

THERMO

300.000 1000.000 5000.000

!THERMO CURRAN

AR G 5/97AR 1 0 0 OG 200.000 6000.00 1000.00

1

2.50000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00

0.00000000E+00 2

-7.45375000E+02 4.37967491E+00 2.50000000E+00 0.00000000E+00

0.00000000E+00 3

0.00000000E+00 0.00000000E+00-7.45375000E+02 4.37967491E+00

0.00000000E+00 4

XE REF ELEMENT G 1/99XE 1. 0. 0. 0.G 200.000 6000.000 1000.

1

2.50024133E+00-4.69660973E-07 2.96022821E-10-7.40632003E-14 6.36936063E-

18 2

-7.45462934E+02 6.16309761E+00 2.50000000E+00 0.00000000E+00

0.00000000E+00 3

0.00000000E+00 0.00000000E+00-7.45375000E+02 6.16441993E+00

0.00000000E+00 4

NE L10/92NE 1 0 0 OG 200.000 6000.000

1000.00 1

0.25000000E+01 0. 0. 0. 0.

2

-0.74537500E+03 0.33553227E+01 0.25000000E+01 0. 0.

3

0. 0. -0.74537498E+03 0.33553227E+01

0.00000000E+00 4

N2 G 8/02N 2 0 0 OG 200.000 6000.00 1000.00

1

2.95257637E+00 1.39690040E-03-4.92631603E-07 7.86010195E-11-4.60755204E-

15 2

-9.23948688E+02 5.87188762E+00 3.53100528E+00-1.23660988E-04-5.02999433E-

07 3

2.43530612E-09-1.40881235E-12-1.04697628E+03 2.96747038E+00

0.00000000E+00 4

HE G 5/97HE 1 0 0 0 G 200.000 6000.00 1000.00

1

2.50000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00

0.00000000E+00 2

-7.45375000E+02 9.28723974E-01 2.50000000E+00 0.00000000E+00

0.00000000E+00 3

0.00000000E+00 0.00000000E+00-7.45375000E+02 9.28723974E-01

0.00000000E+00 4

H2 TPIS78H 2 0 0 OG 200.000 6000.00 1000.00

1

2.93286575E+00 8.26608026E-04-1.46402364E-07 1.54100414E-11-6.88804800E-

16 2

-8.13065581E+02-1.02432865E+00 2.34433112E+00 7.98052075E-03-1.94781510E-

05 3

2.01572094E-08-7.37611761E-12-9.17935173E+02 6.83010238E-01

0.00000000E+00 4

H L 6/94H 1 0 0 OG 200.000 6000.00 1000.00

1

0.25000000E+01 0.00000000E+00 0.00000000E+00 0.00000000E+00

0.00000000E+00 2

0.25473660E+05-0.44668285E+00 0.25000000E+01 0.00000000E+00
 0.00000000E+00 3
 0.00000000E+00 0.00000000E+00 0.25473660E+05-0.44668285E+00
 0.26219035E+05 4
 O2 RUS 890 2 0 0 0G 200.000 6000.00 1000.00
 1
 3.66096065E+00 6.56365811E-04-1.41149627E-07 2.05797935E-11-1.29913436E-
 15 2
 -1.21597718E+03 3.41536279E+00 3.78245636E+00-2.99673416E-03 9.84730201E-
 06 3
 -9.68129509E-09 3.24372837E-12-1.06394356E+03 3.65767573E+00
 0.00000000E+00 4
 O L 1/900 1 0 0 0G 200.000 6000.00 1000.00
 1
 2.54363697E+00-2.73162486E-05-4.19029520E-09 4.95481845E-12-4.79553694E-
 16 2
 2.92260120E+04 4.92229457E+00 3.16826710E+00-3.27931884E-03 6.64306396E-
 06 3
 -6.12806624E-09 2.11265971E-12 2.91222592E+04 2.05193346E+00
 2.99687009E+04 4
 H2O L 5/89H 2 O 1 0 0G 200.000 6000.00 1000.00
 1
 0.26770389E+01 0.29731816E-02-0.77376889E-06 0.94433514E-10-0.42689991E-
 14 2
 -0.29885894E+05 0.68825500E+01 0.41986352E+01-0.20364017E-02 0.65203416E-
 05 3
 -0.54879269E-08 0.17719680E-11-0.30293726E+05-0.84900901E+00-
 0.29084817E+05 4
 OH IU3/03O 1 H 1 0 0G 200.000 6000.00 1000.00
 1
 2.83853033E+00 1.10741289E-03-2.94000209E-07 4.20698729E-11-2.42289890E-
 15 2
 3.69780808E+03 5.84494652E+00 3.99198424E+00-2.40106655E-03 4.61664033E-
 06 3
 -3.87916306E-09 1.36319502E-12 3.36889836E+03-1.03998477E-01
 4.48613328E+03 4
 OH* 1212860 1H 1 G 0300.00 5000.00 1000.00
 1
 0.02882730E+02 0.10139743E-02-0.02276877E-05 0.02174683E-09-0.05126305E-
 14 2
 5.02650000E+04 0.05595712E+02 0.03637266E+02 0.01850910E-02-0.16761646E-
 05 3
 0.02387202E-07-0.08431442E-11 5.00213000E+04 0.13588605E+01
 4
 H2O2 T 8/03H 2O 2 0 0G 200.000 6000.00 1000.00
 1
 4.57977305E+00 4.05326003E-03-1.29844730E-06 1.98211400E-10-1.13968792E-
 14 2
 -1.80071775E+04 6.64970694E-01 4.31515149E+00-8.47390622E-04 1.76404323E-
 05 3
 -2.26762944E-08 9.08950158E-12-1.77067437E+04 3.27373319E+00-
 1.63425145E+04 4
 HO2 T 1/09H 1O 2 0 0G 200.000 5000.00 1000.00
 1
 4.17228741E+00 1.88117627E-03-3.46277286E-07 1.94657549E-11 1.76256905E-
 16 2
 3.10206839E+01 2.95767672E+00 4.30179807E+00-4.74912097E-03 2.11582905E-
 05 3

-2.42763914E-08 9.29225225E-12 2.64018485E+02 3.71666220E+00
 1.47886045E+03 4
 CO RUS 79C 10 1 0 0G 200.000 6000.00 1000.00
 1
 0.30484859E+01 0.13517281E-02-0.48579405E-06 0.78853644E-10-0.46980746E-
 14 2
 -0.14266117E+05 0.60170977E+01 0.35795335E+01-0.61035369E-03 0.10168143E-
 05 3
 0.90700586E-09-0.90442449E-12-0.14344086E+05 0.35084093E+01-
 0.13293628E+05 4
 CO2 L 7/88C 10 2 0 0G 200.000 6000.00 1000.00
 1
 0.46365111E+01 0.27414569E-02-0.99589759E-06 0.16038666E-09-0.91619857E-
 14 2
 -0.49024904E+05-0.19348955E+01 0.23568130E+01 0.89841299E-02-0.71220632E-
 05 3
 0.24573008E-08-0.14288548E-12-0.48371971E+05 0.99009035E+01-
 0.47328105E+05 4
 HOCO T05/06H 1 C 1 O 2 0 G 200.000 6000.00
 1000.00 1
 5.39206152E+00 4.11221455E-03-1.48194900E-06 2.39875460E-10-1.43903104E-
 14 2
 -2.38606717E+04-2.23529091E+00 2.92207919E+00 7.62453859E-03 3.29884437E-
 06 3
 -1.07135205E-08 5.11587057E-12-2.30281524E+04 1.12925886E+01-
 2.18076591E+04 4
 CH4 G 8/99C 1 H 4 0 0 G 200.000 6000.00 1000.00
 1
 1.65326226E+00 1.00263099E-02-3.31661238E-06 5.36483138E-10-3.14696758E-
 14 2
 -1.00095936E+04 9.90506283E+00 5.14911468E+00-1.36622009E-02 4.91453921E-
 05 3
 -4.84246767E-08 1.66603441E-11-1.02465983E+04-4.63848842E+00-
 8.97226656E+03 4
 CH3 IU0702C 1 H 3 0 0 G 200.000 6000.00 1000.00
 1
 0.29781206E+01 0.57978520E-02-0.19755800E-05 0.30729790E-09-0.17917416E-
 13 2
 0.16509513E+05 0.47224799E+01 0.36571797E+01 0.21265979E-02 0.54583883E-
 05 3
 -0.66181003E-08 0.24657074E-11 0.16422716E+05 0.16735354E+01
 0.17643935E+05 4
 CH2 IU3/03C 1 H 2 0 0 G 200.000 6000.00 1000.00
 1
 3.14631886E+00 3.03671259E-03-9.96474439E-07 1.50483580E-10-8.57335515E-
 15 2
 4.60412605E+04 4.72341711E+00 3.71757846E+00 1.27391260E-03 2.17347251E-
 06 3
 -3.48858500E-09 1.65208866E-12 4.58723866E+04 1.75297945E+00
 4.70504920E+04 4
 CH2(S) IU6/03C 1 H 2 0 0 G 200.000 6000.00 1000.00
 1
 3.13501686E+00 2.89593926E-03-8.16668090E-07 1.13572697E-10-6.36262835E-
 15 2
 5.05040504E+04 4.06030621E+00 4.19331325E+00-2.33105184E-03 8.15676451E-
 06 3
 -6.62985981E-09 1.93233199E-12 5.03662246E+04-7.46734310E-01
 5.15727280E+04 4

C L 7/88C 1 0 0 0G 200.000 6000.00 1000.00
1
0.26055830E+01-0.19593434E-03 0.10673722E-06-0.16423940E-10 0.81870580E-
15 2
0.85411742E+05 0.41923868E+01 0.25542395E+01-0.32153772E-03 0.73379223E-
06 3
-0.73223487E-09 0.26652144E-12 0.85442681E+05 0.45313085E+01
0.86195097E+05 4
CH IU3/03C 1 H 1 0 0 G 200.000 6000.00 1000.00
1
0.25209369E+01 0.17653639E-02-0.46147660E-06 0.59289675E-10-0.33474501E-
14 2
0.70946769E+05 0.74051829E+01 0.34897583E+01 0.32432160E-03-0.16899751E-
05 3
0.31628420E-08-0.14061803E-11 0.70612646E+05 0.20842841E+01
0.71658188E+05 4
CH* 073003C 1H 1 G 0300.00 5000.00 1000.00
1
0.02196223E+02 0.02340381E-01-0.07058201E-05 0.09007582E-09-0.03855040E-
13 2
0.10419559E+06 0.09178373E+02 0.03200202E+02 0.02072875E-01-0.05134431E-
04 3
0.05733890E-07-0.01955533E-10 0.10393714E+06 0.03331587E+02
4
CH3O2H A 7/05C 1 H 4 O 2 0 G 200.000 6000.00 1000.00
1
7.76538058E+00 8.61499712E-03-2.98006935E-06 4.68638071E-10-2.75339255E-
14 2
-1.82979984E+04-1.43992663E+01 2.90540897E+00 1.74994735E-02 5.28243630E-
06 3
-2.52827275E-08 1.34368212E-11-1.68894632E+04 1.13741987E+01-
1.52423685E+04 4
CH3O2 H 3C 1O 2 0G 300.000 5000.000
1374.000 11
6.47970487E+00 7.44401080E-03-2.52348555E-06 3.89577296E-10-2.25182399E-
14 2
-1.56285441E+03-8.19477074E+00 1.97339205E+00 1.53542340E-02-6.37314891E-
06 3
3.19930565E-10 2.82193915E-13 2.54278835E+02 1.69194215E+01
4
CH2O2H 9/ 1/12 C 1H 3O 2 0G 300.000 5000.000
1410.000 21
9.24697852E+00 4.60845541E-03-1.53501472E-06 2.34434830E-10-1.34573106E-
14 2
4.11529953E+03-2.11503248E+01 2.88976454E+00 2.09465776E-02-1.75190772E-
05 3
7.27819787E-09-1.18912344E-12 6.12390620E+03 1.23802076E+01
4
CH3OH T06/02C 1H 4 O 1 0 G 200.000 6000.00 1000.00
1
3.52726795E+00 1.03178783E-02-3.62892944E-06 5.77448016E-10-3.42182632E-
14 2
-2.60028834E+04 5.16758693E+00 5.65851051E+00-1.62983419E-02 6.91938156E-
05 3
-7.58372926E-08 2.80427550E-11-2.56119736E+04-8.97330508E-01-
2.41746056E+04 4
CH3O IU1/03C 1 H 3 O 1 0 G 200.000 6000.00 1000.00
1

4.75779238E+00 7.44142474E-03-2.69705176E-06 4.38090504E-10-2.63537098E-
 14 2
 3.78111940E+02-1.96680028E+00 3.71180502E+00-2.80463306E-03 3.76550971E-
 05 3
 -4.73072089E-08 1.86588420E-11 1.29569760E+03 6.57240864E+00
 2.52571660E+03 4
 CH2OH IU2/03C 1 H 3 O 1 0 G 200.000 6000.00
 1000.00 1
 5.09314370E+00 5.94761260E-03-2.06497460E-06 3.23008173E-10-1.88125902E-
 14 2
 -4.03409640E+03-1.84691493E+00 4.47834367E+00-1.35070310E-03 2.78484980E-
 05 3
 -3.64869060E-08 1.47907450E-11-3.50072890E+03 3.30913500E+00-
 2.04462770E+03 4
 CH2O T 5/11H 2C 1O 1 0G 200.000 6000.00 1000.00
 1
 3.16952665E+00 6.19320560E-03-2.25056366E-06 3.65975660E-10-2.20149458E-
 14 2
 -1.45486831E+04 6.04207898E+00 4.79372312E+00-9.90833322E-03 3.73219990E-
 05 3
 -3.79285237E-08 1.31772641E-11-1.43791953E+04 6.02798058E-01-
 1.31293365E+04 4
 HCO T 5/03C 1 H 1 O 1 0 G 200.000 6000.00 1000.00
 1
 3.92001542E+00 2.52279324E-03-6.71004164E-07 1.05615948E-10-7.43798261E-
 15 2
 3.65342928E+03 3.58077056E+00 4.23754610E+00-3.32075257E-03 1.40030264E-
 05 3
 -1.34239995E-08 4.37416208E-12 3.87241185E+03 3.30834869E+00
 5.08749163E+03 4
 HCOH MAR94 C 1H 2O 1 0G 300. 5000. 1398.
 1
 9.18749272E+00 1.52011152E-03-6.27603516E-07 1.09727989E-10-6.89655128E-
 15 2
 7.81364593E+03-2.73434214E+01-2.82157421E+00 3.57331702E-02-3.80861580E-
 05 3
 1.86205951E-08-3.45957838E-12 1.12956672E+04 3.48487757E+01
 4
 HO2CHO 6/26/95 THERMC 1H 2O 3 0G 300.000 5000.000 1378.00
 21
 9.87503878E+00 4.64663708E-03-1.67230522E-06 2.68624413E-10-1.59595232E-
 14 2
 -3.80502496E+04-2.24939155E+01 2.42464726E+00 2.19706380E-02-1.68705546E-
 05 3
 6.25612194E-09-9.11645843E-13-3.54828006E+04 1.75027796E+01
 4
 HOCH2O2H 9/ 1/12 C 1H 4O 3 0G 300.000 5000.000
 1398.000 21
 1.24531886E+01 7.18221110E-03-2.47029548E-06 3.85611737E-10-2.24774193E-
 14 2
 -4.24862928E+04-3.58745197E+01 5.35189713E-01 3.73266553E-02-3.15299511E-
 05 3
 1.30352583E-08-2.11473264E-12-3.86609415E+04 2.71776082E+01
 4
 HOCH2O2 9/ 1/12 C 1H 3O 3 0G 300.000 5000.000
 1377.000 21
 1.16406115E+01 5.72826040E-03-2.05362036E-06 3.29070695E-10-1.95188360E-
 14 2

-2.53505769E+04-3.07332064E+01 2.82068616E+00 2.47857094E-02-1.66186399E-
 05 3
 4.79633095E-09-4.28087766E-13-2.22077036E+04 1.70599803E+01
 4
 OCH2O2H 7/21/14 THERMC 1H 30 3 0G 300.000 5000.000
 1418.000 31!UPDATED 0722
 1.29622491E+01 4.21948855E-03-1.54275194E-06 2.50413077E-10-1.49855537E-
 14 2
 -1.81326406E+04-3.87016356E+01 4.46349361E-01 3.63049606E-02-3.26130978E-
 05 3
 1.37050551E-08-2.20872791E-12-1.41972598E+04 2.72960376E+01
 4
 HOCH2O 2/16/99 THERMC 1H 30 2 0G 300.000 5000.000
 1452.000 11
 6.39521515E+00 7.43673043E-03-2.50422354E-06 3.84879712E-10-2.21778689E-
 14 2
 -2.41108840E+04-6.63865583E+00 4.11183145E+00 7.53850697E-03 3.77337370E-
 06 3
 -5.38746005E-09 1.45615887E-12-2.28023001E+04 7.46807254E+00
 4
 O2CHO 6/26/95 THERMC 1H 10 3 0G 300.000 5000.000 1368.00
 11
 7.24075139E+00 4.63312951E-03-1.63693995E-06 2.59706693E-10-1.52964699E-
 14 2
 -1.87027618E+04-6.49547212E+00 3.96059309E+00 1.06002279E-02-5.25713351E-
 06 3
 1.01716726E-09-2.87487602E-14-1.73599383E+04 1.17807483E+01
 4
 HOCHO L 8/88H 2C 10 2 0G 200.000 6000.00 1000.00
 1
 0.46138316E+01 0.64496364E-02-0.22908251E-05 0.36716047E-09-0.21873675E-
 13 2
 -0.47514850E+05 0.84788383E+00 0.38983616E+01-0.35587795E-02 0.35520538E-
 04 3
 -0.43849959E-07 0.17107769E-10-0.46770609E+05 0.73495397E+01-
 0.45531246E+05 4
 OCHO ATCT/AC 1 O 2 H 1 0 G 200.000 6000.000 1000.00
 1
 4.14394211E+00 5.59738818E-03-1.99794019E-06 3.16179193E-10-1.85614483E-
 14 2
 -1.72459887E+04 5.07778617E+00 4.68825921E+00-4.14871834E-03 2.55066010E-
 05 3
 -2.84473900E-08 1.04422559E-11-1.69867041E+04 4.28426480E+00-
 1.55992356E+04 4
 C2H6 G 8/88C 2H 6 0 0G 200.000 6000.00 1000.00
 1
 4.04666411E+00 1.53538802E-02-5.47039485E-06 8.77826544E-10-5.23167531E-
 14 2
 -1.24473499E+04-9.68698313E-01 4.29142572E+00-5.50154901E-03 5.99438458E-
 05 3
 -7.08466469E-08 2.68685836E-11-1.15222056E+04 2.66678994E+00-
 1.00849652E+04 4
 C2H5 8/ 4/ 4 THERMC 2H 5 0 0G 300.000 5000.000
 1387.000 11
 5.88784390E+00 1.03076793E-02-3.46844396E-06 5.32499257E-10-3.06512651E-
 14 2
 1.15065499E+04-8.49651771E+00 1.32730217E+00 1.76656753E-02-6.14926558E-
 06 3

-3.01143466E-10 4.38617775E-13 1.34284028E+04 1.71789216E+01
 4
 C2H5O2H 9/ 1/12 C 2H 60 2 0G 300.000 5000.000
 1390.000 31
 1.04823538E+01 1.34779879E-02-4.62179078E-06 7.18618519E-10-4.17307436E-
 14 2
 -2.46578171E+04-2.84294243E+01 1.83755328E+00 3.38053586E-02-2.37548140E-
 05 3
 9.31974865E-09-1.58003428E-12-2.15814086E+04 1.80977584E+01
 4
 C2H5O2 9/ 1/12 C 2H 50 2 0G 300.000 5000.000
 1389.000 21
 9.50282570E+00 1.20429839E-02-4.09491581E-06 6.33049241E-10-3.66133788E-
 14 2
 -7.37069391E+03-2.21717130E+01 3.90351912E+00 2.22599212E-02-1.01610079E-
 05 3
 1.71709751E-09 1.88166738E-14-5.09654081E+03 8.98722750E+00
 4
 C2H4 8/12/15 C 2H 4 0 0G 300.000 5000.000
 1392.000 01
 5.07061289E+00 9.11140768E-03-3.10506692E-06 4.80733851E-10-2.78321396E-
 14 2
 3.66391217E+03-6.64501414E+00 4.81118223E-01 1.83778060E-02-9.99633565E-
 06 3
 2.73211039E-09-3.01837289E-13 5.44386648E+03 1.85867157E+01
 4
 C2H3 8/12/15 C 2H 3 0 0G 300.000 5000.000
 1400.000 01
 4.99675415E+00 6.55838271E-03-2.20921909E-06 3.39300272E-10-1.95316926E-
 14 2
 3.34604382E+04-3.01451097E+00 1.25545094E+00 1.57481597E-02-1.12218328E-
 05 3
 4.50915682E-09-7.74861577E-13 3.47435574E+04 1.69664043E+01
 4
 C2H2 G 1/91C 2 H 2 0 0 G 200.000 6000.00 1000.00
 1
 4.65878489E+00 4.88396667E-03-1.60828888E-06 2.46974544E-10-1.38605959E-
 14 2
 2.57594042E+04-3.99838194E+00 8.08679682E-01 2.33615762E-02-3.55172234E-
 05 3
 2.80152958E-08-8.50075165E-12 2.64289808E+04 1.39396761E+01
 2.74459950E+04 4
 C2H T 5/10C 2 H 1 0 0 G 200.000 6000.00 1000.00
 1
 3.66270248E+00 3.82492252E-03-1.36632500E-06 2.13455040E-10-1.23216848E-
 14 2
 6.71683790E+04 3.92205792E+00 2.89867676E+00 1.32988489E-02-2.80733327E-
 05 3
 2.89484755E-08-1.07502351E-11 6.70616050E+04 6.18547632E+00
 6.83210436E+04 4
 H2CC L12/89H 2C 2 0 0G 200.000 6000.000
 1000.000 1
 0.42780340E+01 0.47562804E-02-0.16301009E-05 0.25462806E-09-0.14886379E-
 13 2
 0.48316688E+05 0.64023701E+00 0.32815483E+01 0.69764791E-02-0.23855244E-
 05 3
 -0.12104432E-08 0.98189545E-12 0.48621794E+05 0.59203910E+01
 0.49887266E+05 4

C2H5OH 8/12/15 C 2H 60 1 0G 300.000 5000.000
1402.000 21
8.14483865E+00 1.28314052E-02-4.29052743E-06 6.55971721E-10-3.76506611E-
14 2
-3.24005526E+04-1.86241126E+01 2.15805861E-01 2.95228396E-02-1.68271048E-
05 3
4.49484797E-09-4.02451543E-13-2.94851823E+04 2.45725052E+01
4
C2H5O 8/12/15 C 2H 50 1 0G 300.000 5000.000
1467.000 11
8.19120635E+00 1.10391986E-02-3.75270536E-06 5.80275784E-10-3.35735146E-
14 2
-5.66847208E+03-1.90131344E+01 2.90353584E+00 1.77256708E-02-2.69624757E-
06 3
-3.45830533E-09 1.25224784E-12-3.28930290E+03 1.13545591E+01
4
PC2H4OH 8/12/15 C 2H 50 1 0G 300.000 5000.000
1395.000 21
8.06750150E+00 1.06143554E-02-3.57999360E-06 5.50363760E-10-3.17051769E-
14 2
-6.92747939E+03-1.53833428E+01 2.59479867E+00 2.27100669E-02-1.39473846E-
05 3
4.70095591E-09-6.90044236E-13-4.91486975E+03 1.43240718E+01
4
SC2H4OH 8/12/15 C 2H 50 1 0G 300.000 5000.000
1385.000 21
8.15007136E+00 1.02549305E-02-3.40137764E-06 5.17509965E-10-2.96128942E-
14 2
-1.05014386E+04-1.73134615E+01 1.46281093E+00 2.39193995E-02-1.30667185E-
05 3
3.10615465E-09-1.85896007E-13-8.00790323E+03 1.92547092E+01
4
O2C2H4OH 9/ 1/12 THERMC 2H 50 3 0G 300.000 5000.000
1506.000 41
1.27503881E+01 1.11514325E-02-3.83473891E-06 5.98155829E-10-3.48372108E-
14 2
-2.52770876E+04-3.54317608E+01 7.04009800E+00 1.59564166E-02 2.21097416E-
06 3
-7.05197355E-09 2.08266026E-12-2.24524432E+04-1.75361758E+00
4
C2H4O2H 9/ 1/12 C 2H 50 2 0G 300.000 5000.000
1389.000 31
1.00590614E+01 1.13378955E-02-3.89403387E-06 6.06090687E-10-3.52212353E-
14 2
4.24048653E+02-2.32086536E+01 2.75788364E+00 2.88271987E-02-2.08302264E-
05 3
8.47401397E-09-1.48617610E-12 3.00153893E+03 1.59921711E+01
4
C2H4O1-2 L 8/88C 2 H 4 O 1 0 G 200.000 6000.00 1000.00
1
0.54887641E+01 0.12046190E-01-0.43336931E-05 0.70028311E-09-0.41949088E-
13 2
-0.91804251E+04-0.70799605E+01 0.37590532E+01-0.94412180E-02 0.80309721E-
04 3
-0.10080788E-06 0.40039921E-10-0.75608143E+04 0.78497475E+01-
0.63304657E+04 4
C2H3O1-2 A 1/05C 2 H 3 O 1 0 G 200.000 6000.00 1000.00
1

