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!
!           This CHEMKIN thermo file is part of the
!
!           Supplemental Material for
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!
!           A model of tetrahydrofuran
!
!           low-temperature oxidation
!
!           based on theoretically calculated rate constants
!
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!
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!
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!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
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```
THERMO
   300.000 1000.000 5000.000
!Carstensen
cy(OCCCC)        111616H   8C   40   1   0g   300.000 2500.0001000.000
1
0.13962569E+01 0.42079657E-01-0.22174640E-04 0.57022138E-08-0.58057004E-
12      2
```

-0.24071602E+05 0.14912234E+02-0.14748075E+01 0.33896927E-01 0.25760606E-04 3
 -0.55893288E-07 0.24138171E-10-0.22632461E+05 0.33312099E+02
 HHC 0 P 4
 cy(OCJCCC) 031417H 7C 40 1 0g 300.000 2500.0001000.000
 1
 0.29826450E+01 0.36683500E-01-0.19384201E-04 0.50059228E-08-0.51240197E-12 2
 -0.32233701E+04 0.77025766E+01-0.17188536E+01 0.39853767E-01 0.40468203E-05 3
 -0.34006568E-07 0.16604185E-10-0.15875396E+04 0.34018620E+02
 HHC 0 P 4
 cy(OCCJCC) 031417H 7C 40 1 0g 300.000 2500.0001000.000
 1
 0.31563146E+01 0.36710650E-01-0.19493855E-04 0.50536126E-08-0.51888886E-12 2
 -0.99790283E+03 0.72754645E+01-0.11309419E+01 0.38155951E-01 0.66731986E-05 3
 -0.35923502E-07 0.17137047E-10 0.55744495E+03 0.31607014E+02
 HHC 0 P 4
 JOOcy(COCCC) 111616H 7C 40 3 0g 300.000 2500.0001000.000
 1
 0.57433567E+01 0.40730312E-01-0.21955842E-04 0.57809717E-08-0.60290428E-12 2
 -0.22352344E+05-0.22813134E+01-0.56596291E+00 0.47225948E-01 0.17061885E-05 3
 -0.37454175E-07 0.18788299E-10-0.20247641E+05 0.32539185E+02
 HHC 1 M 4
 JOOcy(CCOCC) 111616H 7C 40 3 0g 300.000 2500.0001000.000
 1
 0.56679087E+01 0.41005980E-01-0.22189824E-04 0.58624230E-08-0.61328373E-12 2
 -0.18917594E+05-0.11968113E+01-0.60556877E+00 0.47362387E-01 0.16519019E-05 3
 -0.37457042E-07 0.18785931E-10-0.16819537E+05 0.33451588E+02
 HHC 1 M 4
 HOOcy(COCCCJ) 111616H 7C 40 3 0g 300.000 2500.0001000.000
 1
 0.11522829E+02 0.33325672E-01-0.18274461E-04 0.49285083E-08-0.52827003E-12 2
 -0.18546605E+05-0.34088593E+02-0.35817933E+01 0.78291662E-01-0.59221871E-04 3
 0.10949083E-07 0.45408746E-11-0.14794814E+05 0.42484013E+02
 HHC 2 M 4
 HOOcy(COCCJC) 111616H 7C 40 3 0g 300.000 2500.0001000.000
 1
 0.12878942E+02 0.30743873E-01-0.16322343E-04 0.42549244E-08-0.44037780E-12 2
 -0.19336252E+05-0.40679260E+02-0.36155021E+01 0.77105038E-01-0.51422106E-04 3
 -0.48748511E-09 0.95400033E-11-0.15132943E+05 0.43534744E+02
 HHC 2 M 4
 HOOcy(COCJCC) 111616H 7C 40 3 0g 300.000 2500.0001000.000
 1
 0.12581011E+02 0.31392928E-01-0.16868018E-04 0.44557855E-08-0.46755498E-12 2
 -0.20923609E+05-0.40205181E+02-0.34859555E+01 0.73654994E-01-0.41842315E-04 3

-0.10022304E-07 0.12794751E-10-0.16695850E+05 0.42517025E+02
 HHC 2 M 4
 HOCcy (CCJOCC) 111616H 7C 40 3 0g 300.000 2500.0001000.000
 1
 0.94829445E+01 0.35107922E-01-0.18789107E-04 0.49397300E-08-0.51649581E-
 12 2
 -0.16867605E+05-0.21218187E+02-0.27126837E+00 0.60451489E-01-0.32815558E-
 04 3
 -0.52956861E-08 0.81594202E-11-0.14286021E+05 0.29074017E+02
 HHC 2 M 4
 HOCcy (CCOCCJ) 111616H 7C 40 3 0g 300.000 2500.0001000.000
 1
 0.88231239E+01 0.36168601E-01-0.19447638E-04 0.51290581E-08-0.53759384E-
 12 2
 -0.12748683E+05-0.16993429E+02 0.74789482E+00 0.56085795E-01-0.27555030E-
 04 3
 -0.72638340E-08 0.81238037E-11-0.10563645E+05 0.24890392E+02
 HHC 2 M 4
 HOCcy (CCOCJC) 111616H 7C 40 3 0g 300.000 2500.0001000.000
 1
 0.86422272E+01 0.36332101E-01-0.19445259E-04 0.50933981E-08-0.52938377E-
 12 2
 -0.15233667E+05-0.16402325E+02 0.51761115E+00 0.53432688E-01-0.17778606E-
 04 3
 -0.18467802E-07 0.12393003E-10-0.12909073E+05 0.26409758E+02
 HHC 2 M 4
 cy (OC*CCC) 111616H 6C 40 1 0g 300.000 2500.0001000.000
 1
 0.31386127E+01 0.33065617E-01-0.17558106E-04 0.45599839E-08-0.46956102E-
 12 2
 -0.11223865E+05 0.67258730E+01-0.22620840E+01 0.40398996E-01-0.30037829E-
 05 3
 -0.26265864E-07 0.13872826E-10-0.95033135E+04 0.36111713E+02
 HHC 0 P 4
 cy (OCC*CC) 111616H 6C 40 1 0g 300.000 2500.0001000.000
 1
 0.27616191E+01 0.33944465E-01-0.18214221E-04 0.47719451E-08-0.49511816E-
 12 2
 -0.96709648E+04 0.79336481E+01-0.18453888E+01 0.37533920E-01 0.29682560E-
 05 3
 -0.31284099E-07 0.15399610E-10-0.80844453E+04 0.33622036E+02
 HHC 0 P 4
 O*cy (COCCC) 111616H 6C 40 2 0g 300.000 2500.0001000.000
 1
 0.35844150E+01 0.37118524E-01-0.20251804E-04 0.54003237E-08-0.57065594E-
 12 2
 -0.47045520E+05 0.49788489E+01-0.15532407E+01 0.43094985E-01-0.34522275E-
 05 3
 -0.26847520E-07 0.14042144E-10-0.45356551E+05 0.33188351E+02
 HHC 0 P 4
 O*cy (COCC) 111616H 6C 40 2 0g 300.000 2500.0001000.000
 1
 0.38955882E+01 0.36905572E-01-0.20216941E-04 0.54108900E-08-0.57372840E-
 12 2
 -0.37302316E+05 0.37373068E+01-0.13019978E+01 0.43904129E-01-0.64004676E-
 05 3
 -0.23633147E-07 0.12856024E-10-0.35634441E+05 0.32058071E+02
 HHC 0 P 4

bicy(O) (CCOCC) 111716H 6C 40 2 0g 300.000 2500.0001000.000
 1
 0.42743173E+01 0.36129829E-01-0.19637178E-04 0.52151066E-08-0.54861264E-
 12 2
 -0.27323227E+05 0.44318539E+00-0.36951227E+01 0.51708881E-01-0.14158682E-
 04 3
 -0.22089482E-07 0.13671841E-10-0.24987420E+05 0.42722244E+02
 HHC 0 M 4
 bicy(O) (CCCOC) 111716H 6C 40 2 0g 300.000 2500.0001000.000
 1
 0.39936516E+01 0.36734130E-01-0.20054229E-04 0.53384523E-08-0.56207437E-
 12 2
 -0.24081873E+05 0.14374781E+01-0.29909902E+01 0.47281124E-01-0.50386820E-
 05 3
 -0.29954784E-07 0.16157407E-10-0.21896498E+05 0.39215450E+02
 HHC 0 P 4
 CJC(OOH)CCHO 111716H 7C 40 3 0g 300.000 2500.0001000.000
 1
 0.14121294E+02 0.27206797E-01-0.14446630E-04 0.38146633E-08-0.40428097E-
 12 2
 -0.15394168E+05-0.39850266E+02-0.17801756E+00 0.95943727E-01-0.13957282E-
 03 3
 0.10567199E-06-0.31574632E-10-0.12984851E+05 0.26592196E+02
 HHC 5 M 4
 OHCCcy(COC) 111716H 6C 40 2 0g 300.000 2500.0001000.000
 1
 0.56765676E+01 0.32466020E-01-0.17231372E-04 0.44706550E-08-0.45995098E-
 12 2
 -0.25587906E+05 0.69465184E+00 0.59464626E+01 0.17097939E-01 0.31631011E-
 04 3
 -0.49378240E-07 0.19627709E-10-0.25016529E+05 0.26948888E+01
 HHC 2 M 4
 C*CCHO 111716H 4C 30 1 0g 300.000 2500.0001000.000
 1
 0.37032585E+01 0.22451503E-01-0.12543299E-04 0.34092389E-08-0.36630724E-
 12 2
 -0.10330175E+05 0.58010960E+01 0.12733116E+01 0.28454961E-01-0.15366333E-
 04 3
 0.43828921E-09 0.18549665E-11-0.96624629E+04 0.18429632E+02
 HHC 1 P 4
 C*CCOCHO 111716H 6C 40 2 0g 300.000 2500.0001000.000
 1
 0.50865870E+01 0.33445932E-01-0.17921056E-04 0.46989270E-08-0.48893013E-
 12 2
 -0.36560438E+05 0.31250787E+01 0.22685885E+01 0.31602766E-01 0.82603810E-
 05 3
 -0.31978143E-07 0.14670782E-10-0.35410676E+05 0.19779331E+02
 HHC 2 P 4
 OHCCCCHO 111716H 6C 40 2 0g 300.000 2500.0001000.000
 1
 0.76955075E+01 0.29919768E-01-0.16243828E-04 0.43402517E-08-0.46210383E-
 12 2
 -0.39104785E+05-0.10299726E+02-0.20445995E+00 0.69164336E-01-0.89936453E-
 04 3
 0.66025166E-07-0.19800203E-10-0.37816500E+05 0.26145950E+02
 HHC 3 P 4
 Qcy(COC(OOJ)CC) 031417H 7C 40 5 0g 300.000 2500.0001000.000
 1

0.12017854E+02 0.40942602E-01-0.23105275E-04 0.63670171E-08-0.69382450E-
 12 2
 -0.38821922E+05-0.31912525E+02-0.17145114E+01 0.80869675E-01-0.57683617E-
 04 3
 0.93533501E-08 0.47068877E-11-0.35353703E+05 0.37963768E+02
 HHC 3 M 4
 Qcy(COCC(OOJ)C) 031417H 7C 40 5 0g 300.000 2500.0001000.000
 1
 0.13134745E+02 0.38950615E-01-0.21775224E-04 0.59629390E-08-0.64689898E-
 12 2
 -0.36223168E+05-0.37941021E+02 0.58338457E+00 0.71402550E-01-0.40075010E-
 04 3
 -0.60618430E-08 0.97808749E-11-0.32877207E+05 0.26859976E+02
 HHC 3 M 4
 Qcy(COCCC(OOJ)) 031417H 7C 40 5 0g 300.000 2500.0001000.000
 1
 0.12110909E+02 0.39382085E-01-0.21498192E-04 0.57501861E-08-0.61022552E-
 12 2
