1.58717284E+04	-2.45945234E-02	2.85538164E+00	7.27364238E-03	1.65712636E-05	3
5755	-2.70976978E-08	1.16327939E-11	1.66165986E+04	1.02444521E+01	1.78895690E+04	4
5756	CH3NH	T03/10C	1.H 4.N 1.	0.G 200.000 6000.000 1000.	1 !	
	Burcat database (CH3NH radical)					
5757	4.02244380E+00	1.03512061E-02	-3.64560169E-06	5.80491587E-10	-3.44103829E-14	2
5758	1.95050854E+04	1.64483768E+00	4.70973738E+00	-7.31946952E-03	4.95105509E-05	3
5759	-5.72790480E-08	2.16523586E-11	2.00619432E+04	1.85460205E+00	2.14752744E+04	4
5760	!+++++					
5761	!PYRROLE MODULE					
5762	!+++++					
5763	C4H5N	1/16/17	THERMC	4.H 5.N 1.	0.G 300.000 5000.000 1430.000	61 !
	Martoprawiro M., Bacskay G.B. & Mackie J.C., JPCA (1999) 103, 3923-3934					
5764	1.08130186E+01	1.48492978E-02	-4.63893065E-06	6.75632087E-10	-3.74350506E-14	2
5765	7.86128350E+03	-3.62440836E+01	-5.22833031E+00	6.28815185E-02	-5.92617976E-05	3
5766	2.83624834E-08	-5.27666016E-12	1.22545900E+04	4.59560293E+01		4

5767 C4H4N Pyrridyl R T 7/14C 4.H 4.N 1. 0.G 200.000 6000.000 1000. 1 !
Burcat database

5768 9.56455967E+00 1.37100337E-02-4.92563602E-06 7.95650357E-10-4.76637329E-14 2
5769 3.05922716E+04-2.78072307E+01 7.12951232E-01 1.73878483E-02 4.69371029E-05 3
5770 -8.26955853E-08 3.67546269E-11 3.38297439E+04 2.23581694E+01 3.50837627E+04 4
5771 PYRLNE 1/29/99 THERMC 4.H 5N 1 0 300.000 5000.000 1612.000 61 !
Martoprawiro M., Backsay G.B. & Mackie J.C., JPCA (1999) 103, 3923-3934

5772 1.34940533E+01 1.30782225E-02-5.31092725E-06 9.16774974E-10-5.70507480E-14 2
5773 1.25447012E+04-5.29019191E+01 5.18331222E-01 3.05263735E-02-6.96325842E-06 3
5774 -4.74435769E-09 1.85423711E-12 1.85043254E+04 2.16317664E+01 4
5775 PYRLYL 1/29/99 THERMC 4.H 4N 1 0 300.000 5000.000 1441.000 61 !
Martoprawiro M., Backsay G.B. & Mackie J.C., JPCA (1999) 103, 3923-3934

5776 1.42655423E+01 7.16959055E-03-2.61629833E-06 4.24123219E-10-2.53584367E-14 2
5777 2.87282192E+04-5.49876875E+01-3.3777631E+00 4.89860058E-02-3.90370036E-05 3
5778 1.41332646E-08-1.88256423E-12 3.45930525E+04 3.92182224E+01 4
5779 PYROP 1/29/99 THERMC 4.H 5N 1 0 300.000 5000.000 1406.000 61 !
Martoprawiro M., Backsay G.B. & Mackie J.C., JPCA (1999) 103, 3923-3934

5780 2.20116388E+01 2.78736506E-03-1.13805728E-06 1.97996882E-10-1.24211667E-14 2
5781 4.01825790E+04-9.50138981E+01-1.77243194E+01 1.29768946E-01-1.54581953E-04 3
5782 8.22911009E-08-1.62970458E-11 5.03953146E+04 1.05995170E+02 4
5783 HNCPROP 1/29/99 THERMC 4.H 5N 1 0 300.000 5000.000 1423.000 61 !
Martoprawiro M., Backsay G.B. & Mackie J.C., JPCA (1999) 103, 3923-3934

5784 1.57166050E+01 8.54887604E-03-3.10680164E-06 5.02269358E-10-2.99741839E-14 2
5785 2.73052217E+04-5.90784124E+01 7.52279780E-01 3.84264182E-02-2.21149260E-05 3
5786 3.78397494E-09 3.31583656E-13 3.28206971E+04 2.27770410E+01 4
5787 A-C3H4CN 1/29/99 THERMC 4.H 4N 1 0 300.000 5000.000 1340.000 61 !
Martoprawiro M., Backsay G.B. & Mackie J.C., JPCA (1999) 103, 3923-3934