5.60158035E+00 9.17613962E-03-3.28028902E-06 5.27903888E-10-3.15362241E-
 14 2
 1.71446252E+04-5.47228512E+00 3.58349017E+00-6.02275805E-03 6.32426867E-
 05 3
 -8.18540707E-08 3.30444505E-11 1.85681353E+04 9.59725926E+00
 1.97814471E+04 4
 CH3CHO L 8/88C 2 H 4 O 1 0 G 200.000 6000.00 1000.00
 1
 0.54041108E+01 0.11723059E-01-0.42263137E-05 0.68372451E-09-0.40984863E-
 13 2
 -0.22593122E+05-0.34807917E+01 0.47294595E+01-0.31932858E-02 0.47534921E-
 04 3
 -0.57458611E-07 0.21931112E-10-0.21572878E+05 0.41030159E+01-
 0.19987949E+05 4
 CH3CO IU2/03C 2 H 3 O 1 0 G 200.000 6000.00 1000.00
 1
 0.53137165E+01 0.91737793E-02-0.33220386E-05 0.53947456E-09-0.32452368E-
 13 2
 -0.36450414E+04-0.16757558E+01 0.40358705E+01 0.87729487E-03 0.30710010E-
 04 3
 -0.39247565E-07 0.15296869E-10-0.26820738E+04 0.78617682E+01-
 0.12388039E+04 4
 CH2CHO T03/10C 2 H 3 O 1 0 G 200.000 6000.00 1000.00
 1
 6.53928338E+00 7.80238629E-03-2.76413612E-06 4.42098906E-10-2.62954290E-
 14 2
 -1.18858659E+03-8.72091393E+00 2.79502600E+00 1.01099472E-02 1.61750645E-
 05 3
 -3.10303145E-08 1.39436139E-11 1.62944975E+02 1.23646657E+01
 1.53380440E+03 4
 O2CH2CHO BOZ_03C 2H 3O 3 OG 300.000 5000.000
 1393.000 01
 1.11807543E+01 9.14479256E-03-3.15089833E-06 4.91944238E-10-2.86639180E-
 14 2
 -1.55790331E+04-2.87892740E+01-1.29465843E+00 4.44936393E-02-4.26577074E-
 05 3
 2.07391950E-08-3.96828771E-12-1.18275628E+04 3.60778797E+01
 4
 HO2CH2CO BOZ_03C 2H 3O 3 OG 300.000 5000.000
 1386.000 01
 1.04146322E+01 1.12680116E-02-5.17494839E-06 1.00333285E-09-6.68165911E-
 14 2
 -1.40955672E+04-2.27894400E+01 2.22681686E+00 3.56781380E-02-3.26401909E-
 05 3
 1.47651988E-08-2.64794380E-12-1.18735095E+04 1.91581197E+01
 4
 C2H3OH 2/ 3/ 9 THERMC 2H 4O 1 OG 300.000 5000.000
 1410.000 11
 8.32598158E+00 8.03387281E-03-2.63928405E-06 3.98410726E-10-2.26551155E-
 14 2
 -1.83221436E+04-2.02080305E+01-1.27972260E-01 3.38506073E-02-3.30644935E-
 05 3
 1.64858739E-08-3.19935455E-12-1.59914544E+04 2.30438601E+01
 4
 C2H2OH H 3C 2O 1 OG 300.000 5000.000
 1401.000 11
 8.20268447E+00 5.92989165E-03-1.99194448E-06 3.05794341E-10-1.76114732E-
 14 2

1.24881328E+04-1.89670436E+01 6.41642616E-01 2.61903633E-02-2.30385370E-
 05 3
 1.02804704E-08-1.81971416E-12 1.48276951E+04 2.06750999E+01
 4
 CH2CO H 2C 2O 1 OG 300.00 5000.00 1000.00
 1!CHONGWEN 240615
 5.35869367E+00 6.95641586E-03-2.64802637E-06 4.65067592E-10-3.08641820E-
 14 2
 -7.90294013E+03-3.98525731E+00 1.81422511E+00 1.99008590E-02-2.21416008E-
 05 3
 1.45028521E-08-3.98877068E-12-7.05394926E+03 1.36079359E+01
 4
 HCCO T 4/09H 1 C 2 O 1 0 G 200.000 6000.00 1000.00
 1
 5.91479333E+00 3.71408730E-03-1.30137010E-06 2.06473345E-10-1.21476759E-
 14 2
 1.93596301E+04-5.50567269E+00 1.87607969E+00 2.21205418E-02-3.58869325E-
 05 3
 3.05402541E-08-1.01281069E-11 2.01633840E+04 1.36968290E+01
 2.14444387E+04 4
 HCCOH T12/09C 2 H 2 O 1 0 G 200.000 6000.00 1000.00
 1
 6.37509678E+00 5.49429011E-03-1.88136576E-06 2.93803536E-10-1.71771901E-
 14 2
 8.93277676E+03-8.24498007E+00 2.05541154E+00 2.52003372E-02-3.80821654E-
 05 3
 3.09890632E-08-9.89799902E-12 9.76872113E+03 1.22271534E+01
 1.12217316E+04 4
 CH3CO3H 6/26/95 THERMC 2H 4O 3 OG 300.000 5000.000
 1391.000 31
 1.25060485E+01 9.47789695E-03-3.30402246E-06 5.19630793E-10-3.04233568E-
 14 2
 -4.59856703E+04-3.79195947E+01 2.24135876E+00 3.37963514E-02-2.53887482E-
 05 3
 9.67583587E-09-1.49266157E-12-4.24677831E+04 1.70668133E+01
 4
 CH3CO3 4/ 3/ 0 THERMC 2H 3O 3 OG 300.000 5000.000
 1391.000 21
 1.12522498E+01 8.33652672E-03-2.89014530E-06 4.52781734E-10-2.64354456E-
 14 2
 -2.60238584E+04-2.96370457E+01 3.60373432E+00 2.70080341E-02-2.08293438E-
 05 3
 8.50541104E-09-1.43846110E-12-2.34205171E+04 1.12014914E+01
 4
 CH3CO2 2/14/95 THERMC 2H 3O 2 OG 300.000 5000.000
 1395.000 11
 8.54059736E+00 8.32951214E-03-2.84722010E-06 4.41927196E-10-2.56373394E-
 14 2
 -2.97290678E+04-2.03883545E+01 1.37440768E+00 2.49115604E-02-1.74308894E-
 05 3
 6.24799508E-09-9.09516835E-13-2.72330150E+04 1.81405454E+01
 4
 CH3OCH3 2/11/14 THERMC 2H 6O 1 OG 300.000 5000.000
 1999.000 21
 6.03232751E+00 1.56155270E-02-5.50761030E-06 8.75666140E-10-5.17180562E-
 14 2
 -2.52690354E+04-8.25885183E+00 2.05597390E+00 2.07019456E-02-5.00382376E-
 06 3

-1.62279885E-09 6.84330155E-13-2.35494445E+04 1.45029944E+01
 4
 CH3OCH2 2/11/14 THERMC 2H 50 1 0G 300.000 5000.000
 1395.000 11
 6.62621974E+00 1.22219496E-02-4.12416696E-06 6.34127512E-10-3.65317390E-
 14 2
 -3.33965890E+03-8.95305753E+00 1.58874948E+00 2.24414123E-02-1.19434933E-
 05 3
 3.37160213E-09-4.15077249E-13-1.37208255E+03 1.87548958E+01
 4
 CH3OCH2O2H 2/12/14 THERMC 2H 60 3 0G 300.000 5000.000
 1404.000 31
 1.28159161E+01 1.34818095E-02-4.50397729E-06 6.88229286E-10-3.94883680E-
 14 2
 -4.06745921E+04-3.78047802E+01 1.05786981E+00 4.36787095E-02-3.46383899E-
 05 3
 1.44808830E-08-2.46100643E-12-3.68851076E+04 2.43391936E+01
 4
 CH3OCH2O2 2/12/14 THERMC 2H 50 3 0G 300.000 5000.000
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 14 2
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 05 3
 5.76033887E-09-6.16081571E-13-2.04433218E+04 1.39429608E+01
 4
 CH2OCH2O2H 2/12/14 THERMC 2H 50 3 0G 300.000 5000.000
 1418.000 21
 1.23892901E+01 1.11758961E-02-3.59249095E-06 5.34196366E-10-3.00536541E-
 14 2
 -1.80551598E+04-3.29576862E+01 1.62245477E-01 4.76101093E-02-4.52046954E-
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 2.18379311E-08-4.11295947E-12-1.46498100E+04 2.98253164E+01
 4
 O2CH2OCH2O2H 2/12/14 ERMC 2H 50 5 0G 300.000 5000.000
 1433.000 31
 1.77378326E+01 1.13589899E-02-3.67382539E-06 5.49255712E-10-3.10405899E-
 14 2
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 05 3
 2.19792134E-08-3.86106979E-12-3.37824638E+04 2.30683371E+01
 4
 HO2CH2OCHO 2/12/14 THERMC 2H 40 4 0G 300.000 5000.000
 1386.000 31
 1.57136128E+01 9.64430166E-03-3.44136025E-06 5.49722196E-10-3.25360322E-
 14 2
 -6.29409094E+04-5.29505242E+01 1.21909586E+00 4.28858235E-02-3.17634222E-
 05 3
 1.11542676E-08-1.49753153E-12-5.79287926E+04 2.49759193E+01
 4
 OCH2OCHO 5/29/14 THERMC 2H 30 3 0G 300.000 5000.000
 1523.000 21
 1.24013200E+01 7.83738243E-03-2.82992688E-06 4.55558739E-10-2.71061389E-
 14 2
 -4.68453470E+04-3.78084549E+01 1.89539692E+00 2.74118545E-02-1.36476090E-
 05 3
 1.26325603E-09 5.17970476E-13-4.27879440E+04 2.02333278E+01
 4

HOCH2OCO 5/29/14 THERMC 2H 30 3 0G 300.000 5000.000
 1443.000 11
 1.11498410E+01 9.34736520E-03-3.35541548E-06 5.38037115E-10-3.19260183E-
 14 2
 -4.75012119E+04-2.95983867E+01 5.95255071E+00 8.42196282E-03 1.36741678E-
 05 3
 -1.46786275E-08 3.84143533E-12-4.44470269E+04 2.85657217E+00
 4
 CH3OCH2O 5/15/14 THERMC 2H 50 2 0G 300.000 5000.000
 1523.000 31
 9.81288609E+00 1.21313106E-02-4.30285768E-06 6.84443177E-10-4.03862658E-
 14 2
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 05 3
 -1.40497059E-08 3.54625624E-12-2.22825214E+04 1.93588846E+00
 4
 CH3OCHO T 6/08C 2 H 4 O 2 0 G 200.000 6000.00 1000.00
 1
 6.33360880E+00 1.34851485E-02-4.84305805E-06 7.81719241E-10-4.67917447E-
 14 2
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 05 3
 -8.29932227E-08 3.13522917E-11-4.55713267E+04 7.50341113E-01-
 4.37330508E+04 4
 CH3OCO 5/ 8/ 3 THERMC 2H 30 2 0G 300.000 5000.000
 1601.000 21
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 14 2
 -2.36015721E+04-2.36353471E+01 4.16215406E+00 1.38037511E-02-3.08486109E-
 07 3
 -4.56430814E-09 1.46909632E-12-2.10130301E+04 8.64301044E+00
 4
 CH2OCHO 4/15/ 8 THERMC 2H 30 2 0G 300.000 5000.000
 1442.000 21
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 06 3
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 4
 C3H8 8/12/15 C 3H 8 0 0G 300.000 5000.000
 1390.000 21
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 14 2
 -1.75762439E+04-2.77418510E+01 2.40878470E-01 3.39548599E-02-1.60930874E-
 05 3
 2.83480628E-09 2.78195172E-14-1.40362853E+04 2.16500800E+01
 4
 IC3H7 8/12/15 C 3H 7 0 0G 300.000 5000.000
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 07 3
 -6.37322722E-09 2.00284148E-12 9.03496678E+03 1.72590353E+01
 4
 NC3H7 8/12/15 C 3H 7 0 0G 300.000 5000.000
 1391.000 21

8.51726970E+00 1.53591153E-02-5.22415895E-06 8.07838904E-10-4.67326294E-
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 NC3H7O2H 8/12/15 C 3H 80 2 OG 300.000 5000.000
 1392.000 41
 1.42246236E+01 1.74340964E-02-5.97063522E-06 9.27753851E-10-5.38585168E-
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 4
 NC3H7O2 8/12/15 C 3H 70 2 OG 300.000 5000.000
 1390.000 31
 1.32753283E+01 1.61303126E-02-5.52348308E-06 8.58197168E-10-4.98172586E-
 14 2
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 4
 IC3H7O2H 8/12/15 C 3H 80 2 OG 300.000 5000.000
 1405.000 41
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 1.31405381E-08-2.06922904E-12-2.63458844E+04 1.77669753E+01
 4
 IC3H7O2 8/12/15 C 3H 70 2 OG 300.000 5000.000
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 05 3
 1.08614807E-08-1.66312005E-12-9.67013161E+03 1.44731300E+01
 4
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 1386.000 21
 1.15279177E+01 1.53775991E-02-5.23946272E-06 8.11382512E-10-4.69927603E-
 14 2
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 4
 IC3H7O 8/12/15 C 3H 70 1 OG 300.000 5000.000
 1527.000 21
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 4.71536901E-09-2.64704937E-13-8.28791395E+03 1.33112436E+01
 4
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 14 2

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 4
 C3H6OOH1-3 9/1/12 C 3H 70 2 0G 300.000 5000.000
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 -3.65650518E+03-4.21532559E+01 1.74271107E+00 4.53733504E-02-3.57580373E-
 05 3
 1.48540053E-08-2.49981756E-12 2.32580844E+02 2.20973041E+01
 4
 C3H6OOH2-1 9/ 1/12 C 3H 70 2 0G 300.000 5000.000
 1393.000 41
 1.36645362E+01 1.54329764E-02-5.29285952E-06 8.23001262E-10-4.77931121E-
 14 2
 -5.58295862E+03-4.28758364E+01 2.38465746E+00 4.42928555E-02-3.50977087E-
 05 3
 1.53695144E-08-2.81167824E-12-1.80979612E+03 1.69923285E+01
 4
 C3H6OOH1-2O2 9/1/12 C 3H 70 4 0G 300.000 5000.000
 1404.000 51
 1.91044980E+01 1.44076100E-02-4.72127814E-06 7.12631642E-10-4.05578490E-
 14 2
 -2.50270510E+04-6.63747978E+01 3.99085043E+00 5.31865338E-02-4.28597948E-
 05 3
 1.77187019E-08-2.92768695E-12-2.02143526E+04 1.34150719E+01
 4
 C3H6OOH1-3O2 9/ 1/12 C 3H 70 4 0G 300.000 5000.000
 1416.000 51
 1.81661664E+01 1.47644887E-02-4.74842743E-06 7.06972467E-10-3.98305587E-
 14 2
 -2.26256376E+04-5.93719393E+01 5.56933350E+00 4.68523421E-02-3.58917784E-
 05 3
 1.43314525E-08-2.29776083E-12-1.86065694E+04 7.18655005E+00
 4
 C3H6OOH2-1O2 9/1/12 C 3H 70 4 0G 300.000 5000.000
 1404.000 51
 1.91044980E+01 1.44076100E-02-4.72127814E-06 7.12631642E-10-4.05578490E-
 14 2
 -2.50270510E+04-6.63747978E+01 3.99085043E+00 5.31865338E-02-4.28597948E-
 05 3
 1.77187019E-08-2.92768695E-12-2.02143526E+04 1.34150719E+01
 4
 C3KET12 10/17/12 C 3H 60 3 0G 300.000 5000.000
 1385.000 41
 1.70187760E+01 1.32097361E-02-4.67054741E-06 7.41411770E-10-4.36869787E-
 14 2
 -4.23572589E+04-5.92615939E+01 1.03882879E+00 5.34180080E-02-4.47684141E-
 05 3
 1.94651680E-08-3.45055244E-12-3.70308881E+04 2.56511209E+01
 4
 C3KET13 10/17/12 C 3H 60 3 0G 300.000 5000.000
 1508.000 41
 1.73612692E+01 1.32330813E-02-4.75332110E-06 7.62529227E-10-4.52613717E-
 14 2
 -4.06248060E+04-6.17768199E+01 4.74956819E+00 3.14080991E-02-6.83838427E-
 06 3

-5.67123901E-09 2.27686972E-12-3.51924570E+04 9.83753744E+00
 4
 C3H51-2,3OOH C 3H 70 4 0G 300.000 5000.000
 1386.000 61 !8/26/3THRM
 2.12378169E+01 1.39519596E-02-4.94539222E-06 7.86381389E-10-4.63925564E-
 14 2
 -1.92864584E+04-7.69636561E+01 2.55619708E+00 6.13504487E-02-5.23205391E-
 05 3
 2.28208029E-08-4.02231508E-12-1.31353414E+04 2.21043799E+01
 4
 C3H52-1,3OOH 8/26/3THRMC 3H 70 4 0G 300.000 5000.000
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 14 2
 -1.80085066E+04-7.22688262E+01 4.12253742E+00 5.19553611E-02-3.83733727E-
 05 3
 1.45851637E-08-2.29820536E-12-1.22759164E+04 1.48367359E+01
 4
 C3H501-2OOH-3 10/13THER C 3H 60 3 0G 300.000 5000.000
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 14 2
 -2.77269333E+04-5.51895464E+01-3.25001215E+00 6.65787151E-02-6.18859778E-
 05 3
 2.84638649E-08-5.08511634E-12-2.22371240E+04 4.30381280E+01
 4
 C3H501-3OOH-2 10/13 THERC 3H 60 3 0G 300.000 5000.000
 1434.000 21
 1.44493479E+01 1.36372560E-02-4.25836513E-06 6.20006211E-10-3.43451580E-
 14 2
 -2.77372360E+04-5.06099103E+01-4.43959178E+00 7.16532928E-02-7.15032351E-
 05 3
 3.51737842E-08-6.63682938E-12-2.27250412E+04 4.56394038E+01
 4
 C3H601-2 A01/05C 3 H 6 O 1 0 G 200.000 6000.00 1000.00
 1
 8.01491079E+00 1.73919953E-02-6.26027968E-06 1.01188256E-09-6.06239111E-
 14 2
 -1.51980838E+04-1.88279964E+01 3.42806676E+00 6.25176642E-03 6.13196311E-
 05 3
 -8.60387185E-08 3.51371393E-11-1.28446646E+04 1.04244994E+01-
 1.11564001E+04 4
 C3H601-3 A11/04C 3 H 6 O 1 0 G 200.000 6000.00 1000.00
 1
 6.80716906E+00 1.88824545E-02-6.79082475E-06 1.09713919E-09-6.57154952E-
 14 2
 -1.36547629E+04-1.35382154E+01 5.15283752E+00-1.86401716E-02 1.29980652E-
 04 3
 -1.58629974E-07 6.20668783E-11-1.13243512E+04 4.73561224E+00-
 9.75233898E+03 4
 C3H6 8/12/15 C 3H 6 0 0G 300.000 5000.000
 1387.000 11
 7.96904658E+00 1.37811801E-02-4.69782604E-06 7.27579148E-10-4.21368920E-
 14 2
 -1.72035522E+03-1.98794546E+01 7.64219985E-01 2.74294063E-02-1.34507688E-
 05 3
 2.72030922E-09-9.72000850E-14 1.14259854E+03 2.00145307E+01
 4

C3H5-A 8/12/15 C 3H 5 0 0G 300.000 5000.000
 1373.000 01
 8.76859148E+00 1.08337121E-02-3.65937325E-06 5.64011260E-10-3.25773494E-
 14 2
 1.61205737E+04-2.42574843E+01 4.49521576E-01 2.75404048E-02-1.51792914E-
 05 3
 3.50842115E-09-1.79934287E-13 1.92623564E+04 2.13563160E+01
 4
 C3H5-S 8/12/15 C 3H 5 0 0G 300.000 5000.000
 1390.000 11
 7.95954498E+00 1.11163183E-02-3.75197834E-06 5.77246260E-10-3.32768957E-
 14 2
 2.80567891E+04-1.79800372E+01 1.61793372E+00 2.44803904E-02-1.41856503E-
 05 3
 4.16402233E-09-4.90904795E-13 3.04291037E+04 1.66341443E+01
 4
 C3H5-T 8/12/15 C 3H 5 0 0G 300.000 5000.000
 1376.000 11
 7.69949212E+00 1.17803985E-02-4.07791749E-06 6.38119222E-10-3.72229675E-
 14 2
 2.61747145E+04-1.68305890E+01 2.29256998E+00 1.98527646E-02-6.42635654E-
 06 3
 -5.90016395E-10 5.05491095E-13 2.85773377E+04 1.39407124E+01
 4
 CC3H6 C 3H 60 0 0G 200.000 6000.000 1000.
 1
 6.21663437E+00 1.65393591E-02-5.90075838E-06 9.48095199E-10-5.65661522E-
 14 2
 2.95937491E+03-1.36041009E+01 2.83278674E+00-5.21028618E-03 9.29583210E-
 05 3
 -1.22753194E-07 4.99191366E-11 5.19520048E+03 1.08306333E+01
 6.41047999E+03 4
 C3H5O KPS12 C 3H 50 1 0G 300.000 5000.000
 1402.000 01
 1.02638186E+01 1.17609932E-02-3.89837957E-06 5.92650815E-10-3.38867417E-
 14 2
 7.25938472E+03-2.75108651E+01 8.24068673E-01 3.46749909E-02-2.51786795E-
 05 3
 9.56781953E-09-1.48085302E-12 1.04203725E+04 2.28283070E+01
 4
 CH2CHOCH2 8/ 8/15 C 3H 50 1 0G 300.000 5000.000
 1384.000 21
 1.20076931E+01 1.05055204E-02-3.69920541E-06 5.85629983E-10-3.44431587E-
 14 2
 6.97311613E+03-3.75189859E+01 1.15350351E+00 3.51253596E-02-2.50071619E-
 05 3
 9.00715632E-09-1.32376643E-12 1.08300872E+04 2.10606652E+01
 4
 CH3CHCHO C 3H 50 1 0G 300.000 5000.000
 1424.000 21
 1.06781476E+01 1.12805711E-02-3.89010759E-06 6.07617268E-10-3.54120848E-
 14 2
 -7.73234209E+03-3.24971238E+01 1.47166733E+00 2.69251618E-02-1.00248013E-
 05 3
 -1.13421435E-09 1.03416658E-12-4.04142023E+03 1.88722472E+01
 4
 AC4H7OOH 6/17/13 THERMC 4H 80 2 0G 300.000 5000.000
 1395.000 41

1.47661443E+01 2.12235231E-02-7.09403390E-06 1.08423759E-09-6.22145708E-
 14 2
 -1.35617411E+04-4.77449138E+01 1.33470633E+00 5.27831440E-02-3.58861360E-
 05 3
 1.32495013E-08-2.06619289E-12-8.87891782E+03 2.43857336E+01
 4
 C3H6OH1-2 9/ 1/12 C 3H 70 1 OG 300.000 5000.000
 1395.000 31
 1.00338281E+01 1.60227373E-02-5.41658448E-06 8.34191172E-10-4.81215988E-
 14 2
 -1.27912397E+04-2.39034395E+01 5.05207596E-01 3.63869988E-02-2.15530901E-
 05 3
 6.45584786E-09-7.71267046E-13-9.26980840E+03 2.79804349E+01
 4
 CH3CHCO 03/03/95 THERMC 3H 40 1 OG 300.000 5000.000 1400.00
 41
 1.00219123E+01 9.56966300E-03-3.26221644E-06 5.05231706E-10-2.92593257E-
 14 2
 -1.42482738E+04-2.77829973E+01 1.48380119E+00 3.22203013E-02-2.70250033E-
 05 3
 1.20499164E-08-2.18365931E-12-1.15276540E+04 1.71552068E+01
 4
 AC3H5OOH GOLDSMITH C 3H 60 2 OG 298.0 6000.0
 1000.000 31
 1.20838649E+01 1.47946591E-02-5.13212591E-06 8.07504999E-10-4.74394983E-
 14 2
 -1.02184463E+04-3.36434791E+01 3.18124993E+00 4.35233041E-02-5.16277353E-
 05 3
 4.32011427E-08-1.57714983E-11-7.63521503E+03 1.21725683E+01
 4
 C2H3OOH 4/18/ 8 THERMC 2H 40 2 OG 300.000 5000.000
 1397.000 21
 1.15749951E+01 8.09909174E-03-2.81808668E-06 4.42697954E-10-2.58998042E-
 14 2
 -8.84852664E+03-3.43859117E+01 1.35644398E+00 3.37002447E-02-2.75988500E-
 05 3
 1.14222854E-08-1.89488886E-12-5.49996692E+03 1.98354466E+01
 4
 C2H3OO H 3C 20 2 G 298.150 2000.000 1000.00
 1
 6.04483828E+00 1.45511127E-02-7.50974622E-06 1.83488280E-09-1.66689681E-
 13 2
 1.01699244E+04-3.71144913E+00 1.09784776E+00 2.95333237E-02-2.27744360E-
 05 3
 7.20559155E-09-3.07929092E-13 1.13996101E+04 2.13563583E+01
 4
 CHCHO H 2C 20 1 G 298.150 2000.000 1000.00
 1
 4.92632910E+00 9.71712147E-03-5.54855980E-06 1.53068537E-09-1.64742462E-
 13 2
 2.89499494E+04 5.27874677E-01 2.33256751E+00 1.62952986E-02-9.72052177E-
 06 3
 5.15124155E-10 1.03836514E-12 2.96585452E+04 1.39904923E+01
 4
 C3H6OH2-1 8/9/4 THERMC 3H 70 1 OG 300.000 5000.000
 1392.000 31
 1.12222277E+01 1.36444398E-02-4.51406709E-06 7.10523275E-10-4.22690392E-
 14 2