 -0.34586824E+05-0.30554895E+02 0.17387532E-01 0.70785105E-01-0.38976337E-
 04 3
 -0.66921166E-08 0.10004892E-10-0.31381211E+05 0.31813898E+02
 HHC 3 M 4
 JOOcy(CCOCC(Q)) 031417H 7C 40 5 0g 300.000 2500.0001000.000
 1
 0.12940489E+02 0.39013542E-01-0.21598422E-04 0.58548206E-08-0.62944512E-
 12 2
 -0.38831797E+05-0.36976673E+02-0.12060853E+01 0.80475152E-01-0.57976227E-
 04 3
 0.94712922E-08 0.48203420E-11-0.35284168E+05 0.34903755E+02
 HHC 3 M 4
 JOOcy(COCC(Q)C) 031417H 7C 40 5 0g 300.000 2500.0001000.000
 1
 0.10994226E+02 0.41109066E-01-0.22515134E-04 0.60217937E-08-0.63773260E-
 12 2
 -0.34114160E+05-0.24241552E+02 0.11172258E+01 0.60263988E-01-0.15410520E-
 04 3
 -0.27929065E-07 0.16935299E-10-0.31209719E+05 0.28202818E+02
 HHC 3 M 4
 JOOcy(COCCC(Q)) 031417H 7C 40 5 0g 300.000 2500.0001000.000
 1
 0.11883786E+02 0.39481506E-01-0.21469647E-04 0.57229586E-08-0.60549525E-
 12 2
 -0.33898961E+05-0.29267609E+02 0.22458367E+01 0.60194351E-01-0.21248621E-
 04 3
 -0.19857790E-07 0.13683399E-10-0.31153703E+05 0.21440321E+02
 HHC 3 M 4
 C*COCCHO 111716H 6C 40 2 0g 300.000 2500.0001000.000
 1
 0.92581310E+01 0.27371496E-01-0.14455595E-04 0.37582621E-08-0.39000045E-
 12 2
 -0.28640188E+05-0.19211472E+02-0.13339773E+01 0.70325226E-01-0.80485974E-
 04 3
 0.49067612E-07-0.12029682E-10-0.26514219E+05 0.31824486E+02
 HHC 3 P 4
 C*CCCOH 111616H 8C 40 1 0g 300.000 2500.0001000.000
 1
 0.80262175E+01 0.29798526E-01-0.14765434E-04 0.36552266E-08-0.36564187E-
 12 2

-0.21905115E+05-0.14229634E+02-0.75955737E+00 0.75276412E-01-0.10203850E-
 03 3
 0.77518393E-07-0.23649391E-10-0.20576305E+05 0.25818878E+02
 HHC 3 P 4
 cy(O)13cy(CCCOC) 111517H 6C 40 2 0g 300.000 2500.0001000.000
 1
 0.43273191E+01 0.36129646E-01-0.19668147E-04 0.52296429E-08-0.55057700E-
 12 2
 -0.22222777E+05-0.96174747E+00-0.55757818E+01 0.59615314E-01-0.26442802E-
 04 3
 -0.13596996E-07 0.11472276E-10-0.19502201E+05 0.50617947E+02
 HHC 0 M 4
 C*CCC(OJ)OOH 111517H 7C 40 3 0g 300.000 2500.0001000.000
 1
 0.14307881E+02 0.26477188E-01-0.13362423E-04 0.33197134E-08-0.32834895E-
 12 2
 -0.11012597E+05-0.42839687E+02 0.19610279E+01 0.61840642E-01-0.41418101E-
 04 3
 0.13304854E-08 0.67037686E-11-0.79046948E+04 0.20018787E+02
 HHC 4 M 4
 HC(*O)OOH 111517H 2C 10 3 0g 300.000 2500.0001000.000
 1
 0.74812489E+01 0.85496353E-02-0.41361563E-05 0.99148245E-09-0.95294832E-
 13 2
 -0.37309512E+05-0.12547585E+02-0.11642935E+01 0.45421481E-01-0.63683488E-
 04 3
 0.43901764E-07-0.11683796E-10-0.35660652E+05 0.28669224E+02
 HHC 1 P 4
 !
 !Verdicchion/Tran
 !YF
 C4H5O-2 H 5C 40 1 0g 300.00 5000.00 1000.00
 1
 0.20341429E+02 0.11968300E-02-0.64454362E-07 0.17374489E-11 0.46487352E-
 17 2
 0.27596789E+03-0.87880509E+02 0.16755061E+01 0.36561195E-01-0.22516078E-
 04 3
 0.79847426E-08-0.22298188E-11 0.71937964E+04 0.14817021E+02
 4
 C4H5O-3 H 5C 40 1 0g 300.00 5000.00 1000.00
 1
 0.20181027E+02 0.12747848E-02-0.61260515E-07-0.99676691E-12 0.26328857E-
 15 2
 -0.45709505E+04-0.87036225E+02 0.21551745E+01 0.32899953E-01-0.15094073E-
 04 3
 0.17689651E-08-0.33620218E-12 0.22780576E+04 0.12867317E+02
 4
 C3H6CHO-1 H 7C 40 1 G 0300.00 5000.00 1000.00
 1
 0.10158430E+02 0.20117089E-01-0.73492706E-05 0.12271479E-08-0.77712400E-
 13 2
 -0.43062731E+04-0.22800783E+02 0.58740253E+01 0.20765830E-01 0.12162194E-
 04 3
 -0.23643254E-07 0.89168889E-11-0.24313799E+04 0.24318485E+01
 4
 C2H3OC2H4 H 7C 40 1 G 0300.00 5000.00 1000.00
 1

0.12036350E+02 0.18121399E-01-0.65403442E-05 0.10821506E-08-0.68058704E-
 13 2
 0.38351909E+04-0.33961809E+02 0.14405545E+01 0.51599532E-01-0.48536116E-
 04 3
 0.26079418E-07-0.59518922E-11 0.66179600E+04 0.19889639E+02
 4
 AC3H5OCH2 H 7C 4O 1 G 0300.00 5000.00 1000.00
 1
 0.10737946E+02 0.19378901E-01-0.70236802E-05 0.11653500E-08-0.73421629E-
 13 2
 0.49028997E+04-0.26290571E+02 0.20183141E+01 0.37532926E-01-0.13436096E-
 04 3
 -0.66257608E-08 0.46957117E-11 0.76769419E+04 0.20399448E+02
 4
 CH2CHCH2CH2O C 4H 7O 1 G 0300.00 5000.00 1000.00
 1
 0.10548280E+02 0.20077419E-01-0.73041283E-05 0.12161293E-08-0.76867102E-
 13 2
 0.45279075E+04-0.26380841E+02 0.32536917E+01 0.33363685E-01-0.78266594E-
 05 3
 -0.94734931E-08 0.51436091E-11 0.69818506E+04 0.13241481E+02
 4
 FURAN H 4C 4O 1 0g 300.00 5000.00 1000.00
 1
 0.85330832E+01 0.15491830E-01-0.60538157E-05 0.10841704E-08-0.73011472E-
 13 2
 -0.83189334E+04-0.22484919E+02-0.41408036E+01 0.50094797E-01-0.36077330E-
 04 3
 0.65275725E-08 0.25780211E-11-0.48297488E+04 0.42994755E+02
 4
 FURYL-2 H 3C 4O 1 0g 300.00 5000.00 1000.00
 1
 0.86891037E+01 0.12653736E-01-0.49816218E-05 0.89685293E-09-0.60626683E-
 13 2
 0.25679702E+05-0.21690799E+02-0.30241469E+01 0.45461979E-01-0.35446311E-
 04 3
 0.89781471E-08 0.12277760E-11 0.28865724E+05 0.38629706E+02
 4
 FURYL-3 H 3C 4O 1 0g 300.00 5000.00 1000.00
 1
 0.85786315E+01 0.12760208E-01-0.50240529E-05 0.90456735E-09-0.61152197E-
 13 2
 0.25804085E+05-0.21178320E+02-0.30061794E+01 0.44694120E-01-0.33586282E-
 04 3
 0.72693450E-08 0.17871980E-11 0.28981819E+05 0.38610241E+02
 4
 CH2CCHCHO H 4C 4O 1 0g 300.00 5000.00 1000.00
 1
 0.92593676E+01 0.15220151E-01-0.61588394E-05 0.11267837E-08-0.76935914E-
 13 2
 0.37084077E+04-0.21801022E+02 0.12385215E+01 0.35605465E-01-0.23678689E-
 04 3
 0.59223436E-08 0.28288588E-12 0.61056924E+04 0.20291156E+02
 4
 SC3H5CHO C 4H 6O 1 G 300.0 5000.0 1000.0
 1
 0.17803599E+02 0.85582836E-02-0.24019453E-05 0.33401309E-09-0.18719586E-
 13 2

-0.20829943E+05-0.70165010E+02 0.17147057E+01 0.29294839E-01-0.30107892E-
 05 3
 -0.36980230E-08-0.25501550E-13-0.13897014E+05 0.21886703E+02
 4
 CH3CHCHCO H 5C 4O 1 OG 300.00 5000.00 1000.00
 1
 8.81125400E+00 1.75712453E-02-6.84340804E-06 1.22169069E-09-8.20481975E-
 14 2
 2.94573899E+03-1.81942896E+01 3.18545375E+00 2.63960038E-02-2.38285068E-
 06 3
 -1.30854274E-08 6.52902197E-12 4.91536234E+03 1.27148011E+01
 4
 CH2CHCHCHO H 5C 4O 1 0g 300.00 5000.00 1000.00
 1
 0.11096231E+02 0.11702731E-01-0.30401659E-05 0.40010689E-09-0.21618115E-
 13 2
 0.74015087E+04-0.26680961E+02 0.17160503E+01 0.35177406E-01-0.21606502E-
 04 3
 0.42076911E-08 0.64263948E-12 0.10148383E+05 0.22488266E+02
 4
 CHCHCHCHOH H 5C 4O 1 0g 300.00 5000.00 1000.00
 1
 0.11757640E+02 0.10950322E-01-0.27650015E-05 0.35572298E-09-0.18888174E-
 13 2
 0.20074210E+05-0.29286528E+02 0.18384148E+01 0.40506996E-01-0.37331400E-
 04 3
 0.20034532E-07-0.47687479E-11 0.22767500E+05 0.21587437E+02
 4
 CYC3H5 (CHO) C 4H 6O 1 G 300.0 5000.0 1000.0
 1
 -0.11955712E+02 0.56075636E-01-0.26370582E-04 0.52871254E-08-0.38301220E-
 12 2
 -0.25040184E+04 0.94476106E+02-0.53328362E+01 0.59858471E-01-0.44611817E-
 04 3
 0.10976227E-07 0.17634104E-11-0.67894600E+04 0.51631710E+02
 4
 CH3CH2CHCHO C 4H 7O 1 G 0300.00 5000.00 1000.00
 1
 0.97988671E+01 0.20837478E-01-0.76027695E-05 0.12686137E-08-0.80315237E-
 13 2
 -0.10407399E+05-0.23308714E+02 0.75414127E+00 0.41017368E-01-0.19177402E-
 04 3
 -0.10867682E-08 0.27145350E-11-0.75645322E+04 0.24863880E+02
 4
 CH3CH2CH2CO C 4H 7O 1 G 0300.00 5000.00 1000.00
 1
 0.94488496E+01 0.20664820E-01-0.75248386E-05 0.12529251E-08-0.79152613E-
 13 2
 -0.10420093E+05-0.19039578E+02 0.34064460E+01 0.27859146E-01 0.26138953E-
 05 3
 -0.17534335E-07 0.74174512E-11-0.81569365E+04 0.14824444E+02
 4
 CH3CH2OCCH2 C 4H 7O 1 G 0300.00 5000.00 1000.00
 1
 0.11490076E+02 0.15780743E-01-0.42633196E-05 0.57740784E-09-0.31818179E-
 13 2
 0.62171039E+04-0.29259258E+02 0.33192248E+01 0.27938491E-01 0.15351584E-
 05 3

-0.16288629E-07 0.70488437E-11 0.91766318E+04 0.15977841E+02
 4
 CH3CH2OCHCH C 4H 7O 1 G 0300.00 5000.00 1000.00
 1
 0.12147922E+02 0.15225769E-01-0.40786263E-05 0.54825311E-09-0.30015748E-
 13 2
 0.71014910E+04-0.33420050E+02 0.25366044E+01 0.33215106E-01-0.74701643E-
 05 3
 -0.95264294E-08 0.50581852E-11 0.10349683E+05 0.18765188E+02
 4
 CH3OCHCHCH2 C 4H 7O 1 G 0300.00 5000.00 1000.00
 1
 0.10723846E+02 0.19813880E-01-0.71736376E-05 0.11888750E-08-0.74819897E-
 13 2