5788 1.42039120E+01 9.92550281E-03-4.36878399E-06 7.99265452E-10-5.19044906E-14 2
5789 2.72109716E+04-5.18657327E+01-7.06083475E+00 6.62435950E-02-6.33711883E-05 3
5790 2.93828617E-08-5.33457552E-12 3.39903133E+04 6.00886287E+01 4
5791 C-C3H4CN 1/29/99 THERMC 4.H 4N 1 0 300.000 5000.000 1375.000 61 !
Martoprawiro M., Backsay G.B. & Mackie J.C., JPCA (1999) 103, 3923-3934

5792 1.49368791E+01 6.47668905E-03-2.34750744E-06 3.78853855E-10-2.25817375E-14 2
5793 3.97271995E+04-5.00165292E+01 2.87163948E+00 3.38692899E-02-2.51401129E-05 3
5794 8.54475962E-09-1.06764268E-12 4.39030490E+04 1.49085502E+01 4
5795 C3H4CN 1/29/99 THERMC 4.H 4N 1 0 300.000 5000.000 1396.000 61 !
Martoprawiro M., Backsay G.B. & Mackie J.C., JPCA (1999) 103, 3923-3934

5796 1.56099688E+01 5.90248907E-03-2.14919493E-06 3.47899402E-10-2.07802288E-14 2
5797 3.61529551E+04-5.79376609E+01 1.63184648E+00 3.98358201E-02-3.29800298E-05 3
5798 1.27631797E-08-1.88643021E-12 4.07507474E+04 1.64665197E+01 4
5799 A-C3H5CN 1/16/17 THERMC 4.H 5N 1 2 300.000 5000.000 1430.000 61 !
Doughty, A., & Mackie, J. C., JPCA (1992) 96(1), 272-281.

5800 1.09928614E+01 1.45505248E-02-4.50210949E-06 6.50638889E-10-3.58287304E-14 2
5801 1.43674178E+04-3.11936847E+01 1.20559815E+00 4.33394942E-02-3.68365078E-05 3
5802 1.69025079E-08-3.09307073E-12 1.71119297E+04 1.91618447E+01 4
5803 T-C3H5CN 1/16/17 THERMC 4.H 5N 1 2 300.000 5000.000 1396.000 61 !
Doughty, A., & Mackie, J. C., JPCA (1992) 96(1), 272-281.

5804 1.09017230E+01 1.43290238E-02-5.16465461E-06 9.09557179E-10-5.91701412E-14 2
5805 1.16777269E+04-3.30706603E+01 1.12815965E-02 4.11350983E-02-3.09863686E-05 3
5806 1.24489967E-08-2.06101384E-12 1.53434572E+04 2.49667826E+01 4
5807 C-C3H5CN 1/16/17 THERMC 4.H 5N 1 2 300.000 5000.000 1396.000 61 !
Doughty, A., & Mackie, J. C., JPCA (1992) 96(1), 272-281.

5808 1.07406806E+01 1.44270533E-02-5.17031206E-06 9.06160193E-10-5.87761178E-14 2
5809 1.09006733E+04-3.22136921E+01-2.43844711E-01 4.14247293E-02-3.11365893E-05 3
5810 1.24941464E-08-2.06685041E-12 1.46026566E+04 2.63403254E+01 4
5811 CHCHCN CH=CHCN A12/04C 3.H 2.N 1. 0.G 200.000 6000.000 1000. 1 !
Burcat database (C3H2CN)

5812 6.99670220E+00 7.50618110E-03-2.68300369E-06 4.31684490E-10-2.57821318E-14 2
5813 5.04796219E+04-1.01552187E+01 2.15324611E+00 2.06638717E-02-1.33975241E-05 3
5814 7.77214839E-10 2.02897347E-12 5.18184058E+04 1.48728946E+01 5.32629680E+04 4
5815 CH2CHCN CH2=CHCN A12/04C 3.H 3.N 1. 0.G 200.000 6000.000 1000. 1 !
Burcat database (C3H2CN)

5816 6.52096861E+00 1.05028771E-02-3.73734374E-06 5.99498117E-10-3.57283503E-14 2
5817 1.92525453E+04-9.59580896E+00 3.04396646E+00 1.05333467E-02 1.96574996E-05 3
5818 -3.42001077E-08 1.48155667E-11 2.06456740E+04 1.05816246E+01 2.21344883E+04 4
5819 C4H4N2 SUCCINONITR12/03C 4.H 4.N 2. 0.G 200.000 6000.000 1000. 1
5820 1.14626097E+01 1.43425847E-02-5.26374167E-06 8.61140761E-10-5.20073439E-14 2
5821 2.02962879E+04-3.23404065E+01 2.92554100E+00 2.74517845E-02 9.39908894E-06 3
5822 -3.65605156E-08 1.81346873E-11 2.31092217E+04 1.41181715E+01 2.52209691E+04 4
5823 C4H3N2 1/29/99 THERMC 4.H 3.N 2. 0.G 300.000 5000.000 1537.000 61 !
K Sendt E Ikeda GB Bacskay JC Mackie JPCA 103 (1999) 1054-1072