-1.75350136E+04-3.18911926E+01 1.09670360E+00 3.80727565E-02-2.75022497E-
 05 3
 1.07477493E-08-1.74895773E-12-1.40764487E+04 2.22475799E+01
 4
 TQJC3H6OH C 3H 70 3 0G 300.000 5000.000
 1411.000 41
 1.57530365E+01 1.56289438E-02-5.23690385E-06 8.01741456E-10-4.60590728E-
 14 2
 -3.24130576E+04-5.08911217E+01 2.29728737E+00 4.96725824E-02-3.84714645E-
 05 3
 1.56038090E-08-2.56748169E-12-2.80429510E+04 2.03767936E+01
 4
 TQC3H6OI C 3H 70 3 0G 300.000 5000.000
 1417.000 41
 1.71497525E+01 1.47440875E-02-4.99973196E-06 7.71920259E-10-4.46175680E-
 14 2
 -2.30944769E+04-5.96032656E+01 3.77984842E+00 4.51246380E-02-3.03819021E-
 05 3
 9.92338649E-09-1.22338206E-12-1.84544341E+04 1.23546787E+01
 4
 QC3H5OHP C 3H 70 3 0G 300.000 5000.000
 1415.000 51
 1.65390643E+01 1.45962463E-02-4.89569717E-06 7.50190330E-10-4.31310565E-
 14 2
 -2.47102324E+04-5.34015731E+01 1.76951547E+00 5.23733147E-02-4.19658180E-
 05 3
 1.72471815E-08-2.83710014E-12-1.99859353E+04 2.46273265E+01
 4
 CCY(COC)OH C 3H 60 2 0G 300.000 5000.000
 1427.000 21
 1.37176873E+01 1.33634818E-02-4.51490840E-06 6.95521032E-10-4.01451866E-
 14 2
 -4.07527954E+04-4.74449508E+01-7.68565795E-01 4.79603507E-02-3.53347028E-
 05 3
 1.27934873E-08-1.79555386E-12-3.59177637E+04 2.98848715E+01
 4
 IQJC3H6OH C 3H 70 3 0G 300.000 5000.000
 1408.000 41
 1.55719527E+01 1.57683363E-02-5.28242575E-06 8.08628793E-10-4.64527621E-
 14 2
 -3.23985113E+04-4.97782092E+01 1.74093905E+00 5.10931764E-02-4.02179535E-
 05 3
 1.66120004E-08-2.78425352E-12-2.79317094E+04 2.33734165E+01
 4
 IQC3H6OT C 3H 70 3 0G 300.000 5000.000
 1406.000 41
 1.67044548E+01 1.52497437E-02-5.19996341E-06 8.05676289E-10-4.66785083E-
 14 2
 -2.29660389E+04-5.69717854E+01 2.97554636E+00 4.80962295E-02-3.51787999E-
 05 3
 1.32008460E-08-2.00208137E-12-1.83154710E+04 1.64182550E+01
 4
 CY(COC)COH C 3H 60 2 0G 300.000 5000.000
 1427.000 21
 1.23650178E+01 1.37866121E-02-4.50198310E-06 6.77071535E-10-3.84092609E-
 14 2
 -3.50388267E+04-3.88318770E+01-3.28993462E+00 5.79159124E-02-5.21642132E-
 05 3

2.38463400E-08-4.27986682E-12-3.04628787E+04 4.23855523E+01
 4
 CHOCOHC3 C 3H 60 2 0G 300.000 5000.000
 1379.000 31
 1.36133542E+01 1.38716512E-02-4.87445259E-06 7.70639716E-10-4.52818606E-14 2
 -4.85836793E+04-4.37863752E+01 9.59562607E-01 4.04355781E-02-2.52333819E-05 3
 7.47748757E-09-8.33450351E-13-4.38727633E+04 2.52653125E+01
 4
 CY(CCOC)OH C 3H 60 2 0G 300.000 5000.000
 1433.000 11
 1.16477060E+01 1.42006208E-02-4.52110513E-06 6.68183015E-10-3.74416389E-14 2
 -3.58421461E+04-3.71322765E+01-5.94615865E+00 6.41555008E-02-5.85235665E-05 3
 2.68222743E-08-4.79465381E-12-3.07734013E+04 5.39539327E+01
 4
 TQC3H5OHI C 3H 70 3 0G 300.000 5000.000
 1526.000 51
 1.55469726E+01 1.61841763E-02-5.60787877E-06 8.78452695E-10-5.12904040E-14 2
 -2.63164910E+04-4.81509679E+01 5.58028765E+00 3.00649782E-02-6.38519910E-06 3
 -4.74322634E-09 1.89822226E-12-2.19537872E+04 8.64790031E+00
 4
 TQC3H5OHIO2 C 3H 70 5 0G 300.000 5000.000
 1387.000 61
 2.02916342E+01 1.92145529E-02-8.58823433E-06 1.62509037E-09-1.06225627E-13 2
 -4.85976512E+04-7.10879629E+01 2.11774097E+00 7.25997025E-02-6.81667819E-05 3
 3.13796075E-08-5.68565078E-12-4.35518506E+04 2.23586550E+01
 4
 TQC3H5OHIQ-I C 3H 70 5 0G 300.000 5000.000
 1391.000 61
 2.28708932E+01 1.56658128E-02-6.48662482E-06 1.17068411E-09-7.44373426E-14 2
 -3.97155885E+04-8.61588096E+01 3.46235675E+00 6.98705440E-02-6.48577576E-05 3
 2.96626742E-08-5.34536953E-12-3.39681675E+04 1.47596723E+01
 4
 TQC3H5OHIQ-P C 3H 70 5 0G 300.000 5000.000
 1478.000 71
 2.59345778E+01 6.66525395E-03-1.66651304E-07-4.20552574E-10 5.49726117E-14 2
 -4.21899085E+04-9.90618026E+01 2.45629666E+00 7.08507900E-02-6.43845421E-05 3
 2.79222006E-08-4.68412156E-12-3.56101660E+04 2.27189955E+01
 4
 C2H3COHOH C 3H 60 3 0G 300.000 5000.000
 1393.000 41
 1.69349460E+01 1.32757225E-02-5.30958950E-06 9.43268930E-10-5.97339692E-14 2
 -3.77990580E+04-5.97614008E+01 3.73734021E-01 5.84060291E-02-5.29627415E-05 3
 2.38734015E-08-4.26063052E-12-3.27577137E+04 2.67905679E+01
 4

COHOOHCY (COC) C 3H 60 4 0G 300.000 5000.000
1394.000 41
1.78808618E+01 1.47154928E-02-5.11766843E-06 8.03382779E-10-4.69696797E-14 2
-5.19254526E+04-6.47302080E+01-3.16180219E+00 7.92240221E-02-8.28674521E-05 3
4.32049848E-08-8.69506663E-12-4.59891154E+04 4.31128002E+01
4

OHCY (COCC) OOH C 3H 60 4 0G 300.000 5000.000
1520.000 31
1.88928431E+01 1.38516388E-02-4.73692460E-06 7.36282623E-10-4.27819063E-14 2
-5.31875949E+04-7.05664934E+01-2.13807799E-01 5.79347134E-02-4.16882857E-05 3
1.38590975E-08-1.65613593E-12-4.67090699E+04 3.18890641E+01
4

TQC3H5OHTO2 C 3H 70 5 0G 300.000 5000.000
1387.000 61
2.02916342E+01 1.92145529E-02-8.58823433E-06 1.62509037E-09-1.06225627E-13 2
-4.85976512E+04-7.10879629E+01 2.11774097E+00 7.25997025E-02-6.81667819E-05 3
3.13796075E-08-5.68565078E-12-4.35518506E+04 2.23586550E+01
4

OHCOCOOHCH3 C 3H 60 4 0G 300.000 5000.000
1393.000 51
2.01819586E+01 1.34325042E-02-4.81163867E-06 7.56987137E-10-4.37448189E-14 2
-7.33623538E+04-7.56343874E+01-1.96293682E-01 6.45815031E-02-5.49196882E-05 3
2.34355354E-08-4.01181684E-12-6.66388685E+04 3.25552353E+01
4

IQC3H5OHPJ C 3H 70 3 0G 300.000 5000.000
1409.000 51
1.59552559E+01 1.50895186E-02-5.06382338E-06 7.76108726E-10-4.46235236E-14 2
-2.45035338E+04-4.99018045E+01 1.35929059E+00 5.34300669E-02-4.41305751E-05 3
1.89646022E-08-3.27838412E-12-1.98996889E+04 2.69126449E+01
4

IQC3H5OHPJO2 C 3H 70 5 0G 300.000 5000.000
1407.000 61
2.05841169E+01 1.60145253E-02-5.42436519E-06 8.36749101E-10-4.83324213E-14 2
-4.36087438E+04-7.05205391E+01 2.83411409E+00 6.29377015E-02-5.35228290E-05 3
2.33491916E-08-4.06934890E-12-3.80451295E+04 2.27789799E+01
4

IQC3H5OTQ-I C 3H 70 5 0G 300.000 5000.000
1415.000 61
2.17590493E+01 1.51627633E-02-5.16409734E-06 7.99713840E-10-4.63243290E-14 2
-3.41193762E+04-7.77619217E+01 4.80614714E+00 5.68137508E-02-4.39675105E-05 3
1.70399951E-08-2.61590876E-12-2.85442590E+04 1.23781282E+01
4

CHOCH2OOH C 2H 40 3 0G 300.000 5000.000
1391.000 31

1.51554685E+01 7.57240000E-03-2.72693024E-06 4.38217189E-10-2.60434287E-14 2
 -3.41419680E+04-5.08149884E+01-1.32768631E+00 5.21618601E-02-4.97327645E-05 3
 2.31272366E-08-4.20787867E-12-2.90608844E+04 3.54965675E+01
 4
 IQC3H5OHQ-SJ C 3H 70 5 OG 300.000 5000.000
 1430.000 71
 2.01633063E+01 1.57355922E-02-5.28426264E-06 8.10536228E-10-4.66373245E-14 2
 -3.70242993E+04-6.56524053E+01 3.75150220E+00 5.60926263E-02-4.26964877E-05 3
 1.62818685E-08-2.44662581E-12-3.16549841E+04 2.15564729E+01
 4
 SC3H5OH 2/ 3/ 9 C 3H 60 1 OG 300.000 5000.000
 1404.000 21
 1.11222064E+01 1.27745410E-02-4.25315532E-06 6.48216484E-10-3.71190850E-14 2
 -2.36690795E+04-3.41335182E+01-3.53977226E-02 4.34969453E-02-3.74479918E-05 3
 1.70906074E-08-3.13775054E-12-2.02502608E+04 2.41528201E+01
 4
 IC3H5OH 8/ 1/95 THERMC 3H 60 1 OG 300.000 5000.000 1374.00
 21
 1.07381025E+01 1.31698194E-02-4.41529622E-06 6.77009837E-10-3.89608901E-14 2
 -2.47298321E+04-3.13634050E+01 1.58376391E+00 3.16215366E-02-1.73664942E-05 3
 4.18927663E-09-2.79899620E-13-2.12643496E+04 1.88313766E+01
 4
 C3H5OH T06/10C 3 H 6 O 1 O G 200.000 6000.00 1000.00
 1
 8.72477114E+00 1.63942712E-02-5.90852993E-06 9.53262253E-10-5.70318010E-14 2
 -1.90496618E+04-1.97198674E+01 3.15011905E+00 1.28538274E-02 4.28438434E-05 3
 -6.67818707E-08 2.80408237E-11-1.66413668E+04 1.35066359E+01-
 1.48710589E+04 4
 CH2CCH2OH 9/ 8/95 THERMC 3H 50 1 OG 300.000 5000.000 1372.00
 21
 9.70702027E+00 1.13972660E-02-3.77993962E-06 5.75209277E-10-3.29229125E-14 2
 9.13212884E+03-2.25012933E+01 2.88422544E+00 2.42428071E-02-1.14152268E-05 3
 1.71775334E-09 1.42177454E-13 1.17935615E+04 1.52102335E+01
 4
 CHOCOHCH2OOH C 3H 60 4 OG 300.000 5000.000
 1384.000 51
 1.86816278E+01 1.39658539E-02-4.94259642E-06 7.85147166E-10-4.62881931E-14 2
 -5.97999375E+04-6.41155772E+01 1.90697565E+00 5.29537602E-02-3.95708722E-05 3
 1.48146113E-08-2.23976588E-12-5.39646718E+04 2.60308355E+01
 4
 CHOCHO C 2H 20 2 OG 300.000 5000.000
 1386.000 11
 9.75438561E+00 4.97645947E-03-1.74410483E-06 2.75586994E-10-1.61969892E-14 2

-2.95832896E+04-2.61878329E+01 1.88105120E+00 2.36386368E-02-1.83443295E-
 05 3
 6.84842963E-09-9.92733674E-13-2.69280190E+04 1.59154793E+01
 4
 C3H4-P T 2/90H 4 C 3 0 0 G 200.000 6000.00 1000.00
 1
 0.60252400E+01 0.11336542E-01-0.40223391E-05 0.64376063E-09-0.38299635E-
 13 2
 0.19620942E+05-0.86043785E+01 0.26803869E+01 0.15799651E-01 0.25070596E-
 05 3
 -0.13657623E-07 0.66154285E-11 0.20802374E+05 0.98769351E+01
 0.22302059E+05 4
 C3H4-A L 8/89C 3 H 4 0 0 G 200.000 6000.00 1000.00
 1
 0.63168722E+01 0.11133728E-01-0.39629378E-05 0.63564238E-09-0.37875540E-
 13 2
 0.20117495E+05-0.10995766E+02 0.26130445E+01 0.12122575E-01 0.18539880E-
 04 3
 -0.34525149E-07 0.15335079E-10 0.21541567E+05 0.10226139E+02
 0.22962267E+05 4
 C3H3 T 7/11C 3 H 3 0 0 G 200.000 6000.00
 1000.000 1
 7.14221719E+00 7.61902211E-03-2.67460030E-06 4.24914904E-10-2.51475443E-
 14 2
 3.95709594E+04-1.25848690E+01 1.35110873E+00 3.27411291E-02-4.73827407E-
 05 3
 3.76310220E-08-1.18541128E-11 4.07679941E+04 1.52058598E+01
 4.22762135E+04 4
 CC3H4 T12/81C 3H 4 0 0G 300.000 5000.00 1000.00
 1
 0.66999931E+01 0.10357372E-01-0.34551167E-05 0.50652949E-09-0.26682276E-
 13 2
 0.30199051E+05-0.13378770E+02-0.24621047E-01 0.23197215E-01-0.18474357E-
 05 3
 -0.15927593E-07 0.86846155E-11 0.32334137E+05 0.22729762E+02 0.3332728
 E+05 4
 C3H2 T12/00C 3 H 2 0 0 G 200.000 6000.00 1000.00
 1
 6.67324762E+00 5.57728845E-03-1.99180164E-06 3.20289156E-10-1.91216272E-
 14 2
 7.57571184E+04-9.72894405E+00 2.43417332E+00 1.73013063E-02-1.18294047E-
 05 3
 1.02756396E-09 1.62626314E-12 7.69074892E+04 1.21012230E+01
 7.83005132E+04 4
 H2CCC (S) 0C 3H 2 0 0G 200.000 5000.000 1500.00
 0 1
 0.64888762E+01 0.53112789E-02-0.17809490E-05 0.27252642E-09-0.15619590E-
 13 2
 0.63661864E+05-0.10064283E+02 0.37229726E+01 0.92589854E-02-0.23006191E-
 05 3
 -0.10200808E-08 0.45374357E-12 0.64877289E+05 0.56865936E+01
 4
 C3H2 (S) 0C 3H 2 0 0G 200.000 5000.000 900.00
 0 1
 0.77642570E+01 0.47112774E-02-0.16170637E-05 0.25472406E-09-0.15038572E-
 13 2
 0.66849672E+05-0.15098549E+02 0.52976482E+01 0.16987466E-01-0.24266517E-
 04 3

0.18653681E-07-0.55763001E-11 0.67240466E+05-0.37540041E+01
 4
 C3H2C 0C 3H 2 0 0G 200.000 5000.000 1500.00
 0 1
 0.65632680E+01 0.52363256E-02-0.17544830E-05 0.26866106E-09-0.15428509E-
 13 2
 0.56514618E+05-0.12000607E+02 0.11295888E+01 0.17287401E-01-0.11366823E-
 04 3
 0.34569296E-08-0.36615951E-12 0.58419080E+05 0.17331448E+02
 4
 PC3H4OH-2 4/ 2/13 THERMC 3H 50 1 0G 300.000 5000.000
 1403.000 21
 1.07164095E+01 1.06066461E-02-3.51374060E-06 5.33713932E-10-3.04901511E-
 14 2
 4.98486803E+03-2.98329329E+01 1.42757363E+00 3.64825569E-02-3.18007132E-
 05 3
 1.46914605E-08-2.72331227E-12 7.80342663E+03 1.85890339E+01
 4
 SC3H4OH 3/28/13 C 3H 50 1 0G 300.000 5000.000
 1407.000 21
 1.20968484E+01 9.43976596E-03-3.10773897E-06 4.69609188E-10-2.67165710E-
 14 2
 -3.85854894E+02-3.76795997E+01 1.72870561E+00 4.41015870E-02-4.72013860E-
 05 3
 2.52073596E-08-5.13375710E-12 2.22720503E+03 1.43928257E+01
 4
 C3H3O 2/17/14 CZHOUH 3C 3O 1 G 298.150 2000.000 1000.00
 1
 4.19355696E+00 1.95625103E-02-1.22336450E-05 3.90615061E-09-5.08539231E-
 13 2
 3.14931737E+04 5.03216224E+00 8.75023836E-01 3.51184068E-02-3.89901356E-
 05 3
 2.40255750E-08-6.10883631E-12 3.20427921E+04 2.04717253E+01
 4
 C3H3O2H 1/31/13 C 3H 4O 2 0G 300.000 5000.000
 1385.000 31
 1.38152174E+01 8.62174763E-03-3.06710006E-06 4.88874247E-10-2.88888385E-
 14 2
 6.29182941E+03-4.39151257E+01 1.09787313E+00 4.22717882E-02-3.83969355E-
 05 3
 1.77405069E-08-3.27674312E-12 1.03592314E+04 2.30651783E+01
 4
 C2HCHO 1/31/13 C 3H 2O 1 0G 300.000 5000.000
 2012.000 11
 7.99952054E+00 7.07825497E-03-2.63086819E-06 4.33073185E-10-2.62003284E-
 14 2
 8.71863156E+03-1.57226237E+01 4.20776611E+00 1.34382727E-02-5.15442099E-
 06 3
 -2.24570818E-11 2.74111284E-13 1.02117375E+04 5.43871873E+00
 4
 C2H5CHO 8/12/15 C 3H 6O 1 0G 300.000 5000.000
 1449.000 21
 1.06224453E+01 1.35569132E-02-4.60754771E-06 7.12755462E-10-4.12631683E-
 14 2
 -2.78692266E+04-3.16628752E+01 2.18895588E+00 2.58289987E-02-6.04170058E-
 06 3
 -3.70702654E-09 1.57131095E-12-2.42671146E+04 1.61496330E+01
 4

C2H5CO A10/04C 3 H 5 O 1 0 G 200.000 6000.00 1000.00
1
6.52325448E+00 1.54211952E-02-5.50898157E-06 8.85889862E-10-5.28846399E-
14 2
-7.19631634E+03-5.19862218E+00 6.25722402E+00-9.17612184E-03 7.61190493E-
05 3
-9.05514997E-08 3.46198215E-11-5.91616484E+03 2.23330599E+00-
3.94851891E+03 4
CH2CH2CHO C 3H 5O 1 0G 300.000 5000.000
1437.000 21
1.00673122E+01 1.14971005E-02-3.90137798E-06 6.03029101E-10-3.48958224E-
14 2
-2.75080876E+03-2.58818404E+01 2.55799036E+00 2.23391941E-02-4.89741478E-
06 3
-3.58874384E-09 1.47175030E-12 4.53127696E+02 1.67016285E+01
4
C2H3CHO KPS12 C 3H 4O 1 0G 300.000 5000.000
1398.000 01
9.99155394E+00 9.82348001E-03-3.31203088E-06 5.09524422E-10-2.93821890E-
14 2
-1.25303509E+04-2.85168883E+01 7.33844455E-01 3.17482671E-02-2.29599468E-
05 3
8.42104232E-09-1.23613478E-12-9.38473548E+03 2.10308851E+01
4
C2H3CO KPS12 C 3H 3O 1 0G 300.000 5000.000
1395.000 01
8.86032735E+00 8.48985205E-03-2.90350080E-06 4.50763986E-10-2.61524281E-
14 2
7.73489171E+03-2.06978792E+01 1.65335195E+00 2.57402596E-02-1.89009911E-
05 3
7.29174972E-09-1.16083226E-12 1.02020654E+04 1.78705872E+01
4
CH3COCH3 8/12/15 C 3H 6O 1 0G 300.000 5000.000
1394.000 21
8.87619308E+00 1.45700263E-02-4.84823280E-06 7.38614777E-10-4.22831194E-
14 2
-3.06046242E+04-2.12730484E+01 2.20008426E+00 2.74019559E-02-1.31342003E-
05 3
2.57150371E-09-6.21509091E-14-2.79933966E+04 1.55883508E+01
4
CH3COCH2 2/14/13 THERMC 3H 5O 1 0G 300.000 5000.000
1387.000 21
1.09524298E+01 1.11458668E-02-3.86262877E-06 6.05088857E-10-3.53293362E-
14 2
-9.60833727E+03-3.15622776E+01 1.13381826E+00 3.25095045E-02-2.10424651E-
05 3
6.64421151E-09-8.12618901E-13-6.04868361E+03 2.17158655E+01
4
CH3COCH2O2 2/14/13 THERMC 3H 5O 3 0G 300.000 5000.000
1397.000 31
1.65756401E+01 1.06465489E-02-3.61368681E-06 5.59053564E-10-3.23832271E-
14 2
-2.42541401E+04-5.45304899E+01 1.19378141E+00 4.98027161E-02-4.17999508E-
05 3
1.74527607E-08-2.88198761E-12-1.93244224E+04 2.67877493E+01
4
CH3COCH2O 2/ 8/13 THERMC 3H 5O 2 0G 300.000 5000.000
2002.000 21

9.84061707E+00 1.59181106E-02-5.85164644E-06 9.56160073E-10-5.75477263E-14 2
 -2.11214823E+04-2.12330791E+01 5.85960137E+00 1.78954926E-02 7.41506398E-07 3
 -5.40032753E-09 1.47393197E-12-1.90714739E+04 2.70987883E+00 4
 C3KET21 2/14/13 THERMC 3H 60 3 0G 300.000 5000.000
 1394.000 41
 1.75768076E+01 1.20311704E-02-4.11633942E-06 6.40149366E-10-3.72127562E-14 2
 -4.15502347E+04-6.09097100E+01-8.74352903E-01 6.12501498E-02-5.51474542E-05 3
 2.48491014E-08-4.42613472E-12-3.58060819E+04 3.59306224E+01 4
 4
 ! Yuan
 iC3H5CHO 7/19/95 thermC 4H 60 1 0G 300.000 5000.000
 1396.000 21
 1.36203958e+01 1.37917192e-02-4.73370118e-06 7.36655226e-10-4.20097974e-14 2
 -2.00025274e+04-4.73184531e+01 6.27183793e-01 4.66780254e-02-3.74430631e-05 3
 1.58330542e-08-2.73952155e-12-1.57203117e+04 2.16034294e+01 4
 4
 C4H P 1/93C 4H 1 0 0G 300.000 3000.000
 1
 0.77697593E+01 0.49829976E-02-0.17628546E-05 0.28144284E-09-0.16689869E-13 2
 0.94345900E+05-0.14165274E+02 0.13186295E+01 0.38582956E-01-0.71385623E-04 3
 0.65356359E-07-0.22617666E-10 0.95456106E+05 0.15567583E+02 4
 4
 C4H5-2 H6W/94C 4H 5 0 0G 300.000 3000.000
 1
 1.45381710E+01-8.56770560E-03 2.35595240E-05-1.36763790E-08 2.44369270E-12 2
 3.32590950E+04-4.53694970E+01 2.96962800E+00 2.44422450E-02-9.12514240E-06 3
 -4.24668710E-18 1.63047280E-21 3.55033160E+04 1.20360510E+01 4
 3.73930550E+04 4
 C4H612 A 8/83C 4H 6 0 0G 300. 3000. 1000.0
 1
 0.1781557E+02 -0.4257502E-02 0.1051185E-04 -0.4473844E-08 0.5848138E-12 2
 0.1267342E+05 -0.6982662E+02 0.1023467E+01 0.3495919E-01 -0.2200905E-04 3
 0.6942272E-08 -0.7879187E-12 0.1811799E+05 0.1975066E+02 4
 0.1950807E+05 4
 H2C4O 120189H 2C 40 1 G 0300.00 4000.00 1000.00
 1
 0.01026888E+03 0.04896164E-01-0.04885081E-05-0.02708566E-08 0.05107013E-12 2
 0.02346903E+06-0.02815985E+03 0.04810971E+02 0.01313999E+00 0.09865073E-05 3
 -0.06120720E-07 0.01640003E-10 0.02545803E+06 0.02113424E+02 4
 4
 C4H6-2 A 8/83C 4H 6 0 0G 300. 3000. 1000.0
 1