 -0.33675716E+04-0.27447562E+02 0.19695328E+01 0.36978841E-01-0.10622844E-
 04 3
 -0.94701198E-08 0.56227332E-11-0.52076569E+03 0.19713341E+02
 4
 CH3OCH2CCH2 C 4H 7O 1 G 0300.00 5000.00 1000.00
 1
 0.13245044E+02 0.14407584E-01-0.38382773E-05 0.51474908E-09-0.28185167E-
 13 2
 0.95588378E+04-0.41402060E+02-0.25159642E+00 0.52669890E-01-0.48729209E-
 04 3
 0.27340484E-07-0.67286541E-11 0.13521629E+05 0.28745794E+02
 4
 CH3OCH2CHCH C 4H 7O 1 G 0300.00 5000.00 1000.00
 1
 0.13894682E+02 0.13901142E-01-0.36895572E-05 0.49486820E-09-0.27174431E-
 13 2
 0.10449182E+05-0.45514166E+02-0.11626500E+01 0.58872998E-01-0.59755072E-
 04 3
 0.35947206E-07-0.93285215E-11 0.14706276E+05 0.32066990E+02
 4
 CH2CHOCHCH3 C 4H 7O 1 G 0300.00 5000.00 1000.00
 1
 0.20357282E+02 0.37431144E-02-0.41311509E-06 0.27698477E-10-0.94679839E-
 15 2
 -0.43489084E+04-0.79665394E+02 0.15902214E+01 0.42649258E-01-0.34092656E-
 04 3
 0.19807114E-07-0.62399044E-11 0.24945317E+04 0.22873096E+02
 4
 CH3CHCOCH3 C 4H 7O 1 G 0300.00 5000.00 1000.00
 1
 0.11461209E+02 0.15473572E-01-0.41025501E-05 0.54617372E-09-0.29641396E-
 13 2
 0.63110350E+04-0.29931575E+02 0.41316543E+01 0.29442674E-01-0.15106306E-
 04 3
 0.82455154E-08-0.33647746E-11 0.90661484E+04 0.10499306E+02
 4
 CH3CHCHOCH2 C 4H 7O 1 G 0300.00 5000.00 1000.00
 1
 0.10613587E+02 0.19261209E-01-0.69198450E-05 0.11399695E-08-0.71407317E-
 13 2
 0.30620730E+04-0.24357076E+02 0.45810490E+01 0.28859425E-01-0.32679682E-
 05 3
 -0.11774857E-07 0.56258648E-11 0.51674634E+04 0.87706928E+01
 4

CH3OCHCCH3 C 4H 7O 1 G 0300.00 5000.00 1000.00
 1
 0.11169005E+02 0.16008766E-01-0.43443847E-05 0.59203842E-09-0.32855893E-
 13 2
 0.63708480E+04-0.28442408E+02 0.52595153E+01 0.21384591E-01 0.29311518E-
 05 3
 -0.82697271E-08 0.20870378E-11 0.89587090E+04 0.57892561E+01
 4
 CH3OCHCCH2 C 4H 6O 1 G 0300.00 5000.00 1000.00
 1
 0.80473591E+01 0.20636620E-01-0.74254290E-05 0.12336301E-08-0.78223933E-
 13 2
 0.33826953E+03-0.12861607E+02 0.51919713E+01 0.18104896E-01 0.16389513E-
 04 3
 -0.27442480E-07 0.10170056E-10 0.16405769E+04 0.44836001E+01
 4
 CHCHCHO H 3C 3O 1 0g 300.00 5000.00 1000.00
 1
 0.78607722E+01 0.11813527E-01-0.40297773E-05 0.64490713E-09-0.39853171E-
 13 2
 0.17320589E+05-0.14234727E+02 0.22272190E+00 0.27970692E-01-0.21389089E-
 04 3
 0.14479667E-07-0.50344160E-11 0.20206717E+05 0.27686600E+02
 4
 CHCHCHCO H 3C 4O 1 0G 300.00 5000.00 1000.00
 1
 0.96529160E+01 0.11564829E-01-0.45009049E-05 0.80326262E-09-0.53940879E-
 13 2
 0.29514436E+05-0.22045829E+02 0.73738210E+00 0.43115940E-01-0.49828826E-
 04 3
 0.31920989E-07-0.84793239E-11 0.31669367E+05 0.22387117E+02
 4
 CHCCHCHO H 3C 4O 1 0G 300.00 5000.00 1000.00
 1
 0.10898676E+02 0.74487077E-02-0.17745550E-05 0.21944631E-09-0.11382359E-
 13 2
 0.29408405E+05-0.24302621E+02 0.31362398E+01 0.26003901E-01-0.15521402E-
 04 3
 0.24814786E-08 0.68067546E-12 0.31771607E+05 0.16709595E+02
 4
 CHCCHCHO H 3C 4O 1 0G 300.00 5000.00 1000.00
 1
 0.10898676E+02 0.74487077E-02-0.17745550E-05 0.21944631E-09-0.11382359E-
 13 2
 0.29408405E+05-0.24302621E+02 0.31362398E+01 0.26003901E-01-0.15521402E-
 04 3
 0.24814786E-08 0.68067546E-12 0.31771607E+05 0.16709595E+02
 4
 CHCCHCO H 2C 4O 1 0G 300.00 5000.00 1000.00
 1
 0.92016685E+01 0.90755314E-02-0.35056572E-05 0.62239046E-09-0.41639784E-
 13 2
 0.20206246E+05-0.20238250E+02 0.10350557E+01 0.42421593E-01-0.59252316E-
 04 3
 0.44593993E-07-0.13446033E-10 0.21970026E+05 0.19395878E+02
 4
 CHCHCH2CHO H 5C 4O 1 0G 300.00 5000.00 1000.00
 1

0.97154262E+01 0.16175538E-01-0.62875252E-05 0.11208290E-08-0.75192858E-
 13 2
 0.15365733E+05-0.20762311E+02 0.14874558E+01 0.41217844E-01-0.36123227E-
 04 3
 0.17674503E-07-0.36075005E-11 0.17585828E+05 0.21315225E+02
 4
 CYCC*OCCO 11/ 4/16 THERMC 4H 60 2 0G 300.000 5000.000
 1404.000 01
 1.03220573E+01 2.07533766E-02-6.76562184E-06 1.01726136E-09-5.77272910E-
 14 2
 -4.12425785E+04-2.94221973E+01-1.15648940E+00 4.02598066E-02-1.43154651E-
 05 3
 -1.29084868E-09 1.32215768E-12-3.66508868E+04 3.46067604E+01
 4
 CYCOJCCCO 11/ 4/16 THERMC 4H 70 2 0G 300.000 5000.000
 1426.000 11
 1.50841706E+01 1.79171514E-02-6.13037571E-06 9.52491935E-10-5.53073553E-
 14 2
 -2.91154745E+04-5.62766593E+01-3.98539562E+00 6.04902224E-02-4.04100752E-
 05 3
 1.24738445E-08-1.34708888E-12-2.24607566E+04 4.65618818E+01
 4
 CYCCOJCCO 11/ 4/16 THERMC 4H 70 2 0G 300.000 5000.000
 1410.000 11
 1.58039043E+01 1.70161699E-02-5.76924324E-06 8.91921690E-10-5.16422695E-
 14 2
 -2.43624702E+04-6.11237271E+01-4.52318083E+00 6.09696125E-02-3.88895994E-
 05 3
 1.05505230E-08-7.79414455E-13-1.71781261E+04 4.89179882E+01
 4
 CYCO2HCCCO 11/16 THERMC 4H 80 3 0G 300.000 5000.000
 1427.000 21
 1.95980894E+01 1.87920957E-02-6.44436401E-06 1.00307967E-09-5.83263762E-
 14 2
 -4.70337373E+04-8.20190937E+01-6.47395624E+00 8.21549219E-02-6.40394964E-
 05 3
 2.41575590E-08-3.51833561E-12-3.84638177E+04 5.67324342E+01
 4
 CYCCO2HCCO 11/16 THERMC 4H 80 3 0G 300.000 5000.000
 1474.000 21
 1.74062308E+01 1.87322887E-02-6.01479415E-06 8.94622008E-10-5.03708975E-
 14 2
 -4.22109473E+04-6.62000668E+01-5.51813075E+00 7.98264449E-02-6.74059046E-
 05 3
 2.83741214E-08-4.65773385E-12-3.52715696E+04 5.37914110E+01
 4
 CYC*OCO2HCCO 11/16 THERMC 4H 60 4 0G 300.000 5000.000
 1402.000 21
 2.10866388E+01 1.58658267E-02-5.62916390E-06 8.95925507E-10-5.28961419E-
 14 2
 -6.60607538E+04-8.58963772E+01-6.40798433E+00 8.38333682E-02-6.93856885E-
 05 3
 2.78025314E-08-4.35572784E-12-5.70732752E+04 6.01296293E+01
 4
 CYC*OCCO2HCO 11/16 THERMC 4H 60 4 0G 300.000 5000.000
 1483.000 21
 1.89559320E+01 1.64520276E-02-5.56749644E-06 8.59323304E-10-4.96884777E-
 14 2

-6.66621348E+04-7.44388222E+01-4.36858326E+00 7.26271592E-02-5.56008203E-
 05 3
 2.02790630E-08-2.79605001E-12-5.89919554E+04 4.97919549E+01
 4
 CYC*OCCCO2HO 11/16 THERMC 4H 60 4 0G 300.000 5000.000
 1412.000 21
 2.02708733E+01 1.64243825E-02-5.79823294E-06 9.20332123E-10-5.42516699E-
 14 2
 -7.09520141E+04-8.46295438E+01-6.09836743E-01 5.42062371E-02-2.39072402E-
 05 3
 -4.84458644E-10 1.85570955E-12-6.28868339E+04 3.09378777E+01
 4
 CYCO2HC*OCCO 11/16 THERMC 4H 60 4 0G 300.000 5000.000
 1411.000 21
 1.98805580E+01 1.58636036E-02-5.41188323E-06 8.40253599E-10-4.87980654E-
 14 2
 -5.46161284E+04-7.54810565E+01-4.32462816E+00 7.42809837E-02-5.79681338E-
 05 3
 2.16802200E-08-3.10897003E-12-4.66294738E+04 5.34649878E+01
 4
 CYCC*OCO2HCO 11/16 THERMC 4H 60 4 0G 300.000 5000.000
 1408.000 21
 2.01373161E+01 1.55143133E-02-5.26202226E-06 8.13771251E-10-4.71299888E-
 14 2
 -5.44952744E+04-7.73088526E+01-4.04293243E+00 7.63190047E-02-6.31347309E-
 05 3
 2.55075846E-08-4.02415661E-12-4.67353338E+04 5.06799914E+01
 4
 CYCC*OCCO2HO 11/16 THERMC 4H 60 4 0G 300.000 5000.000
 1393.000 21
 1.82237656E+01 1.74937605E-02-6.44258630E-06 1.07994503E-09-6.62210530E-
 14 2
 -5.82560243E+04-6.98430523E+01-3.91615901E+00 7.53653558E-02-6.53897136E-
 05 3
 2.86648534E-08-5.02042547E-12-5.12208687E+04 4.68185844E+01
 4
 C*CCC(*O)OH 11/16 THERMC 4H 60 2 0G 300.000 5000.000
 1506.000 31
 1.63836994E+01 1.45671151E-02-5.23212300E-06 8.39297432E-10-4.98163710E-
 14 2
 -3.93331310E+04-5.71812234E+01 2.64257442E+00 3.41137440E-02-6.96970763E-
 06 3
 -6.53970811E-09 2.56470121E-12-3.33883665E+04 2.09378713E+01
 4
 O*CYCCJCCO 11/16 THERMC 4H 50 2 0G 300.000 5000.000
 1527.000 01
 1.47074422E+01 1.38997775E-02-4.82660349E-06 7.58145651E-10-4.43809665E-
 14 2
 -3.17376942E+04-5.66418539E+01-4.54537460E+00 5.55272950E-02-3.63858388E-
 05 3
 1.01650768E-08-8.20183058E-13-2.49127062E+04 4.76201639E+01
 4
 O*CYCCCJCO 11/16 THERMC 4H 50 2 0G 300.000 5000.000
 1413.000 01
 1.29008435E+01 1.58570139E-02-5.59016300E-06 8.86160578E-10-5.21808311E-
 14 2
 -3.01783089E+04-4.44519628E+01-3.79305218E+00 4.29848741E-02-1.36243804E-
 05 3

-4.70834530E-09 2.50307862E-12-2.34191429E+04 4.90399676E+01
 4
 O*CYCCCCJO 11/16 THERMC 4H 50 2 0G 300.000 5000.000
 1437.000 01