5824 1.78444927E+01 5.53110368E-03-2.34526416E-06 4.17551812E-10-2.65848486E-14 2
5825 3.76984604E+04-6.79878141E+01 9.52114548E+00 4.46968930E-03 2.25289931E-05 3

5826	-2.13113568E-08	5.36499501E-12	4.27060163E+04	-1.58875908E+01						4	
5827	C4H2N2	1/29/99	THERMC	4.H	2.N	2.	0.G	300.000	5000.000	1679.000	61 !
	K Sendt E Ikeda GB Bacskay JC Mackie JPCA 103 (1999) 1054-1072										
5828	1.46414829E+01	6.34973068E-03	-2.73148192E-06	4.91630086E-10	-3.15448650E-14						2
5829	3.45707689E+04	-5.24954212E+01	3.10223328E+00	3.06140478E-02	-2.00862591E-05						3
5830	5.27139118E-09	-3.96461834E-13	3.86027891E+04	1.01004955E+01							4
5831	C2H5CN	PropionitrA	1/05C	3.H	5.N	1.	0.G	200.000	6000.000	1000.	1 !
	C3H5N in Burcat database										
5832	7.04418234E+00	1.53008159E-02	-5.44095595E-06	8.72156064E-10	-5.19455789E-14						2
5833	3.05885503E+03	-1.15133490E+01	3.62429314E+00	1.26256761E-02	2.47719570E-05						3
5834	-3.99054512E-08	1.66077777E-11	4.60780029E+03	9.10669692E+00	6.39739347E+03						4
5835	CH2CH2CN	1/29/99	THERMC	3.H	4.N	1.	0.G	300.000	5000.000	1254.000	61 !
	K Sendt E Ikeda GB Bacskay JC Mackie JPCA 103 (1999) 1054-1072										
5836	1.08023780E+01	1.04405370E-02	-4.59647366E-06	8.41034552E-10	-5.46218232E-14						2
5837	2.34914821E+04	-3.44545688E+01	-2.06724114E+00	3.61477061E-02	-2.42081177E-05						3
5838	8.12552666E-09	-1.22443630E-12	2.85306905E+04	3.64765218E+01							4
5839	CH3CHCN	1/29/99	THERMC	3.H	4.N	1.	0.G	300.000	5000.000	1681.000	61 !
	K Sendt E Ikeda GB Bacskay JC Mackie JPCA 103 (1999) 1054-1072										
5840	7.99632382E+00	1.34530512E-02	-5.75498001E-06	1.03132613E-09	-6.59477260E-14						2
5841	2.29924034E+04	-1.70967993E+01	6.51512710E+00	4.37286730E-04	2.39394634E-05						3
5842	-1.87713240E-08	4.13145742E-12	2.51173833E+04	-3.19504522E+00							4
5843	RCTN-1	10/13/17	THERMC	4.H	6.N	1.	0.G	300.000	5000.000	1668.000	61
5844	1.22572997E+01	1.50342019E-02	-5.63013229E-06	9.31426214E-10	-5.65460201E-14						2
5845	2.09882388E+04	-3.52340117E+01	1.61914029E+00	3.46673557E-02	-1.60439742E-05						3
5846	1.65803319E-09	3.94529016E-13	2.49591723E+04	2.34363442E+01							4
5847	RCTN-2	10/13/17	THERMC	4.H	6.N	1.	0.G	300.000	5000.000	1394.000	61
5848	1.57305543E+01	1.05609149E-02	-3.68830695E-06	5.81567945E-10	-3.41348142E-14						2
5849	2.56241356E+04	-7.38317310E+01	-1.44504286E+00	4.99903036E-02	-3.67034405E-05						3
5850	1.23812062E-08	-1.51619189E-12	3.14888137E+04	1.83765220E+01							4
5851	ROHCTN-2	10/13/17	THERMC	4.H	6.N	1.O	1.G	300.000	5000.000	1552.000	61
5852	1.89520103E+01	1.10310157E-02	-3.99442651E-06	6.44232539E-10	-3.83826878E-14						2
5853	4.07565042E+03	-7.87112555E+01	1.39609252E+00	4.68050754E-02	-2.83676286E-05						3
5854	6.28313612E-09	-9.63872394E-14	1.05348265E+04	1.71673874E+01							4
5855	RCTN-4	10/13/17	THERMC	4.H	6.N	1.	0.G	300.000	5000.000	2039.000	61
5856	1.35818392E+01	1.37966703E-02	-5.17336426E-06	8.56608335E-10	-5.20359781E-14						2