9.0338133E+00 8.2124510E-03 7.1753952E-06 -5.8834334E-09 1.0343915E-
 12 2
 1.4335068E+04 -2.0985762E+01 2.1373338E+00 2.6486229E-02 -9.0568711E-
 06 3
 -5.5386397E-19 2.1281884E-22 1.5710902E+04 1.3529426E+01
 1.7488676E+04 4
 C4H6 H6W/94C 4H 6 0 OG 300.000 3000.000
 1
 0.88673134E+01 0.14918670E-01-0.31548716E-05-0.41841330E-09 0.15761258E-
 12 2
 0.91338516E+04-0.23328171E+02 0.11284465E+00 0.34369022E-01-0.11107392E-
 04 3
 -0.92106660E-08 0.62065179E-11 0.11802270E+05 0.23089996E+02
 4
 C4H2 G3B3 H 2C 4O ON OG 300.000 3000.000
 1000.000 1
 9.75839793E+00 3.78873223E-03 3.06142015E-07-6.33655024E-10 1.12930032E-
 13 2
 5.22698696E+04-2.79084005E+01 1.73325212E-01 4.53949030E-02-7.30123830E-
 05 3
 5.95251736E-08-1.87484716E-11 5.42239385E+04 1.80184355E+01
 1.39971242E+04 4
 nC4H3 B3LYPTC 4H 3 0 OG 300.000 5000.000 1401.00
 1
 9.68060685E+00 7.69782764E-03-2.60749517E-06 4.02049412E-10-2.32100778E-
 14 2
 6.18601463E+04-2.42366583E+01 1.81168651E+00 3.09453636E-02-2.96345704E-
 05 3
 1.46967737E-08-2.86825941E-12 6.41464329E+04 1.63650520E+01
 4
 iC4H3 B3LYPTC 4H 3 0 OG 300.000 5000.000 1394.00
 1
 9.86963238E+00 7.54543302E-03-2.55699599E-06 3.94402514E-10-2.27749706E-
 14 2
 5.61078099E+04-2.48051715E+01 4.19283792E+00 2.27653540E-02-1.89504974E-
 05 3
 8.64326722E-09-1.61925002E-12 5.79294291E+04 5.06485759E+00
 4
 C4H4 H6W/94C 4H 4 0 OG 300.000 3000.000
 1
 0.66507092E+01 0.16129434E-01-0.71938875E-05 0.14981787E-08-0.11864110E-
 12 2
 0.31195992E+05-0.97952118E+01-0.19152479E+01 0.52750878E-01-0.71655944E-
 04 3
 0.55072423E-07-0.17286228E-10 0.32978504E+05 0.31419983E+02
 4
 C4H5-N G3B3 H 5C 4O ON OG 300.000 3000.000
 1000.000 1
 4.87674639E+00 2.27534299E-02-1.17714698E-05 2.95251455E-09-2.91456566E-
 13 2
 4.11081097E+04 2.21507772E+00-1.16849950E+00 4.79006074E-02-5.12377002E-
 05 3
 3.06244264E-08-7.59906965E-12 4.22787216E+04 3.11630273E+01
 1.56214077E+04 4
 C4H5-I G3B3 H 5C 4O ON OG 300.000 3000.000
 1000.000 1
 4.34643669E+00 2.45761440E-02-1.30953685E-05 3.38848125E-09-3.43519633E-
 13 2

3.58709780E+04 3.29579091E+00-3.31905498E-01 4.40163876E-02-4.27690246E-
 05 3
 2.31284316E-08-5.17171519E-12 3.67510686E+04 2.56362838E+01
 1.55688047E+04 4
 C5H3 20387C 5H 3 G 0300.00 5000.00 1000.00
 1
 0.01078762E+03 0.09539619E-01-0.03206745E-04 0.04733323E-08-0.02512135E-
 12 2
 0.06392904E+06-0.03005444E+03 0.04328720E+02 0.02352480E+00-0.05856723E-
 04 3
 -0.01215449E-06 0.07726478E-10 0.06588531E+06 0.04173259E+02
 4
 cC5H4 T 3/94C 5H 4 0 OG 200.000 6000.000
 1000.000 1
 0.10106809E+02 0.13457466E-01-0.48862383E-05 0.79465424E-09-0.47821691E-
 13 2
 0.61714735E+05-0.30155332E+02 0.98338482E+00 0.21429446E-01 0.33390071E-
 04 3
 -0.66941379E-07 0.30563346E-10 0.64905174E+05 0.20682801E+02
 0.66327982E+05 4
 C5H4 CH2CCHCCHBur00H 4C 5 0 OG 200.000 6000.000 1000.
 1
 0.10270189E+02 0.13073162E-01-0.46889368E-05 0.75613521E-09-0.45229670E-
 13 2
 0.49102428E+05-0.27545396E+02 0.87018870E+00 0.41493544E-01-0.35400870E-
 04 3
 0.13012008E-07-0.60955029E-12 0.51578444E+05 0.20378880E+02
 4
 lC5H5 1Yne3Ene5Y1 A 1/05C 5H 5 0 OG 200.000 6000.000
 1
 1.08989728E+01 1.42904648E-02-5.02395287E-06 7.99341505E-10-4.73687380E-
 14 2
 4.17506605E+04-3.03965620E+01 9.57517375E-02 4.93848014E-02-4.74598143E-
 05 3
 2.22750663E-08-3.37834761E-12 4.44492650E+04 2.40272094E+01
 4.62959333E+04 4
 C5H5 Refitted H 5C 50 ON OG 300.000 3000.000
 1000.000 1
 4.21464919E+00 2.71834728E-02-1.33173209E-05 3.08980119E-09-2.77879873E-
 13 2
 2.88952416E+04-3.05999781E-02-7.37844042E+00 9.72391818E-02-1.69579138E-
 04 3
 1.51818667E-07-5.12075479E-11 3.05514662E+04 5.12829539E+01
 1.52014006E+04 4
 C5H6 T 1/90C 5H 6 0 OG 200.000 6000.000 1000.
 1
 0.99757848E+01 0.18905543E-01-0.68411461E-05 0.11099340E-08-0.66680236E-
 13 2
 0.11081693E+05-0.32209454E+02 0.86108957E+00 0.14804031E-01 0.72108895E-
 04 3
 -0.11338055E-06 0.48689972E-10 0.14801755E+05 0.21353453E+02
 0.16152485E+05 4
 lC5H7 HWZD99C 5H 7 0 OG 300.000 3000.000
 1
 0.22246480E+01 0.39601296E-01-0.22345617E-04 0.60649676E-08-0.63840047E-
 12 2
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 04 3

0.16696418E-07-0.75334899E-12 0.23683646E+05 0.45148109E+02
 4
 C5H30 TAK0905C 5H 30 1 0G 300.000 3500.000 1500.00
 1
 1.19961781E+01 1.34287065E-02-5.90045309E-06 1.22553862E-09-9.86114716E-
 14 2
 2.89592010E+04-4.07548249E+01-3.03242604E+00 5.43937201E-02-4.95018348E-
 05 3
 2.25523751E-08-4.10727920E-12 3.35644081E+04 3.78374823E+01
 4
 C5H5024 Clo-2,4- T 3/10C 5.H 5.O 1. 0.G 200.000 6000.000 1000.
 1
 1.20244667E+01 1.69698914E-02-6.12274609E-06 9.91737990E-10-5.95206422E-
 14 2
 2.05122293E+04-3.95370458E+01 7.74871946E-01 2.53185105E-02 4.65761215E-
 05 3
 -8.92691495E-08 4.04034749E-11 2.44938481E+04 2.34455624E+01
 2.61043645E+04 4
 C5H40 T 8/99C 5.H 4.O 1. 0.G 200.000 6000.000 1000.
 1
 1.00806824E+01 1.61143465E-02-5.83314509E-06 9.46759320E-10-5.68972206E-
 14 2
 1.94364771E+03-2.94521623E+01 2.64576497E-01 3.34873827E-02 1.67738470E-
 06 3
 -2.96207455E-08 1.54431476E-11 5.11159287E+03 2.35409513E+01
 6.64245999E+03 4
 C5H40H T 8/99C 5.H 5.O 1. 0.G 200.000 6000.000 1000.
 1
 1.33741248E+01 1.51996469E-02-5.45685046E-06 8.80944866E-10-5.27493258E-
 14 2
 2.20358027E+03-4.59569069E+01-1.28398054E+00 4.90298511E-02-1.35844414E-
 05 3
 -2.92983743E-08 1.90820619E-11 6.37364803E+03 3.08073591E+01
 8.00114499E+03 4
 C5H50H 5/ 2/91 THE.MC 5H 60 1 0G 300.000 5000.000
 1398.000 11
 1.53433477E+01 1.50754059E-02-5.13553582E-06 7.95807816E-10-4.61311517E-
 14 2
 -1.19645453E+04-5.85204430E+01-4.26822012E+00 6.62446749E-02-5.68494038E-
 05 3
 2.46858526E-08-4.26820696E-12-5.75581338E+03 4.47962850E+01
 4
 C5H5013 loxy-1,3- T09/10C 5.H 5.O 1. 0.G 200.000 6000.000 1000.
 1
 1.14579913E+01 1.74857813E-02-6.31033387E-06 1.02222611E-09-6.13529798E-
 14 2
 -7.47305910E+02-3.63570579E+01 1.02688782E+00 2.49799222E-02 4.13379251E-
 05 3
 -7.92827590E-08 3.55323358E-11 3.01148270E+03 2.22500883E+01
 4.65324451E+03 4
 C5H52 HR 10/00 BLYPC 5H 5 0 0G 300.000 5000.000
 1403.000 1
 1.23503328E+01 1.31278894E-02-4.49680943E-06 6.98998158E-10-4.05941466E-
 14 2
 4.29602305E+04-4.38813502E+01-3.71635176E+00 5.57854643E-02-4.85524520E-
 05 3
 2.15232840E-08-3.80152957E-12 4.79911937E+04 4.05280169E+01
 4

C5H2 20587C 5H 2 G 0300.00 5000.00 1000.00
 1
 0.01132917E+03 0.07424057E-01-0.02628189E-04 0.04082541E-08-0.02301333E-
 12 2
 0.07878706E+06-0.03617117E+03 0.03062322E+02 0.02709998E+00-0.01009170E-
 03 3
 -0.01272745E-06 0.09167219E-10 0.08114969E+06 0.07071078E+02
 4
 A1 G3B3 H 6C 6O 0N 0G 300.000 3000.000
 1000.000 1
 -2.06240612E-01 4.64122440E-02-2.77653536E-05 7.88910537E-09-8.60365259E-
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 8.09883905E+03 2.06566629E+01-5.51558393E+00 6.45453225E-02-4.41402928E-
 05 3
 7.47712161E-09 3.10282254E-12 9.11031457E+03 4.65332293E+01
 1.43778102E+04 4
 A1- G3B3 H 5C 6O 0N 0G 300.000 3000.000
 1000.000 1
 1.38016336E+00 4.04032009E-02-2.42250885E-05 6.88723321E-09-7.50960802E-
 13 2
 3.86973520E+04 1.55220921E+01-4.87654845E+00 6.26805782E-02-4.87402286E-
 05 3
 1.41122287E-08 5.18518312E-13 3.99269438E+04 4.59964173E+01
 1.43462431E+04 4
 l-C6H4 H6W/94C 6H 4 0 0G 300.000 3000.000
 1
 0.12715182E+02 0.13839662E-01-0.43765440E-05 0.31541636E-09 0.46619026E-
 13 2
 0.57031148E+05-0.39464600E+02 0.29590225E+00 0.58053318E-01-0.67766756E-
 04 3
 0.43376762E-07-0.11418864E-10 0.60001371E+05 0.22318970E+02
 4
 o-C6H4 exp C 6H 4 0 0G 300.000 5000.000 1398.00
 1
 1.36413308E+01 1.20276330E-02-4.12103889E-06 6.41090180E-10-3.72635368E-
 14 2
 4.72060501E+04-5.08934640E+01-3.00704505E+00 5.56175465E-02-4.83319980E-
 05 3
 2.11335333E-08-3.66968788E-12 5.24602203E+04 3.67568461E+01
 4
 n-C6H5 HW /94C 6H 5 0 0G 300.000 3000.000
 1
 0.16070068E+02 0.81899539E-02 0.17325165E-05-0.20624185E-08 0.36292345E-
 12 2
 0.64616867E+05-0.56163742E+02-0.61135769E+00 0.65082610E-01-0.78262397E-
 04 3
 0.53030828E-07-0.14946683E-10 0.68805375E+05 0.27635468E+02
 4
 fulvene Fulv T12/10C 6.H 6. 0. 0.G 200.000 6000.000 1000.
 1
 1.14345282E+01 1.99371432E-02-7.13567060E-06 1.14951842E-09-6.87263886E-
 14 2
 2.04411455E+04-3.86799524E+01 5.09714763E-01 2.58195980E-02 5.06504954E-
 05 3
 -9.32593825E-08 4.15963672E-11 2.44318827E+04 2.30638077E+01
 2.60142888E+04 4
 A10 T05/02C 6.H 5.O 1. 0.G 200.000 6000.000 1000.
 1

1.37221720E+01 1.74688771E-02-6.35504520E-06 1.03492308E-09-6.23410504E-
14 2
2.87274751E+02-4.88181680E+01-4.66204455E-01 4.13443975E-02 1.32412991E-
05 3
-5.72872769E-08 2.89763707E-11 4.77858391E+03 2.76990274E+01
6.49467016E+03 4
A1OH L 4/84C 6H 60 1 0G 300.000 5000.000 1000.
1
0.14912073E+02 0.18378135E-01-0.61983128E-05 0.91983221E-09-0.49209565E-
13 2
-0.18375199E+05-0.55924103E+02-0.16956539E+01 0.52271299E-01-0.72024050E-
05 3
-0.35859603E-07 0.20449073E-10-0.13284121E+05 0.32542160E+02-
0.11594207E+05 4
C5H4CH3 A03/05C 6H 7 0 0G 200.000 6000.000
1
1.28996538E+01 2.12183240E-02-7.67565006E-06 1.24495899E-09-7.47731827E-
14 2
2.12053775E+04-4.47534535E+01 5.64034275E-01 3.84201803E-02 1.94958520E-
05 3
-5.95545053E-08 2.86869522E-11 2.53304225E+04 2.27464371E+01
2.72743433E+04 4
O-C6H4O2 AK0405C 6H 40 2 0G 270.000 3000.000 1370.00
1
1.23614349E+01 2.40491397E-02-1.16529057E-05 2.71332785E-09-2.47593219E-
13 2
-1.67079717E+04-4.00310857E+01-2.36179712E+00 6.86058343E-02-6.39129516E-
05 3
3.06903009E-08-5.97357785E-12-1.26704431E+04 3.53724482E+01
4
P-C6H4O2 AK0405C 6H 40 2 0G 270.000 3000.000 1370.00
1
1.23423732E+01 2.40612690E-02-1.16565184E-05 2.71393504E-09-2.47643065E-
13 2
-2.06185312E+04-4.08244024E+01-2.43170113E+00 6.87937608E-02-6.41382837E-
05 3
3.08126855E-08-5.99832072E-12-1.65696994E+04 3.48309430E+01
4
P-OC6H5OJ WKM C 60 2H 5 0G 300.000 5000.000
1400.000 01
1.82799770E+01 1.59280974E-02-5.50765220E-06 8.61649836E-10-5.02677539E-
14 2
-6.25907994E+01-7.25809444E+01-3.29683290E+00 7.27365977E-02-6.36158220E-
05 3
2.80683553E-08-4.92279426E-12 6.73402222E+03 4.09349895E+01
4
O-OC6H5OJ WKM C 60 2H 5 0G 300.000 5000.000
1400.000 01
1.84625733E+01 1.57607263E-02-5.44671499E-06 8.51765760E-10-4.96759541E-
14 2
-1.72770226E+02-7.28742484E+01-2.65459198E+00 7.17179095E-02-6.31552372E-
05 3
2.81132946E-08-4.97463333E-12 6.45283150E+03 3.81123139E+01
4
P-C6H3O2 AK0505C 6H 30 2 0G 270.000 3000.000 1290.00
1
1.22963699E+01 2.15055142E-02-1.07516136E-05 2.57528163E-09-2.41023652E-
13 2

1.15428998E+04-3.72584002E+01-1.57852347E+00 6.55376473E-02-6.50308721E-
 05 3
 3.32026554E-08-6.86665555E-12 1.51750093E+04 3.31518638E+01
 4
 C6H4OH 4/ 9/ 9 THERMC 6H 50 1 0G 300.000 5000.000
 1402.000 11
 1.73187560E+01 1.36366984E-02-4.68316332E-06 7.29071204E-10-4.23805358E-
 14 2
 1.14990276E+04-6.89986593E+01-5.99875435E+00 8.59063379E-02-9.12525636E-
 05 3
 4.72275890E-08-9.35576749E-12 1.78621926E+04 4.99931427E+01
 4
 C6H2 P 1/93C 6H 2 0 0G 300.000 3000.000
 1
 0.13226281E+02 0.73904302E-02-0.22715381E-05 0.25875217E-09-0.55356741E-
 14 2
 0.80565258E+05-0.41201176E+02-0.15932624E+01 0.80530145E-01-0.14800649E-
 03 3
 0.13300031E-06-0.45332313E-10 0.83273227E+05 0.27980873E+02
 4
 C6H3 H6W/94C 6H 3 0 0G 300.000 3000.000
 1
 0.58188343E+01 0.27933408E-01-0.17825427E-04 0.53702536E-08-0.61707627E-
 12 2
 0.85188250E+05-0.92147827E+00 0.11790619E+01 0.55547360E-01-0.73076168E-
 04 3
 0.52076736E-07-0.15046964E-10 0.85647312E+05 0.19179199E+02
 4
 cC6H7 1/19/95 THERMC 6H 7 0 0G 300.000 5000.000
 1397.000 01
 1.45807530E+01 1.90472668E-02-6.57818915E-06 1.02815839E-09-5.99380191E-
 14 2
 1.73949036E+04-5.69992223E+01-6.01550859E+00 6.95380134E-02-5.43113522E-
 05 3
 2.16857946E-08-3.50034432E-12 2.42697461E+04 5.27055540E+01
 4
 lC6H7 5/ 7/91 THERMC 6H 7 0 0G 300.000 5000.000
 1405.000 21
 1.76225860E+01 1.51976235E-02-5.15602211E-06 7.96188268E-10-4.60220066E-
 14 2
 4.12781421E+04-6.76880771E+01-1.68717680E+00 6.97442629E-02-6.51384982E-
 05 3
 3.08028076E-08-5.72894955E-12 4.70145566E+04 3.26256051E+01
 4
 A100 3/26/ 9 THERMC 6H 50 2 0G 300.000 5000.000
 1403.000 11
 1.67078262E+01 1.62326229E-02-5.47969630E-06 8.43510060E-10-4.86562431E-
 14 2
 8.14242915E+03-6.08346973E+01-2.99164672E+00 7.03857150E-02-6.34400574E-
 05 3
 2.91548920E-08-5.30706938E-12 1.41320240E+04 4.20142955E+01
 4
 A10OH 3/26/ 9 THERMC 6H 60 2 0G 300.000 5000.000
 1404.000 21
 1.92317474E+01 1.63154699E-02-5.53448904E-06 8.55059974E-10-4.94583790E-
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 05 3

3.27610696E-08-5.85584239E-12-3.10973017E+03 4.54324978E+01
 4
 PC6H4CH3 C 7H 70 1 G 300.00 5000.00 1000.00
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 -.104378100E+04-.796692700E+01-.415304900E+01 .776998800E-01-.583028700E-
 04 3
 .178677900E-07-.536299700E-12 .896696700E+03 .453288900E+02
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 1
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 14 2
 2.71779724E+04-4.85624908E+01 1.37723080E+00 3.27432725E-02 4.58225372E-
 05 3
 -9.07721756E-08 4.08096948E-11 3.16491191E+04 2.10799820E+01
 3.37597997E+04 4
 C5H5CH2-2 C 6H 70 00 0G 300.000 5000.000
 1396.000 1
 1.52937914E+01 1.84305481E-02-6.35986836E-06 9.93248621E-10-5.78637916E-
 14 2
 1.91962522E+04-5.97458894E+01-5.39417365E+00 7.51043847E-02-6.77690358E-
 05 3
 3.16886723E-08-5.91960482E-12 2.56132529E+04 4.85135887E+01
 4
 C5H5CH2-3 C 6H 70 00 0G 300.000 5000.000
 1397.000 1
 1.53787161E+01 1.83356361E-02-6.32188797E-06 9.86758405E-10-5.74626535E-
 14 2
 2.21778975E+04-6.01469818E+01-5.34257890E+00 7.55933007E-02-6.88888970E-
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 3.24825676E-08-6.10432744E-12 2.85588845E+04 4.81169777E+01
 4
 C5H5CH2-1 C 6H 70 00 0G 300.000 5000.000
 1398.000 1
 1.75854699E+01 1.58083012E-02-5.49671640E-06 8.63067187E-10-5.04754347E-
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 3.08174859E+04-6.78115249E+01-3.42355668E+00 7.05975967E-02-6.11471177E-
 05 3
 2.68157030E-08-4.69274460E-12 3.75067184E+04 4.29354487E+01
 4
 A1CH3 L 6/87C 7H 8 0 0G 200.000 6000.000 1000.
 1
 0.12940034E+02 0.26691287E-01-0.96838505E-05 0.15738629E-08-0.94663601E-
 13 2
 -0.69764908E+03-0.46728785E+02 0.16152663E+01 0.21099438E-01 0.85366018E-
 04 3
 -0.13261066E-06 0.55956604E-10 0.40756300E+04 0.20282210E+02
 0.60135835E+04 4
 A1CH2 IU3/03C 7.H 7. 0. 0.G 250.000 6000.000 1000.
 1
 0.14723052E+02 0.23034244E-01-0.84847359E-05 0.13916962E-08-0.84247967E-
 13 2
 0.17990189E+05-0.55950989E+02-0.12303836E+01 0.48986376E-01 0.13815518E-
 04 3
 -0.62587233E-07 0.31595731E-10 0.23192877E+05 0.30555495E+02
 0.25016622E+05 4

C7H6 G3SX B3LYPTC 7H 6 0 0G 300.000 5000.000 1401.00
1
1.70564548E+01 1.67766601E-02-5.75637904E-06 8.95748927E-10-5.20574674E-
14 2
3.43929834E+04-6.83510071E+01-3.96406850E+00 7.40750426E-02-6.68009279E-
05 3
3.06821623E-08-5.59258820E-12 4.08575050E+04 4.16088550E+01
4
C7H5 G3SX ref819C 7H 5 0 0G 300.000 5000.000 1404.00
1
1.65644050E+01 1.44569152E-02-4.91369020E-06 7.59739947E-10-4.39556749E-
14 2
4.96364603E+04-6.29487260E+01-2.77567748E+00 6.97210344E-02-6.63891369E-
05 3
3.18329494E-08-5.98040634E-12 5.53261073E+04 3.73111448E+01
4
A1CO THERM C 7H 50 1 0G 300.000 5000.000
1392.000 11
1.75116258E+01 1.62650511E-02-5.65051892E-06 8.86922680E-10-5.18657990E-
14 2
4.67641545E+03-6.70531966E+01-1.56729686E+00 5.99817511E-02-4.29153585E-
05 3
1.48666854E-08-1.98938453E-12 1.12873830E+04 3.55490009E+01
4
O-OA1CH3 G3B3 H 7C 70 1N 0G 300.000 3000.000
1000.000 1
4.14521668E+00 5.02784126E-02-2.90785098E-05 8.02843592E-09-8.55794251E-
13 2
-1.22524065E+03 5.33490308E+00-3.88641950E+00 7.84259616E-02-6.20806903E-
05 3
2.17166947E-08-1.65778530E-12 4.71681386E+02 4.48067664E+01
2.12767448E+04 4
P-OA1CH3 G3B3 H 7C 70 1N 0G 300.000 3000.000
1000.000 1
4.14521668E+00 5.02784126E-02-2.90785098E-05 8.02843592E-09-8.55794251E-
13 2
-1.22524065E+03 5.33490308E+00-3.88641950E+00 7.84259616E-02-6.20806903E-
05 3
2.17166947E-08-1.65778530E-12 4.71681386E+02 4.48067664E+01
2.12767448E+04 4
O-C6H4CH3 G3B3 H 7C 70 0N 0G 300.000 3000.000
1000.000 1
5.19780822E-01 5.26219754E-02-3.12983433E-05 8.84817377E-09-9.61252202E-
13 2
3.45681510E+04 2.33397406E+01-3.91657299E+00 6.65870094E-02-3.99725038E-
05 3
2.04680797E-09 4.98559390E-12 3.54243469E+04 4.51374437E+01
1.82014718E+04 4
P-C6H4CH3 G3B3 H 7C 70 0N 0G 300.000 3000.000
1000.000 1
5.19780822E-01 5.26219754E-02-3.12983433E-05 8.84817377E-09-9.61252202E-
13 2
3.45681510E+04 2.33397406E+01-3.91657299E+00 6.65870094E-02-3.99725038E-
05 3
2.04680797E-09 4.98559390E-12 3.54243469E+04 4.51374437E+01
1.82014718E+04 4
A1CH2OH C 7H 8O 1 G 300.00 5000.00 1000.00
1