 1.40286116E+01 1.40002371E-02-4.75807391E-06 7.36857091E-10-4.27173347E-
 14 2
 -3.17916770E+04-5.11510035E+01-6.24758342E+00 6.17326527E-02-4.60444090E-
 05 3
 1.61557703E-08-2.10968379E-12-2.50044829E+04 5.72515769E+01
 4
 C*CC(*O)OCJ 11/16 THERMC 4H 50 2 0G 300.000 5000.000
 1391.000 31
 1.49306390E+01 1.25443177E-02-4.36828422E-06 6.86426821E-10-4.01624230E-
 14 2
 -2.00926474E+04-4.90775656E+01 2.05371136E+00 4.43047219E-02-3.50868922E-
 05 3
 1.45021892E-08-2.45727625E-12-1.57615349E+04 1.95300894E+01
 4
 C*CCOCJ(*O) 11/16 THERMC 4H 50 2 0G 300.000 5000.000
 1674.000 31
 1.32688625E+01 1.54325818E-02-5.76379194E-06 9.51877940E-10-5.77188744E-
 14 2
 -1.68742835E+04-4.01662921E+01 1.90115490E+00 3.75815464E-02-1.92611444E-
 05 3
 3.28027276E-09 9.39489087E-14-1.27429177E+04 2.21115681E+01
 4
 C(*O)CCCJ(*O) 11/16 THERMC 4H 50 2 0G 300.000 5000.000
 1480.000 31
 1.45343350E+01 1.27763247E-02-4.43500179E-06 6.96212029E-10-4.07300473E-
 14 2
 -2.31647799E+04-4.59956870E+01 5.19033008E+00 2.50175393E-02-3.32327159E-
 06 3
 -5.97355878E-09 2.12980104E-12-1.90259307E+04 7.48295559E+00
 4
 C*COC(*O)CJ 11/16 THERMC 4H 50 2 0G 300.000 5000.000
 1373.000 31
 1.55313665E+01 1.24028967E-02-4.40474510E-06 7.01284547E-10-4.14074844E-
 14 2
 -2.01727357E+04-5.23898006E+01 3.03494306E+00 3.86707368E-02-2.47276030E-
 05 3
 7.57404352E-09-8.98756789E-13-1.55098234E+04 1.58157840E+01
 4
 O*CYCC*CCO 11/16 THERMC 4H 40 2 0G 300.000 5000.000
 1393.000 01
 1.48374688E+01 1.15123620E-02-4.05025495E-06 6.40887785E-10-3.76816286E-
 14 2
 -4.02056676E+04-6.94871556E+01-1.30037247E+00 5.36841530E-02-4.72380331E-
 05 3
 2.10478124E-08-3.74640067E-12-3.50481447E+04 1.55988830E+01
 4
 O*CYCCC*CO 11/16 THERMC 4H 40 2 0G 300.000 5000.000
 1370.000 01
 1.48380166E+01 1.18192913E-02-4.22775996E-06 6.76341902E-10-4.00684701E-
 14 2
 -3.76707665E+04-6.83483755E+01 8.26714391E-01 4.13929566E-02-2.68895555E-
 05 3
 8.06486118E-09-8.82868057E-13-3.24983474E+04 8.00963365E+00
 4

O*CCC*C*O 11/14/16 THERMC 4H 40 2 0G 300.000 5000.000
1367.000 21
1.45665786E+01 1.11977169E-02-4.01294252E-06 6.42785307E-10-3.81141124E-
14 2
-3.48353556E+04-5.67430358E+01 6.67208436E-01 3.98288750E-02-2.46812752E-
05 3
6.50730883E-09-4.95614576E-13-2.96701567E+04 1.91939227E+01
4
O*CC*CC*O 11/14/16 THERMC 4H 40 2 0G 300.000 5000.000
1394.000 21
1.55606251E+01 1.00160664E-02-3.52623062E-06 5.58219798E-10-3.28312450E-
14 2
-3.22390217E+04-5.56858972E+01 2.63568435E-01 5.17368641E-02-4.82625488E-
05 3
2.26254297E-08-4.19193081E-12-2.75103144E+04 2.43722030E+01
4
O*CYCCCOHCJO 11/16 THERMC 4H 50 3 0G 300.000 5000.000
1411.000 11
1.88776839E+01 1.06315385E-02-3.85063527E-06 6.21354527E-10-3.70390550E-
14 2
-5.38531080E+04-7.48694342E+01-6.28795018E+00 7.11692260E-02-5.78764684E-
05 3
2.17448565E-08-3.07247604E-12-4.55544668E+04 5.92229746E+01
4
CYCOH*CC*CO 11/16 THERMC 4H 60 2 0G 300.000 5000.000
1415.000 11
1.76649152E+01 1.28531446E-02-4.31334263E-06 6.61660739E-10-3.80847216E-
14 2
-4.48940409E+04-7.27402041E+01-1.07601114E+01 9.85439738E-02-1.02896331E-
04 3
5.13486895E-08-9.77796729E-12-3.71084884E+04 7.28138363E+01
4
O*CYCCJCOHCO 11/16 THERMC 4H 50 3 0G 300.000 5000.000
1545.000 11
1.95552057E+01 1.01490652E-02-3.70436947E-06 6.00594981E-10-3.59133060E-
14 2
-5.36692271E+04-8.00644607E+01-5.33627029E+00 6.86926468E-02-5.40497390E-
05 3
1.91648876E-08-2.46609910E-12-4.53595464E+04 5.29864611E+01
4
O*CYCCJC*CO 11/16 THERMC 4H 30 2 0G 300.000 5000.000
1446.000 01
1.14978754E+01 1.21363991E-02-4.34528923E-06 6.95689412E-10-4.12404734E-
14 2
-1.50594456E+04-3.43280104E+01-1.39654318E+00 3.18756849E-02-8.35843959E-
06 3
-4.91973887E-09 2.18217501E-12-9.67980912E+03 3.83807222E+01
4
O*CYCC*CCJO 11/16 THERMC 4H 30 2 0G 300.000 5000.000
1419.000 01
1.29440953E+01 1.03090214E-02-3.57965472E-06 5.61870162E-10-3.28626599E-
14 2
-1.71011410E+04-4.48244909E+01-5.51689086E+00 5.80124161E-02-5.04464918E-
05 3
2.12685759E-08-3.49206922E-12-1.13033379E+04 5.24383629E+01
4
O*CYCCCJ*CO 11/16 THERMC 4H 30 2 0G 300.000 5000.000
1446.000 01

1.14978754E+01 1.21363991E-02-4.34528923E-06 6.95689412E-10-4.12404734E-
14 2
-1.50594456E+04-3.43280104E+01-1.39654318E+00 3.18756849E-02-8.35843959E-
06 3
-4.91973887E-09 2.18217501E-12-9.67980912E+03 3.83807222E+01
4
O*CJC*CC*O 11/16 THERMC 4H 30 2 0G 300.000 5000.000
1393.000 21
1.47812704E+01 7.84752284E-03-2.72086050E-06 4.26929936E-10-2.49729967E-
14 2
-1.36789173E+04-4.74050764E+01 1.59602246E+00 4.16458007E-02-3.60476075E-
05 3
1.53874761E-08-2.59202905E-12-9.46587007E+03 2.22359759E+01
4
O*C*CC*COJ 11/16 THERMC 4H 30 2 0G 300.000 5000.000
1670.000 21
1.30115965E+01 1.06098307E-02-4.00075231E-06 6.64892715E-10-4.04929769E-
14 2
-1.24280065E+04-4.77439312E+01 2.22753022E+00 3.39273237E-02-2.13725969E-
05 3
5.79903998E-09-5.05914112E-13-8.73833194E+03 1.04983460E+01
4
O*C*CC*COJ 11/16 THERMC 4H 30 2 0G 300.000 5000.000
1670.000 21
1.30115965E+01 1.06098307E-02-4.00075231E-06 6.64892715E-10-4.04929769E-
14 2
-1.24280065E+04-4.77439312E+01 2.22753022E+00 3.39273237E-02-2.13725969E-
05 3
5.79903998E-09-5.05914112E-13-8.73833194E+03 1.04983460E+01
4
O*CYCCJCOJ 11/16 THERMC 4H 50 2 0G 300.000 5000.000
1643.000 01
1.15657987E+01 1.62965858E-02-5.63970679E-06 8.87400190E-10-5.21016399E-
14 2
-1.90381967E+04-3.52517074E+01-2.68118426E+00 5.01490768E-02-3.44657874E-
05 3
1.13394407E-08-1.41273090E-12-1.44885343E+04 4.05510119E+01
4
O*CYCCCJOC 11/16 THERMC 4H 50 2 0G 300.000 5000.000
1437.000 01
1.19659966E+01 1.42850265E-02-4.53195219E-06 6.67763650E-10-3.73254207E-
14 2
-1.94817305E+04-3.55574389E+01-6.65628672E+00 6.89882411E-02-6.55036840E-
05 3
3.09792212E-08-5.67195206E-12-1.43008673E+04 6.02012111E+01
4
O*CYCCCOCJ 11/16 THERMC 4H 50 2 0G 300.000 5000.000
1437.000 01
1.19659966E+01 1.42850265E-02-4.53195219E-06 6.67763650E-10-3.73254207E-
14 2
-1.94817305E+04-3.55574389E+01-6.65628672E+00 6.89882411E-02-6.55036840E-
05 3
3.09792212E-08-5.67195206E-12-1.43008673E+04 6.02012111E+01
4
O*CYCC*COJ 11/16 THERMC 4H 40 2 0G 300.000 5000.000
1364.000 01
1.31104735E+01 1.33062715E-02-4.74539319E-06 7.57658190E-10-4.48250957E-
14 2

-2.84404421E+04-4.56188075E+01-1.18409862E+00 4.08218568E-02-2.19332488E-05 3
 3.94701609E-09 1.42236537E-13-2.29362481E+04 3.31598805E+01
 4
 O*CYCC*COJ 11/16 THERMC 4H 30 2 0G 300.000 5000.000
 1378.000 01
 1.40314190E+01 9.99523165E-03-3.60883360E-06 5.80939075E-10-3.45666742E-14 2
 -6.30982349E+03-4.95327723E+01-3.13199079E+00 4.81867669E-02-3.43530658E-05 3
 1.09948972E-08-1.23668254E-12-2.96495926E+02 4.30933162E+01
 4
 O*CYCCOHCJOC 11/16 THERMC 4H 50 3 0G 300.000 5000.000
 1395.000 11
 1.77249809E+01 1.15542209E-02-4.15268417E-06 6.66513529E-10-3.95786698E-14 2
 -4.16735541E+04-6.47897796E+01-4.33693969E+00 6.52934671E-02-5.36140845E-05 3
 2.10711316E-08-3.21987345E-12-3.43863462E+04 5.26599541E+01
 4
 THFO1-3 11/ 4/16 THERMC 4H 60 2 0G 300.000 5000.000
 1529.000 01
 1.40284823E+01 1.61764401E-02-5.43065391E-06 8.34025528E-10-4.80685093E-14 2
 -3.45614598E+04-5.69406305E+01-8.80511500E+00 7.06628616E-02-5.32247481E-05 3
 1.89478686E-08-2.51630815E-12-2.70165956E+04 6.48310346E+01
 4
 THFO1-4 11/ 4/16 THERMC 4H 60 2 0G 300.000 5000.000
 1660.000 01
 1.21879182E+01 1.93732709E-02-6.95089084E-06 1.11952601E-09-6.67709148E-14 2
 -3.64572691E+04-4.64751545E+01-6.88045775E+00 6.44501317E-02-4.51917575E-05 3
 1.49648080E-08-1.87295632E-12-3.03319013E+04 5.50873213E+01
 4
 CHOCHO 11/16 THERMC 2H 20 2 0G 300.000 5000.000
 1386.000 11
 9.75438561E+00 4.97645947E-03-1.74410483E-06 2.75586994E-10-1.61969892E-14 2
 -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
 CHOCO C 2H 10 20 0G 300.00 5000.00 1000.00
 1
 0.83591970E+01 0.44947090E-02-0.19879570E-05 0.38903890E-09-0.27935380E-13 2
 -0.12406730E+05-0.16767200E+02 0.76697390E+01-0.12908030E-01 0.59528090E-04 3
 -0.69600430E-07 0.26537680E-10-0.11337010E+05-0.86714600E+01
 4
 O*CC(*O)C*CJ 11/16 THERMC 4H 30 2 0G 300.000 5000.000