5857	1.51378351E+04	-4.46954461E+01	1.50058258E+00	3.94849928E-02	-2.39070512E-05						3
5858	6.22397251E-09	-5.09736651E-13	1.93405098E+04	2.07418063E+01							4
5859	RACN-2	10/13/17	THERMC	3.H	4.N	1.	0.G	300.000	5000.000	2009.000	61
5860	8.53593068E+00	1.25826076E-02	-5.32091919E-06	9.45696397E-10	-6.01038282E-14						2
5861	2.67965972E+04	-1.76340230E+01	6.16788913E+00	6.51532085E-03	1.28419462E-05						3
5862	-1.18769620E-08	2.71600712E-12	2.87565365E+04	-7.36582208E-01							4
5863	RACN-3	10/13/17	THERMC	3.H	4.N	1.	0.G	300.000	5000.000	1673.000	61
5864	1.91916189E+01	9.42148865E-05	-4.17164564E-08	7.66087663E-12	-4.99099472E-16						2
5865	2.56934216E+04	-7.83513935E+01	-1.39375456E+01	9.11267828E-02	-9.36690178E-05						3
5866	4.27590291E-08	-7.31476587E-12	3.53056414E+04	9.38719392E+01							4
5867	ROHACN-2	10/13/17	THERMC	3.H	4.N	1.O	1.G	300.000	5000.000	1385.000	61
5868	1.04261603E+01	1.44720939E-02	-6.28846470E-06	1.13964934E-09	-7.34834549E-14						2
5869	8.33074599E+03	-2.60517251E+01	-5.22435850E+00	6.04821849E-02	-6.12785189E-05						3
5870	3.11780721E-08	-6.15937204E-12	1.31467500E+04	5.51702242E+01							4
5871	ROHACN-3	10/13/17	THERMC	3.H	4.N	1.O	1.G	300.000	5000.000	1414.000	61
5872	1.65126224E+01	5.10968792E-03	-1.86986468E-06	3.03683485E-10	-1.81806834E-14						2
5873	8.74417336E+03	-6.75145599E+01	-1.24744838E-01	4.93113982E-02	-4.65483707E-05						3
5874	2.06105205E-08	-3.50635910E-12	1.38341393E+04	1.96889305E+01							4
5875	C4H4NO2	10/17/17	THERMC	4.H	4.N	1.O	2.G	300.000	5000.000	1396.000	61
5876	1.97101004E+01	7.64871349E-03	-2.78308271E-06	4.50304538E-10	-2.68885330E-14						2
5877	-1.34702487E+03	-7.30406448E+01	8.90040219E-01	5.48813020E-02	-4.77276033E-05						3
5878	1.96705384E-08	-3.13854266E-12	4.71031101E+03	2.66244859E+01							4
5879	CH2NH (H2C=NH)	T	8/11C	1.H	3.N	1.	0.G	200.000	6000.000	1000.	1 !
	Burcat database (CH3N)										
5880	3.44258358E+00	8.37600036E-03	-2.97819078E-06	4.77352867E-10	-2.84295062E-14						2
5881	8.97134621E+03	3.95595397E+00	4.79302577E+00	-1.26841692E-02	5.69766521E-05						3
5882	-6.34985251E-08	2.37023330E-11	9.41385818E+03	1.10277996E+00	1.06682174E+04						4
5883	CH2N H2C=N*	T	1/11C	1.H	2.N	1.	0.G	200.000	6000.000	1000.	1 !
	Burcat database										
5884	3.80315578E+00	5.47197362E-03	-1.95314875E-06	3.13362403E-10	-1.86249384E-14						2
5885	2.71302747E+04	3.31759436E+00	3.97799555E+00	-3.43275801E-03	2.59134260E-05						3
5886	-3.04692171E-08	1.16272717E-11	2.74854081E+04	4.43067396E+00	2.86930920E+04						4
5887	NCCH(3)	11/13/17	THERMC	2.H	1.N	1.	2.G	300.000	5000.000	1426.000	61
5888	7.05553318E+00	3.10686608E-03	-2.51794650E-06	8.62579465E-10	-7.93566639E-14						2
5889	4.30297310E+03	-1.45455851E+01	3.37242258E+00	9.03135655E-03	-6.11959285E-06						3
5890	1.99202763E-09	-2.52636007E-13	6.04948556E+03	6.50451437E+00							4
5891	C2N N(CC) cy	T	8/12C	2.N	1.	0.	0.G	200.000	6000.000	1000.	1
5892	5.31957216E+00	1.68318589E-03	-6.50522050E-07	1.10121243E-10	-6.80945770E-15						2