.988928700E+01 .312351700E-01-.110466410E-04 .129795100E-08
 .000000000E+00 2
 -.176276686E+05-.230348046E+02-.469518200E+01 .695108030E-01-.438445020E-
 04 3
 .104046480E-07 .000000000E+00-.135250700E+05 .527988700E+02
 4
 A1CHO 5/16/90 THERMC 7H 60 1 OG 300.000 5000.000
 1386.000 11
 1.74024893E+01 1.89508317E-02-6.58694307E-06 1.03413046E-09-6.04793155E-
 14 2
 -1.31418522E+04-6.83371315E+01-2.37082285E+00 6.28843128E-02-4.26460754E-
 05 3
 1.39416083E-08-1.74474949E-12-6.11656186E+03 3.85478773E+01
 4
 O-HOAlCH3 4/ 3/ 9 THERMC 7H 80 1 OG 300.000 5000.000
 1401.000 21
 2.09408940E+01 2.04158480E-02-7.04323518E-06 1.09988219E-09-6.40750543E-
 14 2
 -2.53662901E+04-8.94615089E+01-5.82611270E+00 9.52301991E-02-8.89715399E-
 05 3
 4.21339354E-08-7.87119970E-12-1.72848417E+04 4.99599069E+01
 4
 P-HOAlCH3 4/ 3/ 9 THERMC 7H 80 1 OG 300.000 5000.000
 1401.000 21
 2.09408940E+01 2.04158480E-02-7.04323518E-06 1.09988219E-09-6.40750543E-
 14 2
 -2.53662901E+04-8.94615089E+01-5.82611270E+00 9.52301991E-02-8.89715399E-
 05 3
 4.21339354E-08-7.87119970E-12-1.72848417E+04 4.99599069E+01
 4
 A1CH T CBSRAD7/01 C 7H 6 0 OG 300.000 5000.000
 1404.000 11
 1.75286289E+01 1.59878206E-02-5.49454979E-06 8.56118588E-10-4.98053729E-
 14 2
 4.73041322E+04-7.15174971E+01-5.94812574E+00 8.03020198E-02-7.38766020E-
 05 3
 3.39798674E-08-6.14844599E-12 5.44384047E+04 5.10879361E+01
 4
 A1CH2O 4/14/94 THE.MC 7H 70 1 OG 300.000 5000.000
 1392.000 1
 1.78843033E+01 2.09011735E-02-7.21832713E-06 1.12839851E-09-6.57955260E-
 14 2
 4.93182818E+03-7.01304667E+01-4.77736690E+00 7.51049308E-02-5.68532831E-
 05 3
 2.18290029E-08-3.38134298E-12 1.26234438E+04 5.10429366E+01
 4
 O-OC6H4CH2 012508C 7H 60 1 G 300.000 5000.000 1000.00
 1
 1.24204756E+01 2.70171830E-02-1.09476851E-05 2.02705529E-09-1.40757462E-
 13 2
 4.49159466E+02-4.10236260E+01-6.21979546E-01 5.14918065E-02-6.11682462E-
 06 3
 -2.88887155E-08 1.45119845E-11 4.44241036E+03 2.88224802E+01
 4
 C5H5CH3 C 6H 8 G 300.00 5000.00 1399.00
 1
 .154352848E+02 .199801707E-01-.680270423E-05 .105349633E-08-.610336727E-
 13 2

.447456576E+04-.636393642E+02-.665320026E+01 .744640477E-01-.582864186E-
04 3
.231603543E-07-.369017129E-11 .117669311E+05 .538162769E+02
4
A1CH2OO QB3-MF11 OC 7H 70 2 G 0300.00 5000.00 1000.00
1
1.71115179E+01 2.68198282E-02-1.06205723E-05 1.91920856E-09-1.30061244E-
13 2
6.71623207E+03-6.12436900E+01-2.24622429E+00 7.26022303E-02-3.67327921E-
05 3
-8.74034681E-09 1.01564683E-11 1.24729027E+04 4.07042530E+01
4
A1CH2OOH 3/ 4/94 THE.MC 7H 80 2 OG 300.000 5000.000
1390.000 31
2.21951256E+01 2.19901041E-02-7.70452728E-06 1.21574282E-09-7.13427270E-
14 2
-1.43966742E+04-9.07483698E+01-3.39515159E+00 8.45306884E-02-6.70634097E-
05 3
2.72113250E-08-4.48289693E-12-5.78730853E+03 4.57078979E+01
4
O-HOA1CH2 4/ 3/ 9 C 7H 70 1 OG 300.000 5000.000
1402.000 11
2.17284618E+01 1.76293589E-02-6.08300560E-06 9.50072743E-10-5.53543698E-
14 2
-6.69606412E+03-9.33418136E+01-5.63197903E+00 9.80964869E-02-9.82672860E-
05 3
4.87967928E-08-9.40191047E-12 1.17027222E+03 4.77626938E+01
4
P-HOA1CH2 4/ 3/ 9 C 7H 70 1 OG 300.000 5000.000
1402.000 11
2.17284618E+01 1.76293589E-02-6.08300560E-06 9.50072743E-10-5.53543698E-
14 2
-6.69606412E+03-9.33418136E+01-5.63197903E+00 9.80964869E-02-9.82672860E-
05 3
4.87967928E-08-9.40191047E-12 1.17027222E+03 4.77626938E+01
4
eC7H6 G3SX B3LYPTC 7H 6 0 OG 300.000 5000.000 1401.00
1
1.70697845E+01 1.67433678E-02-5.73958594E-06 8.92538887E-10-5.18456003E-
14 2
3.55856416E+04-6.74573770E+01-3.27536620E+00 7.22646827E-02-6.50419941E-
05 3
2.99258499E-08-5.47141606E-12 4.18458582E+04 3.89631961E+01
4
HOA1CH2OOH 7/ 9 THERMC 7H 80 3 OG 300.000 5000.000
1400.000 41
2.69433208E+01 1.98821379E-02-6.93248136E-06 1.09047819E-09-6.38542299E-
14 2
-3.68197020E+04-1.15455122E+02-4.27079330E+00 1.06702301E-01-1.01178433E-
04 3
4.78041859E-08-8.86088235E-12-2.74014110E+04 4.72010210E+01
4
HOA1CH2OO 7/ 9 THERMC 7H 70 3 OG 300.000 5000.000
1399.000 31
2.44885871E+01 1.96975788E-02-6.83424042E-06 1.07136180E-09-6.25824039E-
14 2
-1.85023219E+04-1.00503843E+02-3.30404252E+00 9.78488428E-02-9.29726683E-
05 3

4.44795179E-08-8.36613586E-12-1.01504226E+04 4.41069184E+01
 4
 HOA1CH2O 4/ 7/ 9 THERMC 7H 70 2 OG 300.000 5000.000
 1404.000 21
 2.27674826E+01 1.87580416E-02-6.44936609E-06 1.00501306E-09-5.84671446E-
 14 2
 -1.70289222E+04-9.48170837E+01-4.96646915E+00 9.69128605E-02-9.21049352E-
 05 3
 4.37042315E-08-8.11979451E-12-8.78398897E+03 4.93062368E+01
 4
 HOA1CHO 4/ 7/ 9 THERMC 7H 60 2 OG 300.000 5000.000
 1406.000 21
 2.37586619E+01 1.47270064E-02-4.93265699E-06 7.56306242E-10-4.35377695E-
 14 2
 -3.62468602E+04-1.01187561E+02-4.84031481E+00 9.73663695E-02-9.68302168E-
 05 3
 4.68381956E-08-8.74560771E-12-2.80359046E+04 4.65623414E+01
 4
 HOA1CO 4/ 7/ 9 THERMC 7H 50 2 OG 300.000 5000.000
 1407.000 11
 2.36196074E+01 1.29565163E-02-4.36676042E-06 6.72106801E-10-3.87861042E-
 14 2
 -1.85293338E+04-1.01120435E+02-2.64255595E+00 9.00208969E-02-9.13086471E-
 05 3
 4.48102851E-08-8.45769190E-12-1.10970627E+04 3.41553760E+01
 4
 A1CC HW /94C 8H 5 0 OG 300.000 3000.000
 1
 0.28686157E+02-0.13869863E-01 0.22721186E-04-0.99882271E-08 0.14085851E-
 11 2
 0.56047309E+05-0.12750334E+03-0.29324217E+01 0.66043675E-01-0.39500475E-
 04 3
 -0.31830381E-08 0.85300387E-11 0.65324043E+05 0.38058685E+02
 4
 A1C2H- HW /94C 8H 5 0 OG 300.000 3000.000
 1
 0.12359501E+02 0.25453357E-01-0.10606554E-04 0.18914603E-08-0.10630622E-
 12 2
 0.60930461E+05-0.40900208E+02-0.44495859E+01 0.76995067E-01-0.66617038E-
 04 3
 0.25038682E-07-0.19756601E-11 0.65225926E+05 0.44427948E+02
 4
 C6H3C2H C 8H 4 G 300.000 5000.000 1000.00
 1
 8.98848900E+00 2.80770877E-02-1.07254066E-05 1.90108784E-09-1.27777716E-
 13 2
 7.80045676E+04-2.03200448E+01-1.04246987E+00 6.23596981E-02-5.33874845E-
 05 3
 2.45012480E-08-4.31751147E-12 8.03028206E+04 2.95338396E+01
 4
 A1C2H HW /94C 8H 6 0 OG 300.000 3000.000 1000.0
 1
 0.24090759E+02 0.78232400E-03 0.11453964E-04-0.61620504E-08 0.93346685E-
 12 2
 0.27429445E+05-0.10499631E+03-0.52645016E+01 0.84511042E-01-0.76597848E-
 04 3
 0.33216978E-07-0.47673063E-11 0.35566242E+05 0.46378815E+02
 4

AlcC2H2 BenzocybuT08/06C 8.H 6. 0. 0.G 200.000 6000.000 1000.
 1
 1.46814136E+01 2.27435710E-02-8.23048840E-06 1.33587753E-09-8.02909523E-
 14 2
 4.22562172E+04-5.65249193E+01-4.49261004E-01 3.77029460E-02 4.69708193E-
 05 3
 -9.90233463E-08 4.52489247E-11 4.75307311E+04 2.75548196E+01
 4.93132204E+04 4
 AlCCH2 4/ 3/ 9 THERMC 8H 7 0 0G 300.000 5000.000
 1387.000 11
 1.92154972E+01 2.02185937E-02-7.07970746E-06 1.11666465E-09-6.55073301E-
 14 2
 2.44567929E+04-8.09621525E+01-1.75677703E+00 6.93776528E-02-5.15140526E-
 05 3
 1.96075933E-08-3.05640961E-12 3.17432364E+04 3.16482133E+01
 4
 AlCHCH 4/ 3/ 9 THERMC 8H 7 0 0G 300.000 5000.000
 1397.000 11
 1.90927875E+01 1.98909822E-02-6.86981799E-06 1.07370754E-09-6.25902921E-
 14 2
 3.82661147E+04-7.72000251E+01-3.64383962E+00 7.85604460E-02-6.60358335E-
 05 3
 2.85738243E-08-4.98068485E-12 4.55975302E+04 4.29246209E+01
 4
 O-C6H4C2H3 HW /94C 8H 7 0 0G 300.000 3000.000
 1
 0.11563599E+02 0.30210810E-01-0.11545593E-04 0.17302320E-08-0.52379765E-
 13 2
 0.40498492E+05-0.34882965E+02-0.38868685E+01 0.68168961E-01-0.34805875E-
 04 3
 -0.56410254E-08 0.80714758E-11 0.44941359E+05 0.45943188E+02
 4
 P-C6H4C2H3 HW /94C 8H 7 0 0G 300.000 3000.000
 1
 0.11563599E+02 0.30210810E-01-0.11545593E-04 0.17302320E-08-0.52379765E-
 13 2
 0.40498492E+05-0.34882965E+02-0.38868685E+01 0.68168961E-01-0.34805875E-
 04 3
 -0.56410254E-08 0.80714758E-11 0.44941359E+05 0.45943188E+02
 4
 AlC2H5 3/19/ 9 THERMC 8H 10 0 0G 300.000 5000.000
 1396.000 21
 2.02158866E+01 2.57181400E-02-8.78778587E-06 1.36387819E-09-7.91252430E-
 14 2
 -6.87601990E+03-8.53188987E+01-5.70126210E+00 8.90606644E-02-6.84365242E-
 05 3
 2.70624855E-08-4.33907755E-12 1.79229957E+03 5.27926555E+01
 4
 AlCH2CH2 4/ 7/ 9 C 8H 9 0 0G 300.000 5000.000
 1397.000 11
 1.97367479E+01 2.34359910E-02-7.88460514E-06 1.21151657E-09-6.98141943E-
 14 2
 1.82775793E+04-7.90373183E+01-5.03883577E+00 8.49439879E-02-6.65114973E-
 05 3
 2.66531641E-08-4.29645325E-12 2.64218438E+04 5.25744447E+01
 4
 AlCHCH3 4/ 3/ 9 THERMC 8H 9 0 0G 300.000 5000.000
 1395.000 11

2.03767475E+01 2.34923061E-02-8.02742753E-06 1.24595589E-09-7.22895395E-
 14 2
 1.07287463E+04-8.69308644E+01-3.62245458E+00 8.22327387E-02-6.34562719E-
 05 3
 2.51893798E-08-4.05353192E-12 1.87480811E+04 4.09318172E+01
 4
 A1C2H3 HW /94C 8H 8 0 OG 300.000 3000.000
 1
 0.11303213E+02 0.33709887E-01-0.13208885E-04 0.21140962E-08-0.87311377E-
 13 2
 0.11725388E+05-0.34737919E+02-0.38678493E+01 0.67947865E-01-0.25230333E-
 04 3
 -0.18017145E-07 0.12998470E-10 0.16200269E+05 0.45271770E+02
 4
 C6H4C2H5 C 8H 9 G 300.000 5000.000 1000.00
 1
 1.18902439E+01 3.61059407E-02-1.45474090E-05 2.68142778E-09-1.85537692E-
 13 2
 2.83533550E+04-3.78397523E+01 2.02243922E-01 4.63944836E-02 2.47149622E-
 05 3
 -5.99569435E-08 2.45899194E-11 3.25141279E+04 2.76639557E+01
 4
 A1CHCH3OOH MThERGAS C 8H 100 2 G 0300.00 5000.00
 1000.00 1
 -0.31565318E+01 0.72488472E-01-0.31781656E-04 0.60659939E-08-0.42418182E-
 12 2
 -0.75729609E+04 0.52722046E+02-0.80470219E+01 0.11141342E+00-0.84831234E-
 04 3
 0.23181402E-07 0.13341983E-11-0.90922773E+04 0.67959465E+02
 4
 A1CHCH3O MThERGAS C 8H 90 1 G 0300.00 5000.00
 1000.00 1
 -0.26841152E+01 0.63683085E-01-0.26554239E-04 0.48910964E-08-0.33337355E-
 12 2
 0.11209342E+05 0.45193958E+02-0.10515040E+02 0.10946906E+00-0.87473454E-
 04 3
 0.28099876E-07-0.67344112E-12 0.10719505E+05 0.76310471E+02
 4
 C8H8O FOURNET OC 8H 80 1 G 0300.00 5000.00 1000.00
 1
 1.50839842E+01 3.25092066E-02-1.28403261E-05 2.31578474E-09-1.56702946E-
 13 2
 -1.33912799E+04-5.85151857E+01-5.96220908E+00 8.15010579E-02-3.93920844E-
 05 3
 -1.07682941E-08 1.14611472E-11-7.06811930E+03 5.25774976E+01
 4
 C8H7O ThERGAS OC 8H 70 1 G 0300.00 5000.00 1000.00
 1
 0.39498155E+01 0.47736809E-01-0.19333373E-04 0.34884815E-08-0.23430105E-
 12 2
 0.10867305E+05-0.46506844E+01-0.64320035E+01 0.91989711E-01-0.72167728E-
 04 3
 0.22816783E-07-0.66101562E-12 0.11987392E+05 0.42892570E+02
 4
 C8H7O-1 ThERGAS OC 8H 70 1 G 0300.00 5000.00 1000.00
 1
 0.36577377E+01 0.48040181E-01-0.19457286E-04 0.35114045E-08-0.23589068E-
 12 2

0.52084609E+04-0.30909843E+01-0.60815744E+01 0.89198485E-01-0.67060450E-
 04 3
 0.19099829E-07 0.30027036E-12 0.62320034E+04 0.41498894E+02
 4
 C8H6O BURCAT OC 8H 60 1 G 200.000 6000.00 1000.00
 1
 1.61267559E+01 2.42942790E-02-8.82919089E-06 1.43722155E-09-8.65592465E-
 14 2
 -5.74867958E+03-6.40564836E+01-7.85221476E-01 3.96432449E-02 5.69751746E-
 05 3
 -1.14831806E-07 5.19411145E-11 2.15748538E+02 3.02655928E+01
 4
 C9H7 CBS-QB3C 9H 7 0 OG 300.000 5000.000 1402.00
 1
 2.14687522E+01 2.07965192E-02-7.17407428E-06 1.12057673E-09-6.53011343E-
 14 2
 2.40692659E+04-9.49478593E+01-8.14633421E+00 1.00848853E-01-9.12829918E-
 05 3
 4.14776610E-08-7.44411121E-12 3.31887832E+04 6.01173664E+01
 4
 C9H8 CBS-QB3C 9H 8 0 OG 300.000 5000.000 1400.00
 1
 2.15521509E+01 2.33026261E-02-8.04544454E-06 1.25734902E-09-7.32968859E-
 14 2
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 05 3
 3.81992613E-08-6.64553508E-12 1.80975505E+04 6.18917173E+01
 4
 C9H6O 000000N OH 60 1C 9G 300 3000 1000
 1
 4.65659248E+00 5.70055822E-02-3.43174199E-05 9.76177442E-09-1.06334037E-
 12 2
 4.57857140E+03-7.03868477E-01-6.53928778E+00 9.69323286E-02-8.17698656E-
 05 3
 2.96699474E-08-2.24993392E-12 6.88883578E+03 5.40945996E+01
 4
 C9H9-1 CNRS2000 C 9H 90 0 G 0300.00 5000.00 1000.00
 1
 3.44881E+00 1.15524E-02 -4.20795E-06 7.01596E-10 -4.44089E-14
 2
 4.43492E+03 2.75478E+00 1.06964E+00 1.63341E-02 -7.77930E-06
 3
 2.51462E-09 -7.05979E-13 5.29277E+03 1.57546E+01
 4
 C9H10 T 1/96C 9H 100 0 G 298.150 5000.000 1000.
 1
 0.18890862E+02 0.31553549E-01-0.12056696E-04 0.21436164E-08-0.14430356E-
 12 2
 0.43332577E+04-0.75568080E+02 0.58431766E+01 0.17489030E-01 0.12112118E-
 03 3
 -0.17951022E-06 0.75443868E-10 0.10316404E+05 0.36919595E+01
 4
 0.13586850E+05
 O-CH2AlC2H3 Pousse2010 C 9H 90 0 G 0300.00 5000.00 1000.00
 1
 1.70648122E+01 3.28892095E-02-1.28323249E-05 2.29479720E-09-1.54348164E-
 13 2
 2.48599234E+04-6.61223497E+01-5.67362805E+00 9.67482623E-02-7.49811328E-
 05 3

2.31114824E-08-1.30018265E-14 3.11297550E+04 5.11628285E+01
 4
 P-CH2A1C2H3 Pousse2010 C 9H 90 0 G 0300.00 5000.00 1000.00
 1
 1.70648122E+01 3.28892095E-02-1.28323249E-05 2.29479720E-09-1.54348164E-
 13 2
 2.48599234E+04-6.61223497E+01-5.67362805E+00 9.67482623E-02-7.49811328E-
 05 3
 2.31114824E-08-1.30018265E-14 3.11297550E+04 5.11628285E+01
 4
 O-CH3A1C2H3 Pousse2010 C 9H 100 0 G 0300.00 5000.00 1000.00
 1
 -0.64905424E+01 0.74284628E-01-0.32960350E-04 0.63375678E-08-0.44518054E-
 12 2
 0.15234238E+05 0.65877571E+02-0.45196443E+01 0.92458449E-01-0.64155669E-
 04 3
 0.13829308E-07 0.29229772E-11 0.12028299E+05 0.46347641E+02
 4
 P-CH3A1C2H3 Pousse2010 C 9H 100 0 G 0300.00 5000.00 1000.00
 1
 -0.64905424E+01 0.74284628E-01-0.32960350E-04 0.63375678E-08-0.44518054E-
 12 2
 0.15234238E+05 0.65877571E+02-0.45196443E+01 0.92458449E-01-0.64155669E-
 04 3
 0.13829308E-07 0.29229772E-11 0.12028299E+05 0.46347641E+02
 4
 A1C3H2 1/17/ 0 THERMC 9H 7 0 OG 300.000 5000.000
 1383.000 11
 2.05632118E+01 2.18474960E-02-7.69371038E-06 1.21810939E-09-7.16463859E-
 14 2
 4.65470757E+04-8.26412428E+01-2.26779736E+00 7.34853337E-02-5.21100716E-
 05 3
 1.85954603E-08-2.69498985E-12 5.46642559E+04 4.06118884E+01
 4
 A2 LLYe/11C 10H 8 G 300.000 5000.000 1000.00
 1
 1.46974627E+01 3.68553332E-02-1.50204389E-05 2.79212645E-09-1.94420767E-
 13 2
 9.63935752E+03-5.69348623E+01-4.06639664E+00 7.02480560E-02-2.61545121E-
 06 3
 -4.71405800E-08 2.27044345E-11 1.54752651E+04 4.40055913E+01
 4
 A2-1 HW /94C 10H 7 0 OG 300.000 3000.000
 1
 0.38380905E+02-0.23157451E-01 0.35479272E-04-0.15395457E-07 0.21609069E-
 11 2
 0.32698469E+05-0.18106512E+03-0.85287294E+01 0.10334599E+00-0.91922702E-
 04 3
 0.43147448E-07-0.85738135E-11 0.46335004E+05 0.63342224E+02
 4
 A2-2 HW /94C 10H 7 0 OG 300.000 3000.000
 1
 0.37326401E+02-0.20478070E-01 0.33183067E-04-0.14576987E-07 0.20569137E-
 11 2
 0.32840301E+05-0.17537704E+03-0.38448524E+01 0.70514679E-01-0.93748040E-
 05 3
 -0.44051607E-07 0.24267865E-10 0.45627656E+05 0.43582001E+02
 4

A2T2 HR12/99BLYP00C 10H 6 0 0G 300.000 5000.000
1401.000 01
2.27563525E+01 1.97983673E-02-6.85196907E-06 1.07269721E-09-6.26130244E-
14 2
4.98909571E+04-1.00848492E+02-5.71085200E+00 9.46608203E-02-8.30702095E-
05 3
3.64968043E-08-6.35095707E-12 5.88368563E+04 4.88989311E+01
4
A2T1 HR12/99 BLYP C 10H 6 0 0G 300.000 5000.000
1401.000 01
2.26743828E+01 1.98529546E-02-6.86764509E-06 1.07482892E-09-6.27247999E-
14 2
4.86149947E+04-9.97586064E+01-5.91383758E+00 9.53032669E-02-8.40320825E-
05 3
3.71175012E-08-6.49277297E-12 5.75780222E+04 5.05400652E+01
4
A1 (C2H)2 HW /94C 10H 6 0 0G 300.000 3000.000
1
0.39766785E+02-0.24939798E-01 0.34210185E-04-0.14473258E-07 0.20104023E-
11 2
0.50136750E+05-0.18657632E+03-0.75570364E+01 0.12159592E+00-0.15138849E-
03 3
0.10287488E-06-0.28950911E-10 0.62914168E+05 0.55213287E+02
4
C9H7CH2 Matsugi2013 C 10H 9 0 0G 300.000 5000.000 1400.00
1
2.48973930E+01 2.55147986E-02-8.79922194E-06 1.37404921E-09-8.00535169E-
14 2
1.83072953E+04-1.12654689E+02-8.02975915E+00 1.12889393E-01-9.91274443E-
05 3
4.41732177E-08-7.83596047E-12 2.86367245E+04 6.03761192E+01
4
C9H6CH2 Matsugi2013 C 10H 8 0 0G 300.000 5000.000 1401.00
1
2.37888939E+01 2.39146033E-02-8.24877665E-06 1.28829948E-09-7.50678039E-
14 2
1.43968777E+04-1.07094280E+02-8.01337918E+00 1.08401947E-01-9.55671696E-
05 3
4.25996671E-08-7.54462202E-12 2.43488603E+04 5.99659944E+01
4
C2H2A1C2H HW /94C 10H 7 0 0G 300.000 3000.000
1
0.37523422E+02-0.17028838E-01 0.28777416E-04-0.12719674E-07 0.17976818E-
11 2
0.61041488E+05-0.17188731E+03-0.63184557E+01 0.11657917E+00-0.13638573E-
03 3
0.88823526E-07-0.24348468E-10 0.72977062E+05 0.52624207E+02
4
A20-1 HR 6/99 BLYP C 10H 70 1 0G 300.000 5000.000
1401.000 01
2.55199785E+01 2.25375617E-02-7.79622686E-06 1.22014387E-09-7.12043903E-
14 2
-9.13287721E+02-1.15169184E+02-7.45889821E+00 1.10408595E-01-9.86444941E-
05 3
4.41246608E-08-7.80459565E-12 9.35231821E+03 5.79329757E+01
4
A20-2 HR 6/99 BLYP C 10H 70 1 0G 300.000 5000.000
1403.000 01