 1387.000 21
 1.42603990E+01 8.63754117E-03-3.06553209E-06 4.87882832E-10-2.88004125E-14 2
 1.24572307E+03-4.49927293E+01 2.04374226E+00 3.96027283E-02-3.38308937E-05 3

1.46540861E-08-2.55411718E-12 5.25437455E+03 1.97742891E+01
 4
 CHCHCOCH3 8/18/15 THERMC 4H 50 1 0G 300.000 5000.000
 1395.000 11
 1.14010549E+01 1.34548885E-02-4.59299710E-06 7.11920609E-10-4.12505114E-
 14 2
 8.80627955E+03-3.18999700E+01 1.43580644E+00 3.95510343E-02-3.21091166E-
 05 3
 1.43398918E-08-2.65215250E-12 1.20715975E+04 2.07642148E+01
 4
 C4H5O-3OJ 12/16 THERMC 4H 50 2 0G 300.000 5000.000
 1683.000 11
 1.34315979E+01 1.60039462E-02-5.92985163E-06 9.74552533E-10-5.89069446E-
 14 2
 -6.91217839E+03-4.57309522E+01-2.95279971E+00 5.38570560E-02-3.71914760E-
 05 3
 1.19365458E-08-1.43382960E-12-1.54491961E+03 4.18839855E+01
 4
 C4H5O-3O2H 12/16 THERMC 4H 60 3 0G 300.000 5000.000
 1408.000 21
 1.91194553E+01 1.47120122E-02-5.16801307E-06 8.17211291E-10-4.80355529E-
 14 2
 -2.60886188E+04-7.72847543E+01-6.26374375E+00 7.93440575E-02-6.79495622E-
 05 3
 2.83567636E-08-4.63512505E-12-1.79822329E+04 5.68539097E+01
 4
 C4H5O-2OJ 12/16 THERMC 4H 50 2 0G 300.000 5000.000
 1465.000 11
 1.65617402E+01 1.26406856E-02-4.55052701E-06 7.31117959E-10-4.34448926E-
 14 2
 -1.19608893E+04-6.43380269E+01-1.37713322E+00 4.75365220E-02-2.58071246E-
 05 3
 3.84827193E-09 5.29002214E-13-5.21134770E+03 3.41914752E+01
 4
 C4H5O-2O2H 12/16 THERMC 4H 60 3 0G 300.000 5000.000
 1451.000 21
 1.93323674E+01 1.39271914E-02-4.77166787E-06 7.42868746E-10-4.32204665E-
 14 2
 -3.10573226E+04-7.91381067E+01-5.09653555E+00 7.45364227E-02-6.09481584E-
 05 3
 2.37414540E-08-3.54002092E-12-2.31974849E+04 5.03528704E+01
 4
 O*CCCC*O 12/ 9/16 THERMC 4H 60 2 0G 300.000 5000.000
 1422.000 31
 1.54605801E+01 1.43034469E-02-4.91419273E-06 7.66379858E-10-4.46383637E-
 14 2
 -4.23989669E+04-5.36790327E+01 3.81644561E+00 3.05493478E-02-4.90714738E-
 06 3
 -7.02780832E-09 2.63088668E-12-3.74170481E+04 1.24820303E+01
 4
 O*CYCCCCO2O 12/16 THERMC 4H 50 4 0G 300.000 5000.000
 1419.000 21
 2.03217600E+01 1.43845554E-02-5.21555091E-06 8.41904585E-10-5.01898476E-
 14 2
 -5.42743570E+04-8.47305576E+01 2.16121638E-01 4.76248152E-02-1.59612583E-
 05 3
 -5.21412385E-09 2.87955229E-12-4.62084009E+04 2.76391696E+01
 4

O*CYCCCO2HC*OO 16 THERMC 4H 40 5 0G 300.000 5000.000
1433.000 21
2.39134020E+01 1.12102479E-02-4.09224518E-06 6.63540785E-10-3.96796786E-
14 2
-7.78156031E+04-8.84874709E+01-4.45990295E+00 7.92415342E-02-6.43399269E-
05 3
2.38950675E-08-3.30276453E-12-6.84586712E+04 6.27389300E+01
4
O*CYCCCO2CO2HO 16 THERMC 4H 50 6 0G 300.000 5000.000
1394.000 41
2.44355447E+01 1.49968277E-02-5.61392881E-06 9.30501414E-10-5.60162739E-
14 2
-6.65016191E+04-1.00630882E+02-3.87253641E+00 9.20142532E-02-8.70388800E-
05 3
4.02380707E-08-7.28702084E-12-5.78436535E+04 4.74026982E+01
4
O*CYCCJCCO2HO 16 THERMC 4H 50 4 0G 300.000 5000.000
1509.000 21
1.81755461E+01 1.61057875E-02-5.78390324E-06 9.27742297E-10-5.50639900E-
14 2
-4.67592556E+04-6.97612263E+01 2.04240787E-01 4.67341170E-02-1.84321988E-
05 3
-1.67839542E-09 1.77890668E-12-3.95167914E+04 3.05645102E+01
4
O*CYCCO2HCC*OO 16 THERMC 4H 40 5 0G 300.000 5000.000
1414.000 21
2.20697495E+01 1.28456127E-02-4.67229594E-06 7.55785553E-10-4.51210545E-
14 2
-8.01017613E+04-8.80335222E+01-1.35536734E+00 6.02089856E-02-3.55705096E-
05 3
6.62259627E-09 3.66300995E-13-7.15381827E+04 3.98735641E+01
4
O*CYCCO2CCO2HO 16 THERMC 4H 50 6 0G 300.000 5000.000
1402.000 41
2.77806648E+01 1.22340930E-02-4.45995844E-06 7.22522147E-10-4.31802729E-
14 2
-6.63542912E+04-1.18863445E+02-4.19951783E+00 9.28213765E-02-8.12860902E-
05 3
3.35525369E-08-5.34017604E-12-5.61195143E+04 5.03344014E+01
4
O*CYCCCJCO2HO 16 THERMC 4H 50 4 0G 300.000 5000.000
1392.000 21
1.83830081E+01 1.58142103E-02-5.65800801E-06 9.04290478E-10-5.33888631E-
14 2
-4.63443484E+04-7.07361559E+01-4.13933200E+00 7.37127620E-02-6.37047836E-
05 3
2.77055993E-08-4.81731735E-12-3.90758457E+04 4.83096974E+01
4
AC3H5CHO 2/29/96 THERMC 4H 60 1 0G 300.000 5000.000
1390.000 21
1.22811161E+01 1.50167397E-02-5.17605303E-06 8.07796972E-10-4.70379360E-
14 2
-1.50985283E+04-3.72055710E+01 1.59653121E-01 4.25761347E-02-2.91900593E-
05 3
1.04044255E-08-1.53682904E-12-1.07859656E+04 2.82087323E+01
4
AC3H5CO 2/29/96 THERMC 4H 50 1 0G 300.000 5000.000
1389.000 21

1.18646590E+01 1.28852832E-02-4.45460888E-06 6.96613045E-10-4.06215490E-
 14 2
 3.86344452E+03-3.32989999E+01 9.34300027E-01 3.77751824E-02-2.61384581E-
 05 3
 9.34041036E-09-1.37598294E-12 7.74223639E+03 2.56636231E+01
 4
 C*COCJCHO 3/29/17 THERMC 4H 50 2 0G 300.000 5000.000
 1384.000 31
 1.56094419E+01 1.22117369E-02-4.30946552E-06 6.83219915E-10-4.02221737E-
 14 2
 -7.81235606E+03-5.10353772E+01 1.95974816E+00 4.56618473E-02-3.67147501E-
 05 3
 1.54134932E-08-2.66334566E-12-3.16918340E+03 2.18191444E+01
 4
 C*COCCJO 3/29/17 THERMC 4H 50 2 0G 300.000 5000.000
 1363.000 31
 1.49302879E+01 1.29296153E-02-4.58991128E-06 7.30539994E-10-4.31248679E-
 14 2
 -1.07328474E+04-4.76873343E+01 4.66210244E+00 3.10216312E-02-1.42373891E-
 05 3
 1.65283659E-09 3.03447957E-13-6.52163161E+03 9.64719483E+00
 4
 C3H6CHO1O2 06/09/10 C 4H 70 30 0G 300.00 4000.00 1000.00
 1
 0.76516471E+01 0.30303048E-01-0.10537738E-04 0.17096293E-08-0.10666237E-
 12 2
 -0.20773410E+05-0.20829773E+01 0.16193655E+01 0.57815064E-01-0.45736811E-
 04 3
 0.16852578E-07-0.15469613E-11-0.20261789E+05 0.24986498E+02
 4
 C3H6CHO1Q4J THERGAS C 4H 70 3 0G 300. 3000. 1000.0
 1
 0.78843960E+01 0.28832970E-01-0.97068470E-05 0.15386720E-08-0.94436950E-
 13 2
 -0.21040150E+05 0.20824430E+00 0.31975170E+01 0.53235020E-01-0.44077750E-
 04 3
 0.18986560E-07-0.28947850E-11-0.20899230E+05 0.20251580E+02
 4
 C3H6CHO1Q3J 23/01/11 C 4H 70 30 0G 300.00 4000.00 1000.00
 1
 0.82190475E+01 0.29392142E-01-0.10119235E-04 0.16311542E-08-0.10136340E-
 12 2
 -0.17143785E+05-0.35358276E+01 0.21094601E+01 0.62394403E-01-0.61374361E-
 04 3
 0.32821017E-07-0.69357675E-11-0.16880871E+05 0.22604990E+02
 4
 C3H6CHO1Q2J 23/01/11 C 4H 70 30 0G 300.00 4000.00 1000.00
 1
 0.84472122E+01 0.27956562E-01-0.93132521E-05 0.14660149E-08-0.89581242E-
 13 2
 -0.14952375E+05-0.21901779E+01 0.17000396E+01 0.66549122E-01-0.74351592E-
 04 3
 0.45983111E-07-0.11410838E-10-0.14687058E+05 0.26335529E+02
 4
 C3H6CHO1Q4O2 THERGAS C 4H 70 5 0G 300. 3000. 1000.0
 1
 -0.33120900E+01 0.55561010E-01-0.22539740E-04 0.40718710E-08-0.27371860E-
 12 2

-0.28975330E+05 0.66721420E+02-0.59506310E+00 0.78808660E-01-0.68392400E-
 04 3
 0.24548300E-07-0.93355860E-12-0.33019100E+05 0.40971030E+02
 4
 C3H6CHO1Q3O2 23/01/11 C 4H 7O 50 OG 300.00 4000.00 1000.00
 1
 0.10600700E+02 0.33690017E-01-0.11905188E-04 0.19515809E-08-0.12253431E-
 12 2
 -0.33136773E+05-0.10341759E+02 0.18372377E+01 0.74184120E-01-0.62999257E-
 04 3
 0.22738030E-07-0.15678122E-11-0.32496564E+05 0.28679533E+02
 4
 C3H6CHO1Q2O2 23/01/11 C 4H 7O 50 OG 300.00 4000.00 1000.00
 1
 0.70948396E+01 0.38953193E-01-0.14366015E-04 0.24279445E-08-0.15577607E-
 12 2
 -0.32348094E+05 0.98069534E+01 0.31312940E+01 0.70406489E-01-0.59712031E-
 04 3
 0.21004311E-07-0.90696781E-12-0.33489711E+05 0.22401546E+02
 4
 C3H6CHO1*O4Q THERGAS C 4H 6O 4 OG 300. 3000. 1000.0
 1
 -0.15708170E+02 0.72698740E-01-0.34097570E-04 0.68283250E-08-0.49448960E-
 12 2
 -0.50362020E+05 0.13113290E+03 0.32927130E+00 0.64104470E-01-0.53073620E-
 04 3
 0.16745830E-07 0.89389390E-12-0.58534040E+05 0.34779550E+02
 4
 C3H6CHO1*O3Q 23/01/11 C 4H 6O 40 OG 300.00 4000.00 1000.00
 1
 0.84472122E+01 0.27956562E-01-0.93132521E-05 0.14660149E-08-0.89581242E-
 13 2
 -0.14952375E+05-0.21901779E+01 0.17000396E+01 0.66549122E-01-0.74351592E-
 04 3
 0.45983111E-07-0.11410838E-10-0.14687058E+05 0.26335529E+02
 4
 C3H6CHO1*O2Q 23/01/11 C 4H 6O 40 OG 300.00 4000.00 1000.00
 1
 0.84472122E+01 0.27956562E-01-0.93132521E-05 0.14660149E-08-0.89581242E-
 13 2
 -0.14952375E+05-0.21901779E+01 0.17000396E+01 0.66549122E-01-0.74351592E-