2.55976281E+01 2.24775925E-02-7.77612184E-06 1.21700823E-09-7.10201185E-
 14 2
 9.06605861E+02-1.15554102E+02-7.30371611E+00 1.10120287E-01-9.82564465E-
 05 3
 4.38428145E-08-7.73044601E-12 1.11390084E+04 5.71293774E+01
 4
 C9H8CH3 C 10H 11 G 300.000 5000.000 5000.00
 1
 5.89344512E+01 0.00000000E+00 0.00000000E+00 0.00000000E+00
 0.00000000E+00 2
 -2.21709548E+04-3.29232464E+02 1.57041459E+00 6.95644403E-02-3.28229474E-
 05 3
 6.86333912E-09-5.24482994E-13 1.81216645E+04 1.77907635E+01
 4
 C9H7CH3 A03/05C 10H 100 0 G 200.000 6000.000
 1
 1.86540860E+01 3.48863580E-02-1.26166897E-05 2.04645995E-09-1.22929258E-
 13 2
 1.15449258E+04-7.76150716E+01 1.18875957E+00 4.18832401E-02 8.16146240E-
 05 3
 -1.44935702E-07 6.30963635E-11 1.82030553E+04 2.21078212E+01
 2.08834916E+04 4
 CH2A1C3H5 C 10H 11 G 300.000 5000.000 1000.00
 1
 1.67483463E+01 4.28772793E-02-1.72330966E-05 3.17171024E-09-2.19256527E-
 13 2
 2.32349897E+04-6.31821545E+01-1.76504593E+00 7.66199814E-02-7.38084916E-
 06 3
 -4.37073217E-08 2.15782182E-11 2.89532115E+04 3.62119782E+01
 4
 C2H4A1C2H3 C 10H 11 G 300.000 5000.000 1000.00
 1
 1.70180043E+01 4.26012995E-02-1.71156353E-05 3.14899603E-09-2.17621781E-
 13 2
 2.82025965E+04-6.33261200E+01 3.25517974E-03 7.05322722E-02 1.17994144E-
 06 3
 -4.91760790E-08 2.28956529E-11 3.36119476E+04 2.87922152E+01
 4
 A1 (C2H3) 2 C 10H 10 G 300.000 5000.000 5000.00
 1
 5.60848905E+01 0.00000000E+00 0.00000000E+00 0.00000000E+00
 0.00000000E+00 2
 -1.44640324E+04-3.08906342E+02 3.54769133E+00 6.32681160E-02-2.97482733E-
 05 3
 6.21023998E-09-4.74202473E-13 2.29084499E+04 9.41010680E+00
 4
 H2A2 T 7/98C 10H 100 0 G 200.000 6000.000
 1
 1.92211178E+01 3.51247274E-02-1.27719042E-05 2.07903232E-09-1.25191968E-
 13 2
 4.39595221E+03-8.19390283E+01-1.92135165E-01 4.50394780E-02 8.64482370E-
 05 3
 -1.56640588E-07 6.88727900E-11 1.16587583E+04 2.82951960E+01
 1.40900666E+04 4
 C5H5-C5H5 6/22/94 THERMC 10H 10 0 OG 300.000 5000.000
 1390.000 01
 2.37376593E+01 3.04584890E-02-1.08284032E-05 1.72545836E-09-1.01947418E-
 13 2

1.46634901E+04-1.07726856E+02-2.04390488E+01 1.33899523E-01-1.01916956E-
04 3
3.75374041E-08-5.40373749E-12 2.97634367E+04 1.29084476E+02
4
C5H5-C5H4 9/ 2/93 THERMC 10H 9 0 0G 300.000 5000.000
1399.000 01
2.45083550E+01 2.64757146E-02-9.27286602E-06 1.46300495E-09-8.58478665E-
14 2
3.23863450E+04-1.13439904E+02-1.34109066E+01 1.24639346E-01-1.07874970E-
04 3
4.68295361E-08-8.08624375E-12 4.44966038E+04 8.66451589E+01
4
A2OH-1 HR 6/99 BLYP C 10H 80 1 0G 300.000 5000.000
1395.000 11
2.61461217E+01 2.46035266E-02-8.61118350E-06 1.35779500E-09-7.96351828E-
14 2
-1.62253653E+04-1.17940723E+02-7.42523947E+00 1.15882243E-01-1.06394867E-
04 3
4.96248553E-08-9.19061783E-12-5.79458155E+03 5.78975921E+01
4
A2OH-2 HR 6/99 BLYP C 10H 80 1 0G 300.000 5000.000
1394.000 11
2.60758935E+01 2.46910885E-02-8.64754101E-06 1.36410864E-09-8.00285533E-
14 2
-1.61139144E+04-1.18755598E+02-8.31179579E+00 1.19635782E-01-1.12084722E-
04 3
5.32313499E-08-1.00013101E-11-5.54787579E+03 6.08896927E+01
4
A2CH3-1 HR 6/99 BLYP C 11H 10 0 0G 300.000 5000.000
1394.000 11
2.69620791E+01 2.88172394E-02-1.00254209E-05 1.57466721E-09-9.21126923E-
14 2
5.87059336E+02-1.25204688E+02-7.98962224E+00 1.17448428E-01-9.76360478E-
05 3
4.14932114E-08-7.10609396E-12 1.20022223E+04 5.99922187E+01
4
A2CH2-1 HR 6/99 BLYP C 11H 9 0 0G 300.000 5000.000
1393.000 11
2.67591143E+01 2.66944366E-02-9.34672512E-06 1.47411301E-09-8.64694573E-
14 2
1.79163708E+04-1.23291372E+02-9.42561321E+00 1.26956297E-01-1.19253218E-
04 3
5.69889164E-08-1.07817848E-11 2.90341851E+04 6.56750520E+01
4
C11H8 C9H7C2H C 11H 8 G 300.000 5000.000 1000.00
1
1.87462390E+01 3.59986303E-02-1.47206334E-05 2.74279891E-09-1.91308882E-
13 2
3.93705507E+04-7.54378047E+01-3.18972441E+00 8.77617597E-02-3.83942409E-
05 3
-1.74555204E-08 1.38534520E-11 4.55567796E+04 3.93857196E+01
4
C11H7 C9H6C2H C 11H 7 G 300.000 5000.000 1000.00
1
1.91382170E+01 3.27122733E-02-1.34043269E-05 2.50156852E-09-1.74701818E-
13 2
4.96079143E+04-7.64018259E+01-2.83251519E+00 8.73710500E-02-4.55562638E-
05 3

-9.28795908E-09 1.10787181E-11 5.56632684E+04 3.79002949E+01
 4
 A2CH3-2 HR 6/99 BLYP C 11H 10 0 0G 300.000 5000.000
 1394.000 11
 2.69193347E+01 2.88860474E-02-1.00554939E-05 1.57995341E-09-9.24422986E-
 14 2
 5.52025831E+02-1.23762368E+02-7.79722831E+00 1.17384742E-01-9.81964263E-
 05 3
 4.20963921E-08-7.27587265E-12 1.18609409E+04 6.00521996E+01
 4
 A2CH2-2 HR 6/99 BLYP C 11H 9 0 0G 300.000 5000.000
 1393.000 11
 2.67837993E+01 2.67091735E-02-9.35972813E-06 1.47696837E-09-8.66691339E-
 14 2
 1.80361580E+04-1.23392042E+02-9.37163916E+00 1.27337620E-01-1.20319319E-
 04 3
 5.78670534E-08-1.10107665E-11 2.91224235E+04 6.53001580E+01
 4
 P2 th1011corrC 12H 10 0 0G 300.000 5000.000 1399.00
 1
 2.80048847E+01 3.04182301E-02-1.05632235E-05 1.65703989E-09-9.68431697E-
 14 2
 7.60008446E+03-1.30404203E+02-1.06222431E+01 1.30784097E-01-1.12105297E-
 04 3
 4.88250011E-08-8.50243029E-12 1.99380068E+04 7.33482812E+01
 4
 P2- HW /94C 12H 9 0 0G 300.000 3000.000
 1
 0.44711853E+02-0.22851825E-01 0.39102117E-04-0.17352100E-07 0.24579375E-
 11 2
 0.33714000E+05-0.21220692E+03-0.11851097E+02 0.13545156E+00-0.13310938E-
 03 3
 0.73769911E-07-0.18193003E-10 0.49878781E+05 0.81107361E+02
 4
 BIPHEN HR 4/99 BLYP00C 12H 8 0 0G 300.000 5000.000 1397.00
 1
 2.81058000E+01 2.51442945E-02-8.64168611E-06 1.34737570E-09-7.84473915E-
 14 2
 3.65344197E+04-1.32106002E+02-9.50452662E+00 1.23502500E-01-1.08069883E-
 04 3
 4.72089337E-08-8.16189729E-12 4.83910029E+04 6.59052149E+01
 4
 A2C2HA HW /94C 12H 8 0 0G 300.000 3000.000
 1
 0.49453674E+02-0.33857111E-01 0.46505607E-04-0.19681195E-07 0.27340769E-
 11 2
 0.26851051E+05-0.23933099E+03-0.11530450E+02 0.14741433E+00-0.17302344E-
 03 3
 0.11500390E-06-0.32709183E-10 0.43793129E+05 0.74391754E+02
 4
 A2C2HA* HW /94C 12H 7 0 0G 300.000 3000.000
 1
 0.36614349E+02-0.60314685E-02 0.21614964E-04-0.10579910E-07 0.15563124E-
 11 2
 0.60723898E+05-0.17026691E+03-0.84175968E+01 0.12391680E+00-0.12250672E-
 03 3
 0.64071344E-07-0.13889583E-10 0.73248562E+05 0.61893204E+02
 4

A2C2HB HW /94C 12H 8 0 0G 300.000 3000.000
1
0.18184774E+02 0.41343965E-01-0.17302822E-04 0.31004770E-08-0.17580817E-
12 2
0.36171543E+05-0.73466003E+02-0.68233256E+01 0.11382083E+00-0.88584900E-
04 3
0.25930856E-07 0.80712824E-12 0.42797719E+05 0.54592098E+02
4
A2C2HB* HW /94C 12H 7 0 0G 300.000 3000.000
1
0.44933517E+02-0.26026871E-01 0.38589074E-04-0.16646357E-07 0.23321310E-
11 2
0.57926637E+05-0.21417279E+03-0.11824737E+02 0.14904183E+00-0.18618468E-
03 3
0.13129460E-06-0.39145326E-10 0.73385375E+05 0.76273834E+02
4
A2R5 HW /94C 12H 8 0 0G 300.000 3000.000
1
0.45883698E+02-0.27226903E-01 0.41569336E-04-0.18047093E-07 0.25351396E-
11 2
0.13394574E+05-0.22304584E+03-0.97011614E+01 0.12019449E+00-0.98907694E-
04 3
0.37240884E-07-0.41124578E-11 0.29601926E+05 0.66970596E+02
4
A2R5- P10/91C 12H 7 0 0G 300.000 3000.000
1
0.11953428E+02 0.52386072E-01-0.27695257E-04 0.69858391E-08-0.68493856E-
12 2
0.53199520E+05-0.40392492E+02-0.73380268E+01 0.11196580E+00-0.93282945E-
04 3
0.35866342E-07-0.42660222E-11 0.58059767E+05 0.57350714E+02
4
A2C2H2 HW /94C 12H 9 0 0G 300.000 3000.000
1
0.38449295E+02-0.62794946E-02 0.24404828E-04-0.11968822E-07 0.17586878E-
11 2
0.41090176E+05-0.17668623E+03-0.78516331E+01 0.12104863E+00-0.10531662E-
03 3
0.46280483E-07-0.77963885E-11 0.54316234E+05 0.63654388E+02
4
P2-H HW /94C 12H 11 0 0G 300.000 3000.000
1
0.41542511E+02-0.83502531E-02 0.29097937E-04-0.14148299E-07 0.20728341E-
11 2
0.22772937E+05-0.19578616E+03-0.99978790E+01 0.12279570E+00-0.80112615E-
04 3
0.11102152E-07 0.64273890E-11 0.37960410E+05 0.74195984E+02
4
C12H9 HR 4/99 BLYP00C 12H 9 0 0G 300.000 5000.000
1402.000 1
2.87663424E+01 2.73722766E-02-9.45354931E-06 1.47784724E-09-8.61724077E-
14 2
4.70722218E+04-1.34442577E+02-1.03237782E+01 1.32036012E-01-1.18286026E-
04 3
5.31769275E-08-9.45503080E-12 5.91991673E+04 7.05721752E+01
4
BICYCLO C 12H 10 G 200.000 6000.000 1000.00
1

0.22254488E+02 0.37643162E-01-0.13667443E-04 0.22246959E-08-0.13403330E-
 12 2
 0.32117245E+05-0.99857186E+02-0.38085817E+01 0.73943066E-01 0.33811263E-
 04 3
 -0.97380150E-07 0.41755272E-10 0.40727478E+05 0.42870152E+02
 4
 C13H9 C 13H 9 G 300.000 5000.000 1000.00
 1
 1.99024059E+01 4.38048667E-02-1.79247083E-05 3.34188072E-09-2.33215009E-
 13 2
 3.56237338E+04-8.40981004E+01-5.31476280E+00 9.30601549E-02-1.43875608E-
 05 3
 -5.06296041E-08 2.61630028E-11 4.32478368E+04 5.04635083E+01
 4
 C13H10 HR11/99 BLYP C 13H 10 0 OG 300.000 5000.000
 1400.000 01
 3.04476803E+01 3.11178654E-02-1.07640759E-05 1.68444388E-09-9.82875496E-
 14 2
 5.92347405E+03-1.45855799E+02-1.14291780E+01 1.40625771E-01-1.21919889E-
 04 3
 5.33286885E-08-9.28204948E-12 1.91832070E+04 7.47141338E+01
 4
 C13H12 th1011corrC 13H 12 0 OG 300.000 5000.000 1391.00
 1
 3.09340100E+01 3.57492642E-02-1.25388398E-05 1.97997572E-09-1.16245781E-
 13 2
 3.45809832E+03-1.45318340E+02-9.96702319E+00 1.33907737E-01-1.03445452E-
 04 3
 4.06528413E-08-6.48107478E-12 1.73784372E+04 7.33847060E+01
 4
 p-C13H9 T06/07C 13H 9 G 200.000 6000.000
 1
 2.35179709E+01 3.67313078E-02-1.33789423E-05 2.18093517E-09-1.31476181E-
 13 2
 2.03004536E+04-1.05863041E+02-2.43578513E+00 6.64744455E-02 6.43511201E-
 05 3
 -1.47288149E-07 6.78181636E-11 2.92499630E+04 3.76466027E+01
 3.17878023E+04 4
 C13H11 th1011C 13H 11 0 OG 300.000 5000.000 1390.00
 1
 3.10961477E+01 3.35160687E-02-1.17745038E-05 1.86127950E-09-1.09358735E-
 13 2
 2.15358064E+04-1.45552287E+02-7.87568307E+00 1.26997733E-01-9.83183301E-
 05 3
 3.86754917E-08-6.17018928E-12 3.48061017E+04 6.28552727E+01
 4
 p-C13H10 Phenalen T06/07C 13H 10 0 OG 200.000 6000.000
 1
 2.30587880E+01 3.98725277E-02-1.45204967E-05 2.36649405E-09-1.42632620E-
 13 2
 1.12405240E+04-1.03108891E+02-1.08611198E+00 5.82879410E-02 8.65824731E-
 05 3
 -1.67474671E-07 7.43250497E-11 2.00434823E+04 3.27080726E+01
 2.27794542E+04 4
 A3 HW /94C 14H 10 0 OG 300.000 3000.000
 1
 0.55916473E+02-0.35253201E-01 0.52522926E-04-0.22672634E-07 0.31770584E-
 11 2

0.32654609E+04-0.27604980E+03-0.12275226E+02 0.15032256E+00-0.13862801E-
 03 3
 0.69376767E-07-0.15105445E-10 0.23030492E+05 0.78889145E+02
 4
 A3-1 HW /94C 14H 9 0 0G 300.000 3000.000
 1
 0.51812469E+02-0.28380312E-01 0.45409150E-04-0.19924162E-07 0.28118107E-
 11 2
 0.34357359E+05-0.25257889E+03-0.73971558E+01 0.11464679E+00-0.57456185E-
 04 3
 -0.14070547E-07 0.16005933E-10 0.52239715E+05 0.59582397E+02
 4
 A3-4 HR 6/99BLYP00C 14H 9 0 0G 300.000 5000.000
 1401.000 1
 3.24592632E+01 2.94561329E-02-1.02023235E-05 1.59803996E-09-9.33111464E-
 14 2
 3.82894894E+04-1.54957971E+02-1.09120537E+01 1.44627958E-01-1.28798224E-
 04 3
 5.73715648E-08-1.01060264E-11 5.18219254E+04 7.28191713E+01
 4
 A2 (C2H)2 HW /94C 14H 8 0 0G 300.000 3000.000
 1
 0.23671062E+02 0.42137049E-01-0.17596645E-04 0.31081251E-08-0.16805216E-
 12 2
 0.77926273E+05-0.99615448E+02-0.63029008E+01 0.13745695E+00-0.13055481E-
 03 3
 0.60730663E-07-0.10178345E-10 0.85489430E+05 0.51891548E+02
 4
 C14H14 C 14H 140 0 0G 300.00 3000.00 1000.00
 1
 0.72920350E+01 0.92502000E-01-0.51686410E-04 0.13627090E-07-0.13811480E-
 11 2
 0.10316730E+05-0.11327380E+02-0.13889580E+02 0.17209840E+00-0.17006600E-
 03 3
 0.96018880E-07-0.23732530E-10 0.15032340E+05 0.92707360E+02
 4
 C14H13 C 14H 130 0 0G 300.00 5000.00 1000.00
 1
 0.29929100E+02 0.38304220E-01-0.11866330E-04 0.17730590E-08-0.10447670E-
 12 2
 0.19709960E+05-0.13171330E+03-0.76621550E+01 0.13350520E+00-0.97310320E-
 04 3
 0.34282990E-07-0.47893710E-11 0.30991570E+05 0.65813480E+02
 4
 C14H12 C 14H 12 0 0G 300.00 3000.00 1000.00
 1
 0.26849750E+02 0.42842930E-01-0.15078500E-04 0.24664360E-08-0.15471790E-
 12 2
 0.16421770E+05-0.11741830E+03-0.79270120E+01 0.13207530E+00-0.88117330E-
 04 3
 0.19095230E-07 0.17687960E-11 0.26386720E+05 0.64074330E+02
 4
 C14H11 3/19/ 9 THERMC 14H 11 0 0G 300.000 5000.000
 1395.000 11
 3.27609182E+01 3.39480669E-02-1.17667240E-05 1.84362057E-09-1.07661574E-
 13 2
 2.92915217E+04-1.51883228E+02-6.70772425E+00 1.32788823E-01-1.07842007E-
 04 3

4.47787253E-08-7.50278981E-12 4.22802338E+04 5.76442987E+01
 4
 C14H1300 3/19/ 9 THERMC 14H 130 2 0G 300.000 5000.000
 1394.000 41
 3.76701265E+01 3.91886728E-02-1.36838688E-05 2.15430957E-09-1.26216113E-
 13 2
 4.38748283E+03-1.69872607E+02-9.53800906E+00 1.60095043E-01-1.34982895E-
 04 3
 5.84090458E-08-1.01919995E-11 1.97390228E+04 7.99308597E+01
 4
 C14H1300H 3/19/ 9 THERMC 14H 140 2 0G 300.000 5000.000
 1395.000 51
 4.01427062E+01 3.93395367E-02-1.37664348E-05 2.17056135E-09-1.27304368E-
 13 2
 -1.39277882E+04-1.84904308E+02-1.04261530E+01 1.68709899E-01-1.42892982E-
 04 3
 6.15601039E-08-1.06485940E-11 2.47291567E+03 8.26365480E+01
 4
 C14H1200H 3/19/ 9 THERMC 14H 130 2 0G 300.000 5000.000
 1394.000 41
 4.02968908E+01 3.71210431E-02-1.30088643E-05 2.05309245E-09-1.20495552E-
 13 2
 3.67900543E+03-1.86479334E+02-8.32529422E+00 1.61762848E-01-1.37724101E-
 04 3
 5.95672829E-08-1.03363053E-11 1.94259748E+04 7.06782085E+01
 4
 C14H1202H-102 9/ 9 THERMC 14H 130 4 0G 300.000 5000.000
 1391.000 71
 4.48785960E+01 3.75685709E-02-1.32824040E-05 2.10858085E-09-1.24255944E-
 13 2
 -9.97231472E+03-2.04041648E+02-9.40646930E+00 1.77878119E-01-1.55260847E-
 04 3
 6.84418245E-08-1.20655066E-11 7.52457116E+03 8.27128410E+01
 4
 C14H110-102H 19/ 9 THERMC 14H 120 3 0G 300.000 5000.000
 1393.000 41
 4.03057402E+01 3.72594407E-02-1.30902950E-05 2.06942373E-09-1.21596482E-
 13 2
 -2.78034193E+04-1.82398868E+02-7.77794671E+00 1.57347464E-01-1.29564931E-
 04 3
 5.40605490E-08-9.07699935E-12-1.19364337E+04 7.29984559E+01
 4
 C14H130 3/19/ 9 THERMC 14H 130 1 0G 300.000 5000.000
 1397.000 31
 3.62205336E+01 3.75634484E-02-1.29678295E-05 2.02688785E-09-1.18180078E-
 13 2
 5.74597621E+03-1.65590808E+02-1.19190739E+01 1.59861239E-01-1.33105430E-
 04 3
 5.60228564E-08-9.42896323E-12 2.13328544E+04 8.92151705E+01
 4
 A3L HR 6/99 BLYP C 14H 10 0 0G 300.000 5000.000
 1401.000 01
 3.27305985E+01 3.17099289E-02-1.09656373E-05 1.71571476E-09-1.00103347E-
 13 2
 1.17362521E+04-1.58794553E+02-1.17398193E+01 1.49210569E-01-1.31450144E-
 04 3
 5.81987746E-08-1.02185477E-11 2.56849262E+04 7.49877748E+01
 4

C13H9CH2 CBS-QB3C 14H 11 0 0G 300.000 5000.000 1402.00
 1
 3.35675946E+01 3.29335008E-02-1.12551052E-05 1.74732670E-09-1.01402089E-
 13 2
 2.91973971E+04-1.58421846E+02-1.00563930E+01 1.48339590E-01-1.29515501E-
 04 3
 5.70592278E-08-9.97553162E-12 4.28413950E+04 7.08180720E+01
 4
 C13H8CH2 CBS-QB3C 14H 10 0 0G 300.000 5000.000 1400.00
 1
 3.28469542E+01 3.16630850E-02-1.09601031E-05 1.71588858E-09-1.00153304E-
 13 2
 1.69163469E+04-1.57867490E+02-1.10527644E+01 1.47504519E-01-1.29658655E-
 04 3
 5.73541044E-08-1.00702016E-11 3.07102768E+04 7.29834464E+01
 4
 A2C2H2A G3B3 H 9C 120 0N 0G 300.000 3000.000
 1000.000 1
 8.53385239E+00 6.87542797E-02-4.01750101E-05 1.11481146E-08-1.19062243E-
 12 2
 5.27583345E+04-1.97684170E+01-9.26784872E+00 1.35043130E-01-1.29791842E-
 04 3
 6.27220331E-08-1.16348577E-11 5.64832554E+04 6.71406964E+01
 2.80382524E+04 4
 A2C2H2B G3B3 H 9C 120 0N 0G 300.000 3000.000
 1000.000 1
 7.59341132E+00 7.02776920E-02-4.10737558E-05 1.14009233E-08-1.21860863E-
 12 2
 5.29378620E+04-1.44753573E+01-9.38518818E+00 1.34825796E-01-1.28962273E-
 04 3
 6.14480428E-08-1.09467156E-11 5.63724233E+04 6.79544608E+01
 2.78776314E+04 4
 A3CH3 5/ 3/97 THERMC 15H 12 0 0G 300.000 5000.000
 2025.000 11
 2.86721901E+01 4.57935671E-02-1.67466881E-05 2.72794395E-09-1.63863026E-
 13 2
 6.77859249E+03-1.31269124E+02 2.45407326E-01 1.03437006E-01-5.52427842E-
 05 3
 1.17708807E-08-4.92994185E-13 1.69368456E+04 2.37077261E+01
 4
 A3CH2 5/ 3/97 THERMC 15H 11 0 0G 300.000 5000.000
 2030.000 11
 2.95619587E+01 4.24589619E-02-1.55841596E-05 2.54481062E-09-1.53124916E-
 13 2
 2.56273028E+04-1.36219923E+02 1.33783643E-01 1.04067922E-01-5.92362501E-
 05 3
 1.43179766E-08-9.91637313E-13 3.59458944E+04 2.35063505E+01
 4
 A3C2H HW /94C 16H 10 0 0G 300.000 3000.000
 1
 0.52165146E+02-0.13197318E-01 0.34353056E-04-0.16283892E-07 0.23677362E-
 11 2
 0.34235055E+05-0.25406651E+03-0.11602674E+02 0.16824394E+00-0.16432030E-
 03 3
 0.86394380E-07-0.19310567E-10 0.52172836E+05 0.75515366E+02
 4
 A3C2H-1 HR BLYP-THERMC 16H 9 0 0G 300.000 5000.000
 1397.000 1