 04 3
 0.45983111E-07-0.11410838E-10-0.14687058E+05 0.26335529E+02
 4
 CHOCH2CHO 7/ 6/ 7 THERGC 3H 4O 2 OG 300.000 5000.000
 2041.000 31
 1.01665173E+01 1.26554663E-02-4.72118749E-06 7.79086094E-10-4.72151798E-
 14 2
 -3.85694777E+04-2.39205149E+01 1.05479724E+00 3.10169903E-02-1.69152633E-
 05 3
 3.63174198E-09-1.52155933E-13-3.52900612E+04 2.58148090E+01
 4
 CHOCH2CO 7/ 6/ 7 THERGC 3H 3O 2 OG 300.000 5000.000
 1375.000 31
 1.03839875E+01 8.95653335E-03-3.17495041E-06 5.04859934E-10-2.97835672E-
 14 2
 -2.07847430E+04-2.26918341E+01 1.48700499E+00 2.83963833E-02-1.93510395E-
 05 3

6.68152666E-09-9.54954634E-13-1.75210985E+04 2.56357273E+01
4
THFOOH14J2 4/ 7/17 THERMC 4H 70 5 0G 300.000 5000.000
1040.000 41
1.56221918E+01 2.60691421E-02-7.95477843E-06 7.26281425E-10 2.27811906E-
15 2
-3.51133961E+04-4.91232190E+01-1.00084000E+01 1.25701306E-01-1.49502437E-
04 3
9.09122227E-08-2.25105499E-11-3.01628389E+04 7.46319769E+01
4
THFOOH13J4 4/ 7/17 THERMC 4H 70 5 0G 300.000 5000.000
1001.000 41
3.93576717E+00 4.56589372E-02-1.74030251E-05 2.39357783E-09-9.43671201E-
14 2
-2.86879678E+04 1.70746874E+01-8.92218231E+00 1.24588458E-01-1.50504865E-
04 3
9.23960199E-08-2.30565391E-11-2.88356804E+04 6.92553784E+01
4
THFOOH13J2 4/ 7/17 THERMC 4H 70 5 0G 300.000 5000.000
888.000 41
2.15951358E+01 1.50119028E-02-2.69585523E-06-1.90552564E-10 5.53899065E-
14 2
-3.41936211E+04-8.06896733E+01-8.11911806E+00 1.14250424E-01-1.31026546E-
04 3
7.78079213E-08-1.89725661E-11-2.70043928E+04 6.82653034E+01
4
THFOOH12J3 4/ 7/17 THERMC 4H 70 5 0G 300.000 5000.000
888.000 41
2.15951358E+01 1.50119028E-02-2.69585523E-06-1.90552564E-10 5.53899065E-
14 2
-3.41936211E+04-8.06896733E+01-8.11911806E+00 1.14250424E-01-1.31026546E-
04 3
7.78079213E-08-1.89725661E-11-2.70043928E+04 6.82653034E+01
4
THFOOH23J1 4/ 7/17 THERMC 4H 70 5 0G 300.000 5000.000
1030.000 41
1.38441081E+01 2.73687241E-02-8.16979088E-06 6.58630903E-10 1.52396020E-
14 2
-2.92006349E+04-3.61523883E+01-7.07841006E+00 1.13344247E-01-1.32289189E-
04 3
7.93967332E-08-1.95270304E-11-2.56707560E+04 6.30970363E+01
4
THFOOH1X3 4/ 7/17 THERMC 4H 60 3 0G 300.000 5000.000
1460.000 21
1.84515680E+01 1.48797486E-02-5.14680850E-06 8.06371757E-10-4.71210760E-
14 2
-2.92401481E+04-7.41007801E+01-3.00887712E-01 5.35818562E-02-3.19433593E-
05 3
7.18463623E-09-1.53441840E-13-2.24162959E+04 2.80919916E+01
4
THFOOH2X3 4/ 7/17 THERMC 4H 60 3 0G 300.000 5000.000
1393.000 21
1.87692132E+01 1.45921385E-02-5.04343472E-06 7.89785107E-10-4.61365162E-
14 2
-2.43553361E+04-7.50005559E+01-3.68408324E+00 6.85102424E-02-5.36253334E-
05 3
2.02549081E-08-2.96729572E-12-1.68763785E+04 4.47825338E+01
4

THFOOH1X2 4/ 7/17 THERMC 4H 60 3 0G 300.000 5000.000
 1403.000 21
 1.95946957E+01 1.37095444E-02-4.69897125E-06 7.31855925E-10-4.25952200E-14 2
 -2.65860539E+04-8.01205978E+01-4.88754520E+00 7.75828094E-02-6.84552932E-05 3
 2.95176872E-08-4.98001464E-12-1.89259188E+04 4.87054090E+01
 HOCY(CCJCCO) 04/17 THERMC 4H 70 2 0G 300.000 5000.000
 1422.000 11
 1.43761885E+01 1.79068743E-02-5.99040247E-06 9.16336776E-10-5.26200019E-14 2
 -2.97317472E+04-4.98551562E+01-5.25711758E+00 6.90767815E-02-5.70550981E-05 3
 2.39563677E-08-3.99570665E-12-2.35706366E+04 5.34915669E+01
 4
 HOCY(CCCOCJ) 04/17 THERMC 4H 70 2 0G 300.000 5000.000
 1429.000 11
 1.44578275E+01 1.69543206E-02-5.48404298E-06 8.20103067E-10-4.63605937E-14 2
 -2.82516766E+04-5.01431619E+01-5.55435977E+00 7.03375642E-02-5.96920640E-05 3
 2.55587812E-08-4.30703831E-12-2.21438434E+04 5.46813889E+01
 4
 HOCY(CCJCOC) 04/17 THERMC 4H 70 2 0G 300.000 5000.000
 1426.000 11
 1.45564309E+01 1.68880831E-02-5.46480792E-06 8.17457045E-10-4.62203381E-14 2
 -2.66808344E+04-5.08025116E+01-5.28753918E+00 6.98843954E-02-5.93925777E-05 3
 2.54986508E-08-4.31149830E-12-2.06255073E+04 5.31274798E+01
 4
 O*COCCC*O 4/24/17 THERMC 4H 60 3 0G 300.000 5000.000
 1444.000 41
 1.80620221E+01 1.48609462E-02-5.24225572E-06 8.31235798E-10-4.89523611E-14 2
 -6.82382383E+04-6.68469148E+01 1.45626172E+00 4.56859837E-02-2.17955505E-05 3
 1.52472894E-09 9.91167962E-13-6.18428890E+04 2.48828568E+01
 4
 O*CCOCC*O 4/24/17 THERMC 4H 60 3 0G 300.000 5000.000
 1360.000 41
 1.59840660E+01 1.65048769E-02-5.77812083E-06 9.11271445E-10-5.34551181E-14 2
 -5.55360068E+04-5.21315902E+01 6.11501043E+00 3.11382787E-02-9.43460116E-06 3
 -2.00576690E-09 1.13570453E-12-5.11928782E+04 3.98495960E+00
 4
 JOOCY(CCCOC(OH)) THERMC 4H 70 4 0G 300.000 5000.000
 1431.000 31
 1.98145734E+01 1.76681137E-02-5.94299748E-06 9.12999045E-10-5.26030900E-14 2
 -4.96127369E+04-7.57862745E+01-2.18835895E+00 7.25036863E-02-5.74259593E-05 3
 2.24587248E-08-3.43380672E-12-4.25131594E+04 4.08317066E+01
 4
 JOOCY(CC(OH)CCO) THERMC 4H 70 4 0G 300.000 5000.000
 1037.000 31

1.27990513E+01 2.57356261E-02-7.66343409E-06 6.72035574E-10 5.00446846E-
15 2
-4.62382082E+04-3.63434144E+01-1.04589171E+01 1.16207080E-01-1.35269028E-
04 3
8.10987671E-08-1.99054889E-11-4.18077250E+04 7.58146532E+01
4
JOOCY(CCOCC(OH)) THERMC 4H 70 4 OG 300.000 5000.000
1424.000 31
2.08058266E+01 1.71921668E-02-5.85990063E-06 9.08491545E-10-5.26839100E-
14 2
-4.73466608E+04-8.26061629E+01-6.33448618E+00 8.75489466E-02-7.51679042E-
05 3
3.15869622E-08-5.18231404E-12-3.88519690E+04 6.02927859E+01
4
THF1OH3E 4/24/17 THERMC 4H 60 2 OG 300.000 5000.000
1481.000 11
1.20356276E+01 1.79270140E-02-6.12283958E-06 9.49858669E-10-5.50850723E-
14 2
-3.62571108E+04-3.79905417E+01 1.27992855E+00 3.47929968E-02-1.07135135E-
05 3
-2.64617182E-09 1.50959103E-12-3.17584221E+04 2.25990229E+01
4
THF1OH3E4J 4/24/17 THERMC 4H 50 2 OG 300.000 5000.000
1683.000 11
1.02596160E+01 1.75255698E-02-6.17213292E-06 9.80827158E-10-5.79244851E-
14 2
-1.33262399E+04-2.52350689E+01 1.35128598E+00 3.59363572E-02-1.88104362E-
05 3
4.11641000E-09-2.10843892E-13-1.02013259E+04 2.31767409E+01
4
THF2OH4E 4/24/17 THERMC 4H 60 2 OG 300.000 5000.000
1405.000 11
1.58780281E+01 1.49608516E-02-5.16496515E-06 8.07108816E-10-4.70460974E-
14 2
-3.56926189E+04-5.98820608E+01-5.67337768E+00 7.35284876E-02-6.69485572E-
05 3
3.05230291E-08-5.48518739E-12-2.90951775E+04 5.28370908E+01
4
THF2OH4E4J 4/24/17 THERMC 4H 50 2 OG 300.000 5000.000
1408.000 11
1.56859488E+01 1.24846489E-02-4.29004542E-06 6.68333234E-10-3.88748812E-
14 2
-1.36635435E+04-5.64704062E+01-5.04889738E+00 7.18001262E-02-6.99565918E-
05 3
3.35816045E-08-6.26523642E-12-7.61343996E+03 5.09242227E+01
4
O*COCCC*O 4/24/17 THERMC 4H 50 3 OG 300.000 5000.000
1439.000 41
1.74766304E+01 1.29391352E-02-4.60773363E-06 7.35138078E-10-4.34757383E-
14 2
-4.45001319E+04-6.21461264E+01 2.83604831E+00 3.81075746E-02-1.49072577E-
05 3
-1.68171316E-09 1.57792062E-12-3.86707743E+04 1.94246461E+01
4
O*COCCCJ*O 4/24/17 THERMC 4H 50 3 OG 300.000 5000.000
1439.000 41
1.74766304E+01 1.29391352E-02-4.60773363E-06 7.35138078E-10-4.34757383E-
14 2

-4.92308818E+04-6.20052104E+01 2.83604831E+00 3.81075746E-02-1.49072577E-
05 3
-1.68171316E-09 1.57792062E-12-4.34015242E+04 1.95655620E+01
4
O*CCOCCJ*O 4/24/17 THERMC 4H 50 3 OG 300.000 5000.000
1356.000 41
1.55776921E+01 1.43624873E-02-5.05249270E-06 7.99400165E-10-4.69975934E-
14 2
-3.65788855E+04-4.82842075E+01 6.88849229E+00 2.63373140E-02-6.36719867E-
06 3
-3.08683427E-09 1.30131704E-12-3.26644364E+04 1.44593091E+00
4
CY(OCCOC*C) 17 THERMC 4H 60 2 OG 300.000 5000.000
1456.000 01
1.16422794E+01 1.78986975E-02-5.95641492E-06 9.08885638E-10-5.21325651E-
14 2
-2.84634027E+04-3.92485188E+01-2.29377668E+00 4.46646086E-02-2.17889146E-
05 3
2.87012143E-09 4.98627869E-13-2.31781279E+04 3.74281358E+01
4
CY(OCJCOC*C) 17 THERMC 4H 50 2 OG 300.000 5000.000
1459.000 01
1.15424163E+01 1.55152810E-02-5.14025198E-06 7.81231921E-10-4.46626321E-
14 2
-6.40005538E+03-3.58689747E+01-3.78697774E+00 5.27491252E-02-3.88574905E-
05 3
1.42181531E-08-2.02051671E-12-1.36732853E+03 4.57036053E+01
4
NC3H7CO3 23/01/11 C 4H 70 30 OG 300.00 4000.00 1000.00
1