3.70857649E+01 3.04702886E-02-1.05239953E-05 1.64574966E-09-9.60012998E-
 14 2
 6.46707148E+04-1.75357378E+02-7.64228357E+00 1.48096120E-01-1.30459803E-
 04 3
 5.75544684E-08-1.00616675E-11 7.87427736E+04 5.99568969E+01
 4
 A3C2H-2 HR BLYP-THERMC 16H 9 0 0G 300.000 5000.000
 1398.000 1
 3.67812640E+01 3.10152926E-02-1.07699767E-05 1.68976783E-09-9.87789667E-
 14 2
 6.37587690E+04-1.73313834E+02-7.59050661E+00 1.48490072E-01-1.31806093E-
 04 3
 5.88251124E-08-1.04170126E-11 7.76876714E+04 5.99259097E+01
 4
 A4 HW /94C 16H 10 0 0G 300.000 3000.000
 1
 0.58017273E+02-0.29164989E-01 0.48728383E-04-0.21593682E-07 0.30609786E-
 11 2
 0.43451016E+04-0.29017163E+03-0.13759249E+02 0.16772294E+00-0.15500121E-
 03 3
 0.75759544E-07-0.15674045E-10 0.24996187E+05 0.82853027E+02
 4
 A4-1 HR11/99 BLYP C 16H 9 0 0G 300.000 5000.000
 1401.000 1
 3.63345177E+01 3.13968020E-02-1.09044660E-05 1.71125597E-09-1.00056355E-
 13 2
 4.05143093E+04-1.77494305E+02-1.20603441E+01 1.59247554E-01-1.41562602E-
 04 3
 6.26071650E-08-1.09305161E-11 5.56473533E+04 7.68451211E+01
 4
 A4-2 HR11/99 BLYP C 16H 9 0 0G 300.000 5000.000
 1401.000 1
 3.63627635E+01 3.14148576E-02-1.09190450E-05 1.71432648E-09-1.00264960E-
 13 2
 4.04978572E+04-1.78212405E+02-1.20714675E+01 1.60238508E-01-1.43696791E-
 04 3
 6.41750590E-08-1.13112521E-11 5.55777705E+04 7.60615466E+01
 4
 A4-4 HR11/99 BLYP C 16H 9 0 0G 300.000 5000.000
 1402.000 1
 3.63232136E+01 3.13940645E-02-1.09004163E-05 1.71027067E-09-9.99837591E-
 14 2
 4.04517725E+04-1.77288275E+02-1.19738229E+01 1.59343863E-01-1.42091968E-
 04 3
 6.30656072E-08-1.10480587E-11 5.55239715E+04 7.64192993E+01
 4
 A3C2H2 HW /94C 16H 11 0 0G 300.000 3000.000
 1
 0.47582428E+02-0.12822752E-02 0.25647692E-04-0.13378838E-07 0.20086545E-
 11 2
 0.46191215E+05-0.22653258E+03-0.95893555E+01 0.15080631E+00-0.11617327E-
 03 3
 0.36814228E-07-0.12802901E-11 0.62701906E+05 0.71309311E+02
 4
 FLTHN HR 4/99 BLYP C 16H 10 0 0G 300.000 5000.000
 1401.000 01
 3.65828989E+01 3.36775448E-02-1.16788087E-05 1.83083981E-09-1.06967522E-
 13 2

1.72680575E+04-1.79821482E+02-1.30869351E+01 1.64239769E-01-1.44492135E-
04 3
6.34903784E-08-1.10395110E-11 3.28765164E+04 8.14697326E+01
4
A2R5R5 HR10/99 BLYP C 14H 8 0 OG 300.000 5000.000
1402.000 1
3.28490550E+01 2.60248665E-02-8.91800935E-06 1.38871423E-09-8.08143425E-
14 2
3.45307798E+04-1.62050775E+02-1.32440960E+01 1.46606682E-01-1.29756959E-
04 3
5.62162665E-08-9.53671891E-12 4.89332175E+04 8.03986449E+01
4
C18H12 CJP MM300 C 18H 12 0 OG 300.000 5000.000
1396.000 01
4.03265821E+01 4.07367876E-02-1.41254026E-05 2.21402777E-09-1.29334587E-
13 2
1.44447416E+04-1.98056385E+02-1.09140922E+01 1.70112390E-01-1.40590704E-
04 3
5.88710739E-08-9.88423095E-12 3.11466099E+04 7.34991683E+01
4
CHRYSEN CJP MM300 C 18H 12 0 OG 300.000 5000.000
1396.000 01
4.02767814E+01 4.07664763E-02-1.41327835E-05 2.21487630E-09-1.29371528E-
13 2
1.36797665E+04-1.98070319E+02-1.06837095E+01 1.69184362E-01-1.39372979E-
04 3
5.81858481E-08-9.74318604E-12 3.03145297E+04 7.20877574E+01
4
CHRYSEN-1 MM300-THERM C 18H 11 0 OG 300.000 5000.000
1395.000 1
3.94271918E+01 3.92828136E-02-1.36947073E-05 2.15400475E-09-1.26125737E-
13 2
4.43864722E+04-1.91848271E+02-9.12122835E+00 1.60307896E-01-1.30504730E-
04 3
5.38950856E-08-8.95299337E-12 6.03944025E+04 6.60377334E+01
4
CHRYSEN-4 MM300-THERM C 18H 11 0 OG 300.000 5000.000
1395.000 1
3.94271918E+01 3.92828136E-02-1.36947073E-05 2.15400475E-09-1.26125737E-
13 2
4.43864722E+04-1.91848271E+02-9.12122835E+00 1.60307896E-01-1.30504730E-
04 3
5.38950856E-08-8.95299337E-12 6.03944025E+04 6.60377334E+01
4
CHRYSEN-5 MM300-THERM C 18H 11 0 OG 300.000 5000.000
1395.000 1
3.94271918E+01 3.92828136E-02-1.36947073E-05 2.15400475E-09-1.26125737E-
13 2
4.43864722E+04-1.91848271E+02-9.12122835E+00 1.60307896E-01-1.30504730E-
04 3
5.38950856E-08-8.95299337E-12 6.03944025E+04 6.60377334E+01
4
BIN1A C 20H 16 G 300.00 5000.00 1000.00
1
.228710599E+02 .794839410E-01-.421619700E-04 .106691760E-07-.104891690E-
11 2
.555088663E+05-.100165423E+03-.143921700E+02 .205071170E+00-.201668750E-
03 3

.100637160E-06-.198341200E-10 .644124530E+05 .861129840E+02
4
DIBZFUL C 12H 80 1 G 300.00 5000.00 1000.00
1
.238928699E+02 .342239370E-01-.125916314E-04 .206592304E-08-.125089220E-
12 2
-.481449779E+04-.107327684E+03-.194754604E+01 .663215475E-01 .555418713E-
04 3
-.135401425E-06 .629515620E-10 .401745217E+04 .350605098E+02
4
O-XYL 10/10/17 THERMC 8H 10 0 OG 300.000 5000.000
1394.000 21!!lille therm
1.99603072E+01 2.61557358E-02-8.98445826E-06 1.39910174E-09-8.13519247E-
14 2!!lille therm
-7.93705008E+03-8.56839119E+01-2.23616804E+00 7.47294726E-02-4.80125580E-
05 3!!lille therm
1.49315655E-08-1.75829366E-12 4.06831682E+01 3.45895573E+01
4!!lille therm
O-CH3A1CH2 10/17 THERMC 8H 9 0 OG 300.000 5000.000
1393.000 21!!lille therm
2.10859639E+01 2.31751383E-02-8.07079848E-06 1.26830437E-09-7.42108523E-
14 2!!lille therm
1.10048418E+04-9.08168556E+01-4.85819343E+00 9.01056062E-02-7.61868681E-
05 3!!lille therm
3.34644472E-08-5.95459227E-12 1.94423726E+04 4.63784141E+01
4!!lille therm
CH3C6H3CH3 2/ 9/11 THERMC 8H 9 0 OG 300.0000 5000.0000 1391.00
1
1.77730732e+01 2.56908764e-02-8.87032536e-06 1.38580821e-09-8.07516333e-
14 2
2.33300639e+04-6.98691667e+01-2.46103352e+00 7.29856164e-02-5.34677532e-
05 3
2.22509721e-08-4.19935185e-12 3.04920081e+04 3.90749820e+01
4
O-XYLYLE 12/12/17 THERMC 8H 80 0 OG 300.000 5000.000
1401.000 01
1.91160261E+01 2.24292593E-02-7.65460072E-06 1.18682406E-09-6.87993391E-
14 2
2.02335891E+04-8.10119457E+01-5.65069225E+00 8.76628949E-02-7.47164036E-
05 3
3.28480514E-08-5.79511851E-12 2.80692888E+04 4.93373613E+01
4
O-CHOA1CH2 14/17 THERMC 8H 70 1 OG 300.000 5000.000
1379.000 21
2.25494899E+01 1.92674478E-02-6.71231066E-06 1.05633821E-09-6.19085660E-
14 2
-6.23256096E+02-9.63820984E+01-2.93248047E+00 7.75133321E-02-5.62753938E-
05 3
1.96583417E-08-2.65282085E-12 8.22587937E+03 4.07164262E+01
4
P-CHOA1CH2 14/17 THERMC 8H 70 1 OG 300.000 5000.000
1379.000 21
2.25494899E+01 1.92674478E-02-6.71231066E-06 1.05633821E-09-6.19085660E-
14 2
-6.23256096E+02-9.63820984E+01-2.93248047E+00 7.75133321E-02-5.62753938E-
05 3
1.96583417E-08-2.65282085E-12 8.22587937E+03 4.07164262E+01
4

BZCYBUT 12/12/17 THERMC 8H 80 0 0G 300.000 5000.000
 1388.000 01
 2.14287326E+01 2.03959932E-02-6.95785969E-06 1.08007517E-09-6.27116255E-
 14 2
 -3.46435094E+03-1.09918737E+02-3.91731959E+00 7.77441622E-02-5.42730650E-
 05 3
 1.77310647E-08-2.11679938E-12 5.31444027E+03 2.65179500E+01
 4
 OCH3A1CH3 THERMC 8H 90 1 0G 300.0000 5000.0000 1383.00
 1
 2.15355770e+01 2.51599422e-02-8.81158337e-06 1.38996320e-09-8.15442748e-
 14 2
 -1.28341731e+04-8.86566744e+01-1.58262742e+00 7.65818747e-02-5.36592917e-
 05 3
 2.05498452e-08-3.60804210e-12-4.44936673e+03 3.66388431e+01
 4
 HOCH3A1CH3 THERMC 8H 100 1 0G 300.0000 5000.0000 1394.00
 1
 2.18399583e+01 2.67301470e-02-9.19246244e-06 1.43254548e-09-8.33371290e-
 14 2
 -3.01280408e+04-9.11933874e+01-2.21953089e+00 8.40148551e-02-6.31681643e-
 05 3
 2.59624554e-08-4.67959363e-12-2.18285663e+04 3.77741762e+01
 4
 DMCPD 1/29/14 THERMC 7H 10 0 0G 300.0000 5000.0000 1386.00
 1
 2.00248060e+01 2.43495490e-02-8.53823668e-06 1.34790861e-09-7.91193117e-
 14 2
 -3.09399682e+03-8.84053401e+01-4.82340784e+00 8.50625220e-02-6.89290765e-
 05 3
 3.10077860e-08-6.11095701e-12 5.43505902e+03 4.44497065e+01
 4
 O-CH3A1CHO 2/ 9/11 THERMC 8H 80 1 0G 300.0000 5000.0000 1385.00
 1
 2.15355728e+01 2.21029834e-02-7.56076685e-06 1.17505790e-09-6.82594863e-
 14 2
 -1.90198768e+04-8.99129471e+01-2.01261066e+00 7.67085865e-02-5.62243980e-
 05 3
 2.15014759e-08-3.52919768e-12-1.08536548e+04 3.66499505e+01
 4
 P-CH3A1CHO 2/ 9/11 THERMC 8H 80 1 0G 300.0000 5000.0000 1385.00
 1
 2.15355728e+01 2.21029834e-02-7.56076685e-06 1.17505790e-09-6.82594863e-
 14 2
 -1.90198768e+04-8.99129471e+01-2.01261066e+00 7.67085865e-02-5.62243980e-
 05 3
 2.15014759e-08-3.52919768e-12-1.08536548e+04 3.66499505e+01
 4
 O-CH3A1CH2OO 17 THERMC 8H 90 2 0G 300.000 5000.000
 1432.000 31!!!lille therm
 2.52601197E+01 2.43083934E-02-8.47363414E-06 1.33324628E-09-7.81014775E-
 14 2!!!!lille therm
 -2.34014126E+03-1.09095168E+02 2.22874030E+00 6.41716289E-02-2.52790461E-
 05 3!!!!lille therm
 -2.03922976E-09 2.37421131E-12 6.81017580E+03 1.91395824E+01
 4!!!!lille therm
 O-CH3A1CH2O 11 THERMC 8H 90 1 0G 300.0000 5000.0000 1384.00
 1

2.11703280e+01 2.53464121e-02-8.84886707e-06 1.39299564e-09-8.16090100e-
 14 2
 -9.14077584e+01-8.71618243e+01-2.23641893e+00 7.68626220e-02-5.25804240e-
 05 3
 1.92215845e-08-3.18581528e-12 8.40839885e+03 3.98102663e+01
 4
 P-CH3A1CH2O 11 THERMC 8H 90 1 0G 300.0000 5000.0000 1384.00
 1
 2.11703280e+01 2.53464121e-02-8.84886707e-06 1.39299564e-09-8.16090100e-
 14 2
 -9.14077584e+01-8.71618243e+01-2.23641893e+00 7.68626220e-02-5.25804240e-
 05 3
 1.92215845e-08-3.18581528e-12 8.40839885e+03 3.98102663e+01
 4
 O-CH3A1CH2OOH 17 THERMC 8H 100 2 0G 300.000 5000.000
 1393.000 31!!!lille therm
 2.59195656e+01 2.51783511e-02-8.53268288e-06 1.31779909e-09-7.62164870e-
 14 2!!!lille therm
 -1.91987041e+04-1.12094013e+02-6.01685008e+00 1.14659439e-01-1.07208518e-
 04 3!!!lille therm
 5.12332766e-08-9.67938821e-12-9.53285237e+03 5.42563281e+01
 4!!!lille therm
 O-XYLDIMER 25/17 THERMC 16H 18 0 0G 300.000 5000.000
 1390.000 51!! ADDED BY GOUTHAM..
 4.00434841e+01 4.71143433e-02-1.59247188e-05 2.45519281e-09-1.41832276e-
 13 2!! ADDED BY GOUTHAM..
 -1.08447859e+04-1.86968198e+02-8.13791492e+00 1.59387624e-01-1.14159474e-
 04 3!! ADDED BY GOUTHAM..
 4.07524909e-08-5.74891884e-12 5.68398311e+03 7.15121001e+01
 4!! ADDED BY GOUTHAM..
 O-XYLDIMERJ 25/17 THERMC 16H 17 0 0G 300.000 5000.000
 1390.000 51!! ADDED BY GOUTHAM..
 3.96855071e+01 4.55818273e-02-1.55435754e-05 2.41031908e-09-1.39788706e-
 13 2!! ADDED BY GOUTHAM..
 6.12096981e+03-1.86423185e+02-8.33893130e+00 1.57221631e-01-1.13050885e-
 04 3!! ADDED BY GOUTHAM..!!
 4.03941907e-08-5.70400870e-12 2.26403405e+04 7.13395413e+01
 4!! ADDED BY GOUTHAM..
 O-XYLQOOH 25/17 THERMC 8H 90 2 0G 300.000 5000.000
 1395.000 31!!!lille therm
 2.66241046e+01 2.27862793e-02-7.86216767e-06 1.22830404e-09-7.15905895e-
 14 2!!!lille therm
 5.81136586e+01-1.15045349e+02-8.47305133e+00 1.29787798e-01-1.35531159e-
 04 3!!!lille therm
 7.00830292e-08-1.39726398e-11 9.93179379e+03 6.48913803e+01
 4!!!lille therm
 O-XYLSECO2 25/17 THERMC 8H 90 4 0G 300.000 5000.000
 1382.000 51!!!lille therm
 3.16308876e+01 2.39776943e-02-8.54315998e-06 1.36315554e-09-8.06120464e-
 14 2!!!lille therm
 -1.38388229e+04-1.38606118e+02-1.28236993e+00 1.04842144e-01-8.62520620e-
 05 3!!!lille therm
 3.60624570e-08-6.11523654e-12-2.76358190e+03 3.68269876e+01
 4!!!lille therm
 O-XYLKET 25/17 THERMC 8H 80 3 0G 300.000 5000.000
 1520.000 31!!!lille therm
 2.68434664e+01 2.31245138e-02-8.14802491e-06 1.29478599e-09-7.64498209e-
 14 2!!!lille therm

-2.83909320E+04-1.15294451E+02-1.05489568E+01 1.43460701E-01-1.50564242E-
 04 3!!!!lille therm
 7.42175010E-08-1.36715742E-11-1.91071253E+04 7.30470544E+01
 4!!!!lille therm
 CHOA1CH2OJ 28/17 THERMC 8H 70 2 0G 300.000 5000.000
 1678.000 21
 2.12252029E+01 2.40961633E-02-8.72426435E-06 1.41398462E-09-8.47079390E-
 14 2
 -1.00446613E+04-8.17128494E+01 1.99695499E+00 6.55765802E-02-3.95572024E-
 05 3
 1.05081194E-08-9.08045339E-13-3.45268377E+03 2.21770021E+01
 4
 CHOA1CHO 28/17 THERMC 8H 60 2 0G 300.000 5000.000
 1388.000 21
 2.36436656E+01 1.78856749E-02-6.13624610E-06 9.56104561E-10-5.56559148E-
 14 2
 -3.15793392E+04-9.72449515E+01-1.90286510E-01 7.44633349E-02-5.66655539E-
 05 3
 2.11044189E-08-3.08031209E-12-2.35373852E+04 3.01995277E+01
 4
 CHOA1CO 28/17 THERMC 8H 50 2 0G 300.000 5000.000
 1391.000 21
 2.30302726E+01 1.58214153E-02-5.41380329E-06 8.42086747E-10-4.89611756E-
 14 2
 -1.34005375E+04-9.31495187E+01 1.06784762E+00 6.95439858E-02-5.53641781E-
 05 3
 2.17973904E-08-3.39241094E-12-6.14240079E+03 2.37349962E+01
 4
 O-CH3A1C2H5 4/17 THERMC 9H 12 0 0G 300.000 5000.000
 1390.000 31
 2.28940422E+01 3.00636510E-02-1.01647495E-05 1.56691279E-09-9.04905508E-
 14 2
 -1.20971803E+04-9.82373597E+01-3.76999487E+00 9.01603623E-02-6.04727066E-
 05 3
 2.00689883E-08-2.59783456E-12-2.71964132E+03 4.55742339E+01
 4
 P-CH3A1C2H5 4/17 THERMC 9H 12 0 0G 300.000 5000.000
 1390.000 31
 2.28940422E+01 3.00636510E-02-1.01647495E-05 1.56691279E-09-9.04905508E-
 14 2
 -1.20971803E+04-9.82373597E+01-3.76999487E+00 9.01603623E-02-6.04727066E-
 05 3
 2.00689883E-08-2.59783456E-12-2.71964132E+03 4.55742339E+01
 4
 O-CH3A1CHCH3 4/17 THERMC 9H 11 0 0G 300.000 5000.000
 1388.000 31
 2.31240651E+01 2.79745654E-02-9.58021493E-06 1.48918554E-09-8.64914856E-
 14 2
 5.41076753E+03-1.00395277E+02-1.57321576E+00 8.28014486E-02-5.47579841E-
 05 3
 1.78468955E-08-2.27069978E-12 1.42187488E+04 3.31699113E+01
 4
 P-CH3A1CHCH3 4/17 THERMC 9H 11 0 0G 300.000 5000.000
 1388.000 31
 2.31240651E+01 2.79745654E-02-9.58021493E-06 1.48918554E-09-8.64914856E-
 14 2
 5.41076753E+03-1.00395277E+02-1.57321576E+00 8.28014486E-02-5.47579841E-
 05 3

1.78468955E-08-2.27069978E-12 1.42187488E+04 3.31699113E+01
4
O-CH3A1CHOOCH3 4/17 THERMC 9H 110 2 0G 300.000 5000.000
1386.000 41
2.93703532E+01 2.71662917E-02-9.28295114E-06 1.44239974E-09-8.37986164E-
14 2
-7.51344602E+03-1.28033800E+02-4.05817487E+00 1.06796283E-01-8.11500641E-
05 3
3.06509056E-08-4.59576088E-12 3.78504955E+03 5.06951304E+01
4
P-CH3A1CHOOCH3 4/17 THERMC 9H 110 2 0G 300.000 5000.000
1386.000 41
2.93703532E+01 2.71662917E-02-9.28295114E-06 1.44239974E-09-8.37986164E-
14 2
-7.51344602E+03-1.28033800E+02-4.05817487E+00 1.06796283E-01-8.11500641E-
05 3
3.06509056E-08-4.59576088E-12 3.78504955E+03 5.06951304E+01
4
O-C2H3A1CH2O 4/17 THERMC 9H 90 1 0G 300.000 5000.000
1374.000 21
2.42780301E+01 2.61237974E-02-9.21757448E-06 1.46119682E-09-8.60164803E-
14 2
1.08650948E+04-1.01525616E+02 1.86974735E+00 7.06575657E-02-4.03677059E-
05 3
1.01590337E-08-7.97323353E-13 1.94975553E+04 2.17126382E+01
4
P-C2H3A1CH2O 4/17 THERMC 9H 90 1 0G 300.000 5000.000
1374.000 21
2.42780301E+01 2.61237974E-02-9.21757448E-06 1.46119682E-09-8.60164803E-
14 2
1.08650948E+04-1.01525616E+02 1.86974735E+00 7.06575657E-02-4.03677059E-
05 3
1.01590337E-08-7.97323353E-13 1.94975553E+04 2.17126382E+01
4
O-C2H3A1CHO 4/17 THERMC 9H 80 1 0G 300.000 5000.000
1394.000 21
2.38940932E+01 2.29009823E-02-7.88366855E-06 1.22978218E-09-7.16012687E-
14 2
-8.88575493E+03-1.00098634E+02-1.73204917E+00 8.61320497E-02-6.81195984E-
05 3
2.75190675E-08-4.48866582E-12-3.76814843E+02 3.62469133E+01
4
P-C2H3A1CHO 4/17 THERMC 9H 80 1 0G 300.000 5000.000
1394.000 21
2.38940932E+01 2.29009823E-02-7.88366855E-06 1.22978218E-09-7.16012687E-
14 2
-8.88575493E+03-1.00098634E+02-1.73204917E+00 8.61320497E-02-6.81195984E-
05 3
2.75190675E-08-4.48866582E-12-3.76814843E+02 3.62469133E+01
4
O-C2H3A1CO 4/17 THERMC 9H 70 1 0G 300.000 5000.000
1397.000 11
2.31130455E+01 2.09289316E-02-7.09349717E-06 1.09524474E-09-6.33219416E-
14 2
9.40958160E+03-9.49518485E+01-6.34879254E-01 8.19482088E-02-6.79060098E-
05 3
2.88688468E-08-4.92982514E-12 1.70418435E+04 3.05230003E+01
4

P-C2H3A1CO 4/17 THERMC 9H 70 1 0G 300.000 5000.000
1397.000 11
2.31130455E+01 2.09289316E-02-7.09349717E-06 1.09524474E-09-6.33219416E-
14 2
9.40958160E+03-9.49518485E+01-6.34879254E-01 8.19482088E-02-6.79060098E-
05 3
2.88688468E-08-4.92982514E-12 1.70418435E+04 3.05230003E+01
4
P-XYL 2012 DRAEGC 8H 100 0 0G 298.0000 5000.0000 1393.00
1
1.94360884e+01 2.67127238e-02-9.20115418e-06 1.43547260e-09-8.35723465e-
14 2
-8.13186712e+03-8.21469657e+01-5.48062003e+00 8.68042905e-02-6.68481596e-
05 3
2.81706222e-08-5.18167310e-12 3.96907254e+02 5.11636765e+01
4
P-CH3A1CH2 2012 C 8H 90 0 0G 300.0000 5000.0000 1395.00
1
2.07324230e+01 2.35417931e-02-8.11892856e-06 1.26773140e-09-7.38526644e-
14 2
1.08491884e+04-8.77408764e+01-5.14234891e+00 9.13700369e-02-7.98005008e-
05 3
3.75980712e-08-7.43523350e-12 1.91935309e+04 4.88299768e+01
4
P-XYLYLE 12/12/17 THERMC 8H 80 0 0G 300.000 5000.000
1401.000 01
1.91160261E+01 2.24292593E-02-7.65460072E-06 1.18682406E-09-6.87993391E-
14 2
2.02335891E+04-8.10119457E+01-5.65069225E+00 8.76628949E-02-7.47164036E-
05 3
3.28480514E-08-5.79511851E-12 2.80692888E+04 4.93373613E+01
4
P-CH3A1CH2OO 1 THERMC 8H 90 2 0G 300.0000 5000.0000 1381.00
1
2.29655269e+01 2.61981843e-02-9.19916109e-06 1.45359015e-09-8.53776304e-
14 2
-1.94932777e+03-9.39677964e+01-7.22070594e-01 7.86810365e-02-5.52563254e-
05 3
2.15731903e-08-3.91891453e-12 6.70772379e+03 3.45695675e+01
4
P-CH3A1CH2OOH 11 THERMC 8H 100 2 0G 300.0000 5000.0000 1384.00
1
2.48705290e+01 2.70784794e-02-9.49238562e-06 1.49832155e-09-8.79417225e-
14 2
-1.96027395e+04-1.05034091e+02-1.49161110e+00 8.68329191e-02-6.27487322e-
05 3
2.46475897e-08-4.36606678e-12-1.01740983e+04 3.74090954e+01
4
P-XYLDIMER 25/17 THERMC 16H 18 0 0G 300.000 5000.000
1390.000 51!! ADDED BY GOUTHAM..
4.00434841E+01 4.71143433E-02-1.59247188E-05 2.45519281E-09-1.41832276E-
13 2!! ADDED BY GOUTHAM..
-1.08447859E+04-1.86968198E+02-8.13791492E+00 1.59387624E-01-1.14159474E-
04 3!! ADDED BY GOUTHAM..
4.07524909E-08-5.74891884E-12 5.68398311E+03 7.15121001E+01
4!! ADDED BY GOUTHAM..
P-XYLDIMERJ 25/17 THERMC 16H 17 0 0G 300.000 5000.000
1390.000 51!! ADDED BY GOUTHAM..

3.96855071E+01 4.55818273E-02-1.55435754E-05 2.41031908E-09-1.39788706E-
 13 2!! ADDED BY GOUTHAM..
 6.12096981E+03-1.86423185E+02-8.33893130E+00 1.57221631E-01-1.13050885E-
 04 3!! ADDED BY GOUTHAM..
 4.03941907E-08-5.70400870E-12 2.26403405E+04 7.13395413E+01
 4!! ADDED BY GOUTHAM..
 CH3C9H7 10/11/12 THERMC 10H 10 0 0G 300.0000 5000.0000 1393.00
 1
 2.30571440E+01 2.93786244E-02-1.01727262E-05 1.59279335E-09-9.29698848E-
 14 2
 3.77531679E+03-1.02919126E+02-7.83941264E+00 1.04412020E-01-8.22228301E-
 05 3
 3.47556729E-08-6.32246512E-12 1.42507108E+04 6.21147345E+01
 4
 XYLMETHIDE H 8C 8O 1 G 100.000 5000.000 1079.76
 1!! XYLENE METHIDE
 1.44818737E+01 3.34669122E-02-1.36868631E-05 2.57522021E-09-1.82216877E-
 13 2!! XYLENE METHIDE
 -5.47183783E+03-5.11116513E+01 1.07514336E+00 5.76006785E-02-1.17449569E-
 05 3!! XYLENE METHIDE
 -2.05225703E-08 1.02359399E-11-1.08826150E+03 2.14889776E+01
 4!! XYLENE METHIDE
 O2CH3A1CH3 17 THERMC 8H 9O 2 0G 300.000 5000.000
 1390.000 31
 2.42093572E+01 2.36095730E-02-7.89505982E-06 1.20885000E-09-6.95106329E-
 14 2
 -8.57198510E+03-9.97745150E+01 4.84608036E-01 7.73253481E-02-5.24789059E-
 05 3
 1.71297226E-08-2.09394525E-12-3.32251188E+02 2.79650353E+01
 4
 O-CH3A1CO 11/14/17 THERMC 8H 7O 1 0G 300.000 5000.000
 1391.000 21
 2.06183493E+01 2.09273001E-02-7.27503620E-06 1.14205671E-09-6.67802675E-
 14 2
 -6.24675873E+01-8.49609150E+01-1.22159760E+00 7.20923192E-02-5.30038361E-
 05 3
 1.97157445E-08-2.96244141E-12 7.47491153E+03 3.22281012E+01
 4
 P-CH3A1CO 11/14/17 THERMC 8H 7O 1 0G 300.000 5000.000
 1391.000 21
 2.06183493E+01 2.09273001E-02-7.27503620E-06 1.14205671E-09-6.67802675E-
 14 2
 -6.24675873E+01-8.49609150E+01-1.22159760E+00 7.20923192E-02-5.30038361E-
 05 3
 1.97157445E-08-2.96244141E-12 7.47491153E+03 3.22281012E+01
 4
 DMCPDR 1/29/14 THERMC 7H 9 0 0G 300.0000 5000.0000 1389.00
 1
 2.04343496E+01 2.14241190E-02-7.52207770E-06 1.18852109E-09-6.98061615E-
 14 2
 1.02066345E+04-8.87542108E+01-4.56858075E+00 8.66194326E-02-7.70176077E-
 05 3
 3.71987656E-08-7.58546834E-12 1.83845398E+04 4.34855552E+01
 4
 O-XYLET 10/20/17 C 8H 8O 1 0G 300.000 5000.000
 1399.000 11
 2.01013444E+01 2.43358824E-02-8.45238771E-06 1.32617988E-09-7.75210931E-
 14 2

-1.57928057E+04-8.65702375E+01-6.74255401E+00 8.62499970E-02-6.18331977E-
 05 3
 2.17042299E-08-2.97379814E-12-6.51723709E+03 5.76689647E+01
 4
 C10H10 8/18/17 THERMC 10H 10 0 0G 300.000 5000.000
 1395.000 01
 2.40970279E+01 2.87966072E-02-9.94674330E-06 1.55505858E-09-9.06783454E-
 14 2
 2.63882435E+03-1.11296583E+02-7.51202561E+00 1.03568479E-01-7.70183408E-
 05 3
 2.86680155E-08-4.25720371E-12 1.34056571E+04 5.79383548E+01
 4
 C10H9 8/18/17 THERMC 10H 9 0 0G 300.000 5000.000
 1388.000 01
 2.45424268E+01 2.67866327E-02-9.45749114E-06 1.50005284E-09-8.83433396E-
 14 2
 1.63265244E+04-1.14633515E+02-7.94662027E+00 1.01396120E-01-7.40077012E-
 05 3
 2.65296668E-08-3.76335018E-12 2.76504481E+04 6.01662208E+01
 4

!Species in anisole mech (Buttgen + Wagnon)

A1OCH3 3/02/16 THERMC 7H 80 1 0G 300.000 5000.000
 1393.000 21
 2.03938728E+01 2.09088165E-02-7.22522263E-06 1.12997840E-09-6.59097524E-
 14 2
 -1.85558154E+04-8.62920505E+01-5.40888697E+00 8.73332441E-02-7.39639658E-
 05 3
 3.20208039E-08-5.56946955E-12-1.02318239E+04 5.00696056E+01
 4
 A1OCH2 OC 7H 70 1 0G 300.00 5000.00 1000.00
 1
 0.10423429E+02 0.30678995E-01-0.10676530E-04 0.17271368E-08-0.10722079E-
 12 2
 0.86203691E+04-0.25813568E+02-0.65495462E+01 0.86909175E-01-0.77541947E-
 04 3
 0.35875342E-07-0.66683451E-11 0.12541898E+05 0.58891670E+02
 4
 C6H4OCH3 H 7C 70 1 G 100.000 5000.000 833.31
 1
 1.09323840E+01 3.18789849E-02-1.33572651E-05 2.58331367E-09-1.87763137E-
 13 2
 1.66757775E+04-2.93561643E+01-1.65161413E+00 5.77267148E-02 2.32047549E-
 06 3
 -5.97248620E-08 3.34354025E-11 1.99728791E+04 3.62588512E+01
 4
 A1OCH2O H 7C 70 2 G 100.000 5000.000 843.33
 1
 1.41132246E+01 3.36062397E-02-1.47746102E-05 2.95177088E-09-2.19276262E-
 13 2
 -1.09589128E+04-4.64845067E+01-1.27653531E+00 5.24885448E-02 4.78876661E-
 05 3
 -1.22668285E-07 5.95745391E-11-6.43889286E+03 3.65486404E+01
 4
 A1CYCH2O H 7C 70 1 G 100.000 5000.000 957.15
 1!YF RMG

1.67936521E+01 2.23249048E-02-7.12614366E-06 1.34846653E-09-1.04198083E-
 13 2
 1.04264021E+04-6.58154793E+01 1.69761697E+00 2.76419662E-02 7.50759557E-
 05 3
 -1.18964687E-07 4.77909520E-11 1.59625196E+04 2.01767778E+01
 4
 PC6H4CHO H 7C 7O 1 G 100.000 5000.000 1259.17
 1!YF RMG
 8.19076856E+00 1.41273094E-02 6.73504584E-06-2.42567063E-09 2.11115825E-
 13 2
 9.53813957E+03-3.76974525E+00 3.63170871E-02 8.48291394E-02-1.30854598E-
 04 3
 9.86751208E-08-2.54714104E-11 8.04033384E+03 2.33479868E+01
 4
 A1OCH2OO H 7C 7O 3 G 100.000 5000.000 1339.12
 1
 2.22224177E+01 2.40288898E-02-9.21760930E-06 1.65461055E-09-1.13196848E-
 13 2
 -1.37447149E+04-8.82807078E+01-1.02695328E+01 1.32943408E-01-1.44501602E-
 04 3
 7.56178851E-08-1.51560630E-11-6.10597934E+03 7.39917694E+01
 4
 OOA1OCH3 H 7C 7O 3 G 100.000 5000.000 1683.17
 1
 1.16641156E+01 3.75973281E-02-1.46919230E-05 2.18675911E-09-1.20674453E-
 13 2
 -4.78856300E+03-2.59986169E+01-1.06553299E+00 8.45822321E-02-7.14759914E-
 05 3
 3.05840888E-08-5.21578103E-12-2.87365946E+03 3.50013836E+01
 4
 A1OCH2OOH H 8C 7O 3 G 100.000 5000.000 939.16
 1
 3.11037833E+01 9.94651207E-03-3.96567829E-07 5.92500861E-11-1.78288716E-
 14 2
 -3.48760699E+04-1.37950185E+02-3.52369864E-01 6.42532666E-02 4.01103602E-
 05 3
 -1.19018961E-07 5.57239541E-11-2.54540886E+04 3.05386187E+01
 4
 A1OCHO H 6C 7O 2 G 100.000 5000.000 893.02
 1
 1.30193589E+01 3.32396379E-02-1.48471882E-05 2.97227971E-09-2.20234046E-
 13 2
 -3.39079600E+04-4.25372187E+01-2.10782382E+00 5.57035836E-02 2.34989104E-
 05 3
 -8.24488971E-08 3.95928264E-11-2.94001298E+04 3.88431377E+01
 4
 A1OCO H 5C 7O 2 G 100.000 5000.000 926.95
 1
 1.41226465E+01 2.87979892E-02-1.26709105E-05 2.50431900E-09-1.83782224E-
 13 2
 -1.02661941E+04-4.79227711E+01-4.14181647E+00 7.75800261E-02-4.30106670E-
 05 3
 -1.06281871E-08 1.27848992E-11-5.58985306E+03 4.57671000E+01
 4
 O-HOAlC2H5 4/ 7/16 THERMC 8H 10O 1 OG 300.000 5000.000
 1401.000 31
 2.32385961E+01 2.47039297E-02-8.31885791E-06 1.27881842E-09-7.37088145E-
 14 2

-2.87622749E+04-9.85445539E+01-4.36287991E+00 9.53449314E-02-7.80414708E-05 3
 3.26598714E-08-5.47508824E-12-1.99038201E+04 4.73218583E+01
 4
 P-HOAlC2H5 4/ 7/16 THERMC 8H 100 1 OG 300.000 5000.000
 1401.000 31
 2.32385961E+01 2.47039297E-02-8.31885791E-06 1.27881842E-09-7.37088145E-14 2
 -2.87622749E+04-9.85445539E+01-4.36287991E+00 9.53449314E-02-7.80414708E-05 3
 3.26598714E-08-5.47508824E-12-1.99038201E+04 4.73218583E+01
 4
 O-HOAlC2H4 4/ 7/16 THERMC 8H 90 1 OG 300.000 5000.000
 1402.000 31
 2.25726154E+01 2.28419432E-02-7.70112596E-06 1.18479282E-09-6.83261183E-14 2
 -3.60718390E+03-9.21564163E+01-3.97149212E+00 9.18069363E-02-7.69431901E-05 3
 3.29030287E-08-5.62032074E-12 4.81208076E+03 4.77618934E+01
 4
 P-HOAlC2H4 4/ 7/16 THERMC 8H 90 1 OG 300.000 5000.000
 1402.000 31
 2.25726154E+01 2.28419432E-02-7.70112596E-06 1.18479282E-09-6.83261183E-14 2
 -3.60718390E+03-9.21564163E+01-3.97149212E+00 9.18069363E-02-7.69431901E-05 3
 3.29030287E-08-5.62032074E-12 4.81208076E+03 4.77618934E+01
 4
 O-HOAlC2H4-S 17 THERMC 8H 90 1 OG 300.000 5000.000
 1400.000 21
 2.34117347E+01 2.24617271E-02-7.55225345E-06 1.15991128E-09-6.68169255E-14 2
 -1.11642027E+04-9.98259851E+01-2.26199952E+00 8.84141554E-02-7.29063784E-05 3
 3.06919837E-08-5.16930289E-12-2.95123843E+03 3.57624548E+01
 4
 P-HOAlC2H4-S 17 THERMC 8H 90 1 OG 300.000 5000.000
 1400.000 21
 2.34117347E+01 2.24617271E-02-7.55225345E-06 1.15991128E-09-6.68169255E-14 2
 -1.11642027E+04-9.98259851E+01-2.26199952E+00 8.84141554E-02-7.29063784E-05 3
 3.06919837E-08-5.16930289E-12-2.95123843E+03 3.57624548E+01
 4
 O-HOAlC2H3 THERMC 8H 80 1 OG 300.0000 5000.0000 1402.00
 1
 2.22088861E+01 2.15221137E-02-7.34732595E-06 1.13952632E-09-6.60747160E-14 2
 -1.40752329E+04-9.28164913E+01-4.07517261E+00 9.34032742E-02-8.56414492E-05 3
 4.12714256E-08-8.13954281E-12-5.96652954E+03 4.47322744E+01
 4
 P-HOAlC2H3 THERMC 8H 80 1 OG 300.0000 5000.0000 1402.00
 1
 2.22088861E+01 2.15221137E-02-7.34732595E-06 1.13952632E-09-6.60747160E-14 2
 -1.40752329E+04-9.28164913E+01-4.07517261E+00 9.34032742E-02-8.56414492E-05 3

4.12714256E-08-8.13954281E-12-5.96652954E+03 4.47322744E+01
4
O-CH3A1OCH3 4/19/16THERMC 8H 100 1 0G 300.000 5000.000
1390.000 31
2.28987853E+01 2.57645011E-02-8.85080215E-06 1.37879998E-09-8.02057157E-
14 2
-2.38370876E+04-9.75854705E+01-3.78203348E+00 9.01065160E-02-6.86742138E-
05 3
2.68915016E-08-4.28245421E-12-1.48028548E+04 4.49448230E+01
4
P-CH3A1OCH3 4/19/16THERMC 8H 100 1 0G 300.000 5000.000
1390.000 31
2.28987853E+01 2.57645011E-02-8.85080215E-06 1.37879998E-09-8.02057157E-
14 2
-2.38370876E+04-9.75854705E+01-3.78203348E+00 9.01065160E-02-6.86742138E-
05 3
2.68915016E-08-4.28245421E-12-1.48028548E+04 4.49448230E+01
4
O-CH3A1OCH2 4/19/16THERMC 8H 90 1 0G 300.000 5000.000
1402.000 31
2.19320611E+01 2.37525615E-02-8.08851911E-06 1.25229366E-09-7.25226103E-
14 2
7.78178451E+02-9.08800845E+01-2.40051606E+00 8.52209896E-02-6.82103557E-
05 3
2.81890609E-08-4.70598579E-12 8.71007166E+03 3.80660567E+01
4
P-CH3A1OCH2 4/19/16THERMC 8H 90 1 0G 300.000 5000.000
1402.000 31
2.19320611E+01 2.37525615E-02-8.08851911E-06 1.25229366E-09-7.25226103E-
14 2
7.78178451E+02-9.08800845E+01-2.40051606E+00 8.52209896E-02-6.82103557E-
05 3
2.81890609E-08-4.70598579E-12 8.71007166E+03 3.80660567E+01
4
O-CH2A1OCH3 4/19/16THERMC 8H 90 1 0G 300.000 5000.000
1391.000 31
2.39276824E+01 2.28070518E-02-7.92985169E-06 1.24510705E-09-7.28199051E-
14 2
-5.32326370E+03-1.03645858E+02-3.44967088E+00 9.23107726E-02-7.69334125E-
05 3
3.29120379E-08-5.68689346E-12 3.63252327E+03 4.14272943E+01
4
P-CH2A1OCH3 4/19/16THERMC 8H 90 1 0G 300.000 5000.000
1391.000 31
2.39276824E+01 2.28070518E-02-7.92985169E-06 1.24510705E-09-7.28199051E-
14 2
-5.32326370E+03-1.03645858E+02-3.44967088E+00 9.23107726E-02-7.69334125E-
05 3
3.29120379E-08-5.68689346E-12 3.63252327E+03 4.14272943E+01
4
O-CH3A1CYCH2O 28/17THERMC 8H 90 1 0G 300.000 5000.000
1400.000 01
2.09828421E+01 2.58300368E-02-8.80342968E-06 1.36362157E-09-7.89915086E-
14 2
5.73989469E+03-8.80915698E+01-4.41651363E+00 9.07414913E-02-7.35234368E-
05 3
3.10856456E-08-5.33261303E-12 1.39890160E+04 4.63165461E+01
4

P-CH3A1CYCH2O 28/17THERMC 8H 90 1 0G 300.000 5000.000
1400.000 01
2.09828421E+01 2.58300368E-02-8.80342968E-06 1.36362157E-09-7.89915086E-
14 2
5.73989469E+03-8.80915698E+01-4.41651363E+00 9.07414913E-02-7.35234368E-
05 3
3.10856456E-08-5.33261303E-12 1.39890160E+04 4.63165461E+01
4

O-CH3A1OCH2OO 71416 THERC 8H 90 3 0G 300.000 5000.000
1396.000 41
2.76880205E+01 2.42111858E-02-8.39875610E-06 1.31675575E-09-7.69314121E-
14 2
-2.13142534E+04-1.15621908E+02-3.94078056E+00 1.06647963E-01-9.21966025E-
05 3
4.04762406E-08-7.10221381E-12-1.12269063E+04 5.11439362E+01
4

P-CH3A1OCH2OO 71416 THERC 8H 90 3 0G 300.000 5000.000
1396.000 41
2.76880205E+01 2.42111858E-02-8.39875610E-06 1.31675575E-09-7.69314121E-
14 2
-2.13142534E+04-1.15621908E+02-3.94078056E+00 1.06647963E-01-9.21966025E-
05 3
4.04762406E-08-7.10221381E-12-1.12269063E+04 5.11439362E+01
4

O-CH3A1OCH2OOH 16 THERMC 8H 100 3 0G 300.000 5000.000
1398.000 41
2.82183755E+01 2.60230269E-02-8.96080235E-06 1.39795157E-09-8.13953512E-
14 2
-3.83187191E+04-1.19100714E+02-4.78238320E+00 1.13042024E-01-9.84018646E-
05 3
4.35818105E-08-7.70115097E-12-2.79047177E+04 5.45237801E+01
4

P-CH3A1OCH2OOH 16 THERMC 8H 100 3 0G 300.000 5000.000
1398.000 41
2.82183755E+01 2.60230269E-02-8.96080235E-06 1.39795157E-09-8.13953512E-
14 2
-3.83187191E+04-1.19100714E+02-4.78238320E+00 1.13042024E-01-9.84018646E-
05 3
4.35818105E-08-7.70115097E-12-2.79047177E+04 5.45237801E+01
4

! species in guaiacol mech

HOA1OCH3 H 8C 7O 2 0g 300.00 5000.00 1000.00
1
1.61510010E+01 3.08602336E-02-1.20305311E-05 2.15078810E-09-1.44654722E-
13 2
-3.82738517E+04-6.06312387E+01-2.29319889E+00 7.49731154E-02-3.92562995E-
05 3
-4.81599827E-09 8.31405011E-12-3.27827558E+04 3.64581013E+01
4

HOA1OCH2 H 7C 7O 2 0g 300.00 5000.00 1000.00
1
1.72628598E+01 2.68503641E-02-1.04320420E-05 1.86100044E-09-1.24985754E-
13 2
-1.48215056E+04-6.58621198E+01-3.31726685E+00 8.60800466E-02-7.08460179E-
05 3

2.49967154E-08-1.55373855E-12-9.23517098E+03 3.99003831E+01
 4
 OA1OCH3 H 7C 70 2 0g 300.00 5000.00 1000.00
 1
 1.58640126E+01 2.87463715E-02-1.13183786E-05 2.03699237E-09-1.37635862E-
 13 2
 -2.04846067E+04-5.88275830E+01-1.71830165E+00 6.90520205E-02-3.21785437E-
 05 3
 -9.69080525E-09 9.66299405E-12-1.51516340E+04 3.41841827E+01
 4
 HOA1OH H 6C 60 2 0g 300.00 5000.00 1000.00
 1
 1.51238150E+01 2.29726531E-02-8.86194695E-06 1.57380573E-09-1.05385588E-
 13 2
 -3.95660562E+04-5.53275434E+01-3.18083661E+00 7.54574099E-02-6.14648164E-
 05 3
 2.05311309E-08-6.87184992E-13-3.46082334E+04 3.87405670E+01
 4
 HOA1OHCH3-4 H 8C 70 2 0g 300.00 5000.00 1000.00
 1 !GM2
 1.71015156E+01 2.95814089E-02-1.14360479E-05 2.03322454E-09-1.36229474E-
 13 2
 -4.42040071E+04-6.35028069E+01-1.28861368E+00 7.65346988E-02-4.74175222E-
 05 3
 4.12341298E-09 5.13154697E-12-3.88928103E+04 3.25314462E+01
 4
 OA1OHCH3-1 H 7C 70 2 0g 300.00 5000.00 1000.00
 1 !GR17
 1.61748973E+01 2.82760041E-02-1.10895671E-05 1.99063968E-09-1.34264403E-
 13 2
 -3.09103522E+04-6.01755311E+01-2.10482169E+00 7.39118395E-02-4.42350375E-
 05 3
 1.83347810E-09 5.74955279E-12-2.55583689E+04 3.55895882E+01
 4
 OA1OHCH3-2 H 7C 70 2 0g 300.00 5000.00 1000.00
 1 !GR16
 1.61670545E+01 2.82878579E-02-1.10954970E-05 1.99187216E-09-1.34355905E-
 13 2
 -3.12735060E+04-5.95498954E+01-2.05239639E+00 7.34657333E-02-4.31677763E-
 05 3
 8.06426548E-10 6.10227670E-12-2.59240738E+04 3.59747810E+01
 4
 OA1CHO H 5C 70 2 0g 300.00 5000.00 1000.00
 1 !GR21
 1.57128932E+01 2.34762967E-02-9.32823881E-06 1.68958415E-09-1.14686475E-
 13 2
 -1.46505373E+04-5.72637304E+01-1.88621841E+00 6.73987767E-02-4.10955419E-
 05 3
 1.36455522E-09 5.59794784E-12-9.50402208E+03 3.49248979E+01
 4
 C5H4CHO H 5C 60 1 0g 300.00 5000.00 1000.00
 1 !GR22
 1.28380541E+01 2.01276337E-02-7.91091062E-06 1.42215338E-09-9.60214471E-
 14 2
 1.12592672E+04-4.27638280E+01-2.50849132E+00 6.25096025E-02-4.76211962E-
 05 3
 1.31673235E-08 7.88515679E-13 1.55233114E+04 3.65652064E+01
 4

OC5H3CH3 H 6C 60 1 0g 300.00 5000.00 1000.00
 1 !GM10
 1.23365398E+01 2.33352741E-02-9.13525276E-06 1.63740164E-09-1.10309620E-
 13 2
 -3.44460322E+03-4.02099211E+01-1.77795935E+00 5.95164407E-02-3.79225067E-
 05 3
 5.06137823E-09 3.13523181E-12 6.53356389E+02 3.35293862E+01
 4

HOC5H3CH3 H 7C 60 1 0g 300.00 5000.00 1000.00
 1 !GR19
 1.34947959E+01 2.45948436E-02-9.50700701E-06 1.68963128E-09-1.13161199E-
 13 2
 -1.96499319E+03-4.64388254E+01-2.42375944E+00 6.81333700E-02-4.92552991E-
 05 3
 1.21824565E-08 1.47268918E-12 2.47707716E+03 3.59446665E+01
 4

OC6H3(O)CH3 H 6C 70 2 0g 300.00 5000.00 1000.00
 1 !GM15
 1.55941637E+01 2.62807596E-02-1.03826940E-05 1.87278066E-09-1.26734685E-
 13 2
 -2.16142986E+04-5.55895081E+01-4.40841862E-01 6.52674409E-02-3.75988492E-
 05 3
 1.04204908E-09 4.90628772E-12-1.68195743E+04 2.87922963E+01
 4

OA1OH H 5C 60 2 0g 300.00 5000.00 1000.00
 1
 1.41718387E+01 2.16992179E-02-8.53015380E-06 1.53412649E-09-1.03629451E-
 13 2
 -2.56811298E+04-5.08854417E+01-3.79810725E+00 7.16742679E-02-5.59834086E-
 05 3
 1.62781753E-08 5.50853264E-13-2.07145206E+04 4.18997807E+01
 4

C5H5CO H 5C 60 1 0g 300.00 5000.00 1000.00
 1 !GR23
 1.26822360E+01 2.02317291E-02-7.93985829E-06 1.42585429E-09-9.61986515E-
 14 2
 1.79660382E+04-4.07801049E+01-3.12980966E+00 6.48368957E-02-5.13976992E-
 05 3
 1.58503852E-08 9.95019108E-14 2.23011953E+04 4.06942841E+01
 4

HOA1CYCH2O 28/17THERMC 7H 70 2 0G 300.000 5000.000
 1411.000 01!WAGNON
 2.19976808E+01 1.92971055E-02-6.43123707E-06 9.81629697E-10-5.62952709E-
 14 2!
 -1.11439969E+04-9.20837282E+01-4.85911819E+00 9.45943557E-02-8.78284917E-
 05 3!
 4.07970227E-08-7.41817991E-12-3.20429683E+03 4.74787619E+01
 4!

 !benzodioxole and cinnamaldehyde submech
 A1CYOCH2O1-2 C 7H 60 2 G 100.000 5000.000 928.35
 1! RMG
 2.99108960E+01 1.37299834E-03 4.43051931E-06-8.67370119E-10 4.40422017E-
 14 2
 -3.55412301E+04-1.42325847E+02 9.01933332E-01 3.10493819E-02 1.10486533E-
 04 3
 -1.87622491E-07 8.01185127E-11-2.60478190E+04 1.75904367E+01
 4

A1CYOCHO1-2 C 7H 50 2 G 100.000 5000.000 948.50
1! RMG
 2.18480437E+01 1.36252705E-02-3.35774155E-06 6.27186867E-10-5.30981318E-
14 2
-9.77833021E+03-9.56036576E+01 8.45467473E-01 4.74937929E-02 2.95918676E-
05 3
-8.33377292E-08 3.81048385E-11-3.33346681E+03 1.75826041E+01
4

END