-0.66629653E+01 0.53964116E-01-0.22254402E-04 0.40679011E-08-0.27579084E-
12 2
-0.26180285E+05 0.75498619E+02-0.24077139E+01 0.69231726E-01-0.57902485E-
04 3
0.20644562E-07-0.80081812E-12-0.30225805E+05 0.43266521E+02
4
!
!VERSION: ARAMCOMECH 1.3 C4
!AUTHORS: S. BURKE, C. ZHOU, W. K. METCALFE H. J. CURRAN
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
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
O L 1/90O 1 0 0 OG 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
 O2 RUS 890 2 0 0 OG 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
 OH IU3/030 1 H 1 0 OG 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
 H2O L 5/89H 2 O 1 0 OG 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
 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
 HO2 T 1/09H 1O 2 0 OG 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
 H2O2 T 8/03H 2O 2 0 OG 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
AR G 5/97AR 1 0 0 0G 200.000 6000.00 1000.00
1
2.50000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00
0.00000000E+00 2
-7.45375000E+02 4.37967491E+00 2.50000000E+00 0.00000000E+00
0.00000000E+00 3
0.00000000E+00 0.00000000E+00-7.45375000E+02 4.37967491E+00
0.00000000E+00 4
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
CO RUS 79C 1O 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 1O 2 0 0G 200.000 6000.00 1000.00
1
0.46365111E+01 0.27414569E-02-0.99589759E-06 0.16038666E-09-0.91619857E-
14 2
-0.49024904E+05-0.19348955E+01 0.23568130E+01 0.89841299E-02-0.71220632E-
05 3
0.24573008E-08-0.14288548E-12-0.48371971E+05 0.99009035E+01-
0.47328105E+05 4
HCO T 5/03C 1H 1O 1 0G 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
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
O2CHO 6/26/95 THERMC 1H 1O 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
 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
 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
 HOCH2O2H 9/ 1/12 C 1H 40 3 0G 300.000 5000.000
 1398.000 21
 1.24531886E+01 7.18221110E-03-2.47029548E-06 3.85611737E-10-2.24774193E-
 14 2
 -4.24862928E+04-3.58745197E+01 5.35189713E-01 3.73266553E-02-3.15299511E-
 05 3
 1.30352583E-08-2.11473264E-12-3.86609415E+04 2.71776082E+01
 4
 HOCH2O2 9/ 1/12 C 1H 30 3 0G 300.000 5000.000
 1377.000 21
 1.16406115E+01 5.72826040E-03-2.05362036E-06 3.29070695E-10-1.95188360E-
 14 2
 -2.53505769E+04-3.07332064E+01 2.82068616E+00 2.47857094E-02-1.66186399E-
 05 3
 4.79633095E-09-4.28087766E-13-2.22077036E+04 1.70599803E+01
 4
 OCH2O2H 9/ 1/12 C 1H 30 3 0G 300.000 5000.000
 997.000 21
 2.22488435E+00 1.70328727E-02-6.24631476E-06 8.37499249E-10-3.22096209E-
 14 2
 6.04759781E+03 2.33052848E+01 1.92120102E+00 3.09717915E-02-3.38215757E-
 05 3
 1.93739647E-08-4.63932897E-12 4.86086899E+03 2.02247107E+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

HOCH2O2H 4/ 9/98 THERMC 1H 40 3 0G 300.000 5000.000
 1422.000 31
 1.16303827E+01 7.15133688E-03-2.39035030E-06 3.65772791E-10-2.10199524E-
 14 2
 -4.31079242E+04-3.24276725E+01 1.85716693E+00 3.23153132E-02-2.69928902E-
 05 3
 1.11694484E-08-1.81284103E-12-4.00314471E+04 1.90917729E+01
 4
 HOCH2O2 4/ 9/98 THERMC 1H 30 3 0G 300.000 5000.000
 1412.000 21
 9.04545938E+00 7.15223373E-03-2.37005676E-06 3.60083481E-10-2.05750228E-
 14 2
 -2.49414886E+04-1.74210530E+01 2.85441621E+00 2.33663535E-02-1.88115990E-
 05 3
 7.96709515E-09-1.36346618E-12-2.29866196E+04 1.51730565E+01
 4
 OCH2O2H 4/ 9/98 THERMC 1H 30 3 0G 300.000 5000.000
 1420.000 21
 1.15398246E+01 5.34291432E-03-1.81878917E-06 2.81968625E-10-1.63584348E-
 14 2
 -1.68237489E+04-3.20700633E+01 1.93823075E+00 3.01465730E-02-2.61053152E-
 05 3
 1.09463562E-08-1.78312692E-12-1.38166625E+04 1.85042002E+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
 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
 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
 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 300.00 5000.00 1000.00
 1

4.80390863E+00 9.95844638E-03-3.85301026E-06 6.84740497E-10-4.58402955E-
 14 2
 -7.47135460E+02 1.45281400E+00 3.62497097E+00 3.59397933E-03 2.26538097E-
 05 3
 -2.95391947E-08 1.11977570E-11 7.93040410E+01 9.96382194E+00
 4
 CH2O2H 9/ 1/12 C 1H 30 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
 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
 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
 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
 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
 C2H4 G 1/00C 2 H 4 0 0 G 200.000 6000.00 1000.00
 1
 3.99182724E+00 1.04833908E-02-3.71721342E-06 5.94628366E-10-3.53630386E-
 14 2
 4.26865851E+03-2.69081762E-01 3.95920063E+00-7.57051373E-03 5.70989993E-
 05 3
 -6.91588352E-08 2.69884190E-11 5.08977598E+03 4.09730213E+00
 6.31426266E+03 4
 C2H3 ATCT/AC 2 H 3 0 0 G 200.000 6000.00 1000.00
 1
 4.15026763E+00 7.54021341E-03-2.62997847E-06 4.15974048E-10-2.45407509E-
 14 2
 3.38566380E+04 1.72812235E+00 3.36377642E+00 2.65765722E-04 2.79620704E-
 05 3
 -3.72986942E-08 1.51590176E-11 3.44749589E+04 7.91510092E+00
 3.56701718E+04 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
 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
 CH2CO H 2C 2O 1 0G 300.000 5000.000
 1391.000 01
 6.60179400E+00 5.23168519E-03-1.79376283E-06 2.82183642E-10-1.65610107E-
 14 2
 -8.61085819E+03-1.13932316E+01 1.65982341E+00 1.74426787E-02-1.35629541E-
 05 3
 5.53065784E-09-9.24027432E-13-6.95849922E+03 1.49168757E+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 0G 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 30 3 0G 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 30 2 0G 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
 C2H5OH L 8/88C 2 H 6 O 1 0 G 200.000 6000.00 1000.00
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 0.65624365E+01 0.15204222E-01-0.53896795E-05 0.86225011E-09-0.51289787E-
 13 2
 -0.31525621E+05-0.94730202E+01 0.48586957E+01-0.37401726E-02 0.69555378E-
 04 3
 -0.88654796E-07 0.35168835E-10-0.29996132E+05 0.48018545E+01-
 0.28257829E+05 4
 PC2H4OH T12/01C 2 H 5 O 1 0 G 200.000 6000.00 1000.00
 1
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 -5.92493321E+03-9.40355948E+00 4.47893092E+00 7.59782301E-03 2.81794908E-
 05 3
 -4.26953487E-08 1.78878934E-11-4.71446256E+03 6.38921206E+00-
 2.86833500E+03 4
 SC2H4OH T10/04C 2 H 5 O 1 0 G 200.000 6000.00 1000.00
 1
 6.35842302E+00 1.24356276E-02-4.33096839E-06 6.84530381E-10-4.03713238E-
 14 2
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 05 3
 -4.91943637E-08 2.01183723E-11-8.20503939E+03 8.01675700E+00-
 6.49827831E+03 4
 C2H5O IU2/03C 2 H 5 O 1 0 G 200.000 6000.00 1000.00
 1
 0.66889982E+01 0.13125676E-01-0.47038840E-05 0.75858552E-09-0.45413306E-
 13 2
 -0.47457832E+04-0.96983755E+01 0.43074268E+01 0.64147205E-02 0.31139714E-
 04 3
 -0.43314083E-07 0.17276184E-10-0.34027524E+04 0.59025837E+01-
 0.16357022E+04 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
 C2H5O2H 9/ 1/12 C 2H 6O 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 5O 2 OG 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
 C2H4O2H 9/ 1/12 C 2H 5O 2 OG 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
 CH3CHO2H 9/ 1/12 C 2H 5O 2 OG 300.000 5000.000
 1386.000 31
 9.94166406E+00 1.14384962E-02-3.92847407E-06 6.11402143E-10-3.55267132E-
 14 2
 -2.02545876E+03-2.22163407E+01 4.16440687E+00 2.38795950E-02-1.46887446E-
 05 3
 5.18066666E-09-8.37968487E-13 1.87348817E+02 9.35429162E+00
 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-
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 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
 CH3COCH3 ATCT AC 3 H 6 O 1 0 G 200.000 6000.00 1000.00
 1
 7.29796974E+00 1.75656913E-02-6.31678065E-06 1.02025553E-09-6.10903592E-
 14 2
 -2.95368927E+04-1.27591704E+01 5.55638920E+00-2.83863547E-03 7.05722951E-
 05 3
 -8.78130984E-08 3.40290951E-11-2.78325393E+04 2.31960221E+00-
 2.58360384E+04 4
 CH3COCH2 A10/04C 3 H 5 O 1 0 G 200.000 6000.00 1000.00
 1
 7.54410697E+00 1.43443222E-02-5.08381081E-06 8.13200521E-10-4.83673315E-
 14 2

-7.48672286E+03-1.14792587E+01 4.70187196E+00 5.51653762E-03 4.27505858E-
 05 3
 -5.94680816E-08 2.40685378E-11-5.92845491E+03 7.12932590E+00-
 4.00985747E+03 4
 CH3COCH2O2 2/14/95 C 3H 5O 3 OG 300.000 5000.000 1379.00
 31
 1.27690342E+01 1.42554828E-02-4.92821461E-06 7.70448921E-10-4.49110534E-
 14 2
 -2.34798669E+04-3.27155799E+01 5.95535468E+00 2.70255205E-02-1.37385031E-
 05 3
 3.53735851E-09-4.03922557E-13-2.06679464E+04 5.21436049E+00
 4
 CH3COCH2O2H 2/14/95 C 3H 6O 3 OG 300.000 5000.000 1381.00
 41
 1.52372810E+01 1.44114651E-02-5.01290009E-06 7.87071229E-10-4.60225784E-
 14 2
 -4.27564444E+04-4.77383784E+01 4.94789761E+00 3.60474432E-02-2.21719933E-
 05 3
 6.98296874E-09-9.21269260E-13-3.88687178E+04 8.49926130E+00
 4
 CH3COCH2O 4/ 3/ 0 THERMC 3H 5O 2 OG 300.000 5000.000
 1370.000 21
 1.14637586E+01 1.32124342E-02-4.56580495E-06 7.13897538E-10-4.16281047E-
 14 2
 -2.23833017E+04-3.15127868E+01 3.72927689E+00 2.63943697E-02-1.09796486E-
 05 3
 8.58185303E-10 3.39474590E-13-1.91551565E+04 1.18505335E+01
 4
 C2H3OCH2 H 5 C 3 O 1 G 298.0 6000.0
 1000.0 1
 1.00397568E+01 1.18952742E-02-4.13512716E-06 6.51590471E-10-3.83196617E-
 14 2
 7.27301530E+03-2.57171542E+01-1.44860882E+00 5.42514911E-02-7.45556749E-
 05 3
 6.03597706E-08-2.01938036E-11 1.01608402E+04 3.16318657E+01
 4
 C2H3CHO KPS12 C 3H 4O 1 OG 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 OG 300.000 5000.000
 1395.000 01
 8.86032735E+00 8.48985205E-03-2.90350080E-06 4.50763986E-10-2.61524281E-
 14 2
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 05 3
 7.29174972E-09-1.16083226E-12 1.02020654E+04 1.78705872E+01
 4
 C3H5O KPS12 C 3H 5O 1 OG 300.000 5000.000
 1402.000 01
 1.02638186E+01 1.17609932E-02-3.89837957E-06 5.92650815E-10-3.38867417E-
 14 2
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 05 3

9.56781953E-09-1.48085302E-12 1.04203725E+04 2.28283070E+01
 4
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 14 2
 -2.60055814E+04-1.44195446E+01 4.24529681E+00 6.68296706E-03 4.93337933E-
 05 3
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 2.22688471E+04 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 8/10/ 4 THERMC 3H 5O 1 0G 300.000 5000.000
 1363.000 21
 9.96855598E+00 1.61917946E-02-6.64161740E-06 1.15444520E-09-7.21981790E-
 14 2
 -4.16450354E+03-2.73971573E+01 8.36272659E+00-3.90712606E-03 3.59751257E-
 05 3
 -2.69209237E-08 5.98920261E-12-7.55243244E+02-9.53140102E+00
 4
 CH3CHCHO 8/10/ 4 THERMC 3H 5O 1 0G 300.000 5000.000
 1253.000 21
 8.27772090E+00 1.95687188E-02-8.47575089E-06 1.53249728E-09-9.86441542E-
 14 2
 -8.34456062E+03-2.17652483E+01-2.72811212E+00 3.80354483E-02-1.96782132E-
 05 3
 5.09554570E-09-7.28789092E-13-3.51122739E+03 4.04496677E+01
 4
 CH3OCH3 1/20/11 C 2H 6O 1 0G 300.000 5000.000
 1367.000 21
 7.36358679E+00 1.38910153E-02-4.74083257E-06 7.34874498E-10-4.25867578E-
 14 2
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 06 3
 -4.28367822E-09 1.36818123E-12-2.36771735E+04 1.28877967E+01
 4
 CH3OCH2 1/20/11 C 2H 5O 1 0G 300.000 5000.000
 1389.000 21
 6.73134670E+00 1.18022530E-02-4.00104434E-06 6.17227325E-10-3.56435023E-
 14 2
 -3.34933412E+03-9.40782513E+00 2.19172957E+00 1.90390966E-02-6.81450700E-
 06 3
 8.63577609E-11 3.23902492E-13-1.38948253E+03 1.62440756E+01
 4
 CH3OCH2O2 1/20/11 C 2H 5O 3 0G 300.000 5000.000
 1399.000 31
 1.22024149E+01 1.19225104E-02-4.06624713E-06 6.30079576E-10-3.65065312E-
 14 2
 -2.40327175E+04-3.38665462E+01 1.72101041E+00 3.78155492E-02-2.89668870E-
 05 3
 1.16796117E-08-1.93234479E-12-2.05308597E+04 2.19296296E+01
 4

CH2OCH2O2H 1/20/11 C 2H 50 3 0G 300.000 5000.000
 1419.000 41
 1.51031233E+01 9.18263324E-03-3.15895361E-06 4.92789411E-10-2.87001298E-
 14 2
 -1.96611854E+04-4.85172618E+01 9.08332173E-01 4.47997444E-02-3.69441578E-
 05 3
 1.48366604E-08-2.32279459E-12-1.50992319E+04 2.66419885E+01
 4
 CH3OCH2O2H 1/20/11 C 2H 60 3 0G 300.000 5000.000
 1402.000 41
 1.46617126E+01 1.20544674E-02-4.13604704E-06 6.43721637E-10-3.74188832E-
 14 2
 -4.18896186E+04-4.81293252E+01 7.37369081E-01 4.67410003E-02-3.73051936E-
 05 3
 1.50735309E-08-2.43781978E-12-3.73260287E+04 2.57932851E+01
 4
 CH3OCH2O 2/ 9/96 THERMC 2H 50 2 0G 300.000 5000.000
 2012.000 21
 8.60261845E+00 1.35772195E-02-4.84661602E-06 7.77766193E-10-4.62633624E-
 14 2
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 06 3
 -2.41484158E-10 4.51914496E-13-1.92377212E+04 1.23680069E+01
 4
 O2CH2OCH2O2H 1/20/11 C 2H 50 5 0G 300.000 5000.000
 1411.000 51
 1.96207800E+01 9.96131702E-03-3.41480475E-06 5.31364852E-10-3.08902100E-
 14 2
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 05 3
 3.13441786E-08-5.79042960E-12-3.41530358E+04 3.49112501E+01
 4
 HO2CH2OCHO 1/20/11 C 2H 40 4 0G 300.000 5000.000
 1428.000 41
 1.78528337E+01 7.54042388E-03-2.74895624E-06 4.45343367E-10-2.66154007E-
 14 2
 -6.41380252E+04-6.47357373E+01 5.15432996E-01 4.76081860E-02-3.63877925E-
 05 3
 1.24225089E-08-1.50813145E-12-5.82730214E+04 2.81992694E+01
 4
 OCH2OCHO 1/20/11 C 2H 30 3 0G 300.000 5000.000
 1426.000 21
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 14 2
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 07 3
 -6.94060480E-09 2.32311215E-12-4.07070844E+04 1.02048630E+01
 4
 HOCH2OCO 8/31/99 THERMC 2H 30 3 0G 300.000 5000.000
 1603.000 31
 1.13737391E+01 8.17663898E-03-2.92034021E-06 4.66695616E-10-2.76276823E-
 14 2
 -4.65575743E+04-2.86035265E+01 6.08180801E+00 1.28768359E-02 2.04419418E-
 06 3
 -6.10154921E-09 1.79820559E-12-4.39526183E+04 2.54054449E+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
-4.68316521E+04-6.91542601E+00 5.96757028E+00-9.38085425E-03 7.07648417E-
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
9.73659803E+00 7.42432713E-03-2.65641779E-06 4.25031143E-10-2.51824924E-
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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14 2
-2.36389018E+04-2.71144175E+01 2.31031671E+00 1.80474065E-02-2.71519637E-
06 3
-4.60918579E-09 1.70037078E-12-2.02910878E+04 1.71549722E+01
4
HE G 5/97HE 1 0 0 0 G 200.000 6000.00 1000.00
1
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0.00000000E+00 2
-7.45375000E+02 9.28723974E-01 2.50000000E+00 0.00000000E+00
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0.00000000E+00 0.00000000E+00-7.45375000E+02 9.28723974E-01
0.00000000E+00 4
C3H8 G 2/00C 3 H 8 0 0 G 200.000 6000.00 1000.00
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6.66919760E+00 2.06108751E-02-7.36512349E-06 1.18434262E-09-7.06914630E-
14 2
-1.62754066E+04-1.31943379E+01 4.21093013E+00 1.70886504E-03 7.06530164E-
05 3
-9.20060565E-08 3.64618453E-11-1.43810883E+04 5.61004451E+00-
1.25900384E+04 4
NC3H7 A 5/05C 3 H 7 0 0 G 200.000 6000.00 1000.00
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6.49636579E+00 1.77337992E-02-6.24898046E-06 9.95389495E-10-5.90199770E-
14 2
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05 3
-6.99343598E-08 2.81819493E-11 1.04074558E+04 8.39534919E+00
1.21859256E+04 4
IC3H7 A 5/05C 3 H 7 0 0 G 200.000 6000.00 1000.00
1
5.30597255E+00 1.89854588E-02-6.74315384E-06 1.07993730E-09-6.42785036E-
14 2
7.78748910E+03-2.23233935E+00 5.47421257E+00-8.42536682E-03 8.04607759E-
05 3
-9.49287824E-08 3.59830971E-11 9.04939013E+03 3.40542323E+00
1.08473019E+04 4
C3H6 G 2/00C 3 H 6 0 0 G 200.000 6000.00 1000.00
1
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14 2

-7.41715057E+02-8.43825992E+00 3.83464468E+00 3.29078952E-03 5.05228001E-05 3
-6.66251176E-08 2.63707473E-11 7.88717123E+02 7.53408013E+00
2.40543339E+03 4
C3H5-A PD5/98C 3H 5 0 0G 300.000 3000.00 1000.00
1
0.65007877E+01 0.14324731E-01-0.56781632E-05 0.11080801E-08-0.90363887E-13 2
0.17482449E+05-0.11243050E+02 0.13631835E+01 0.19813821E-01 0.12497060E-04 3
-0.33355555E-07 0.15846571E-10 0.19245629E+05 0.17173214E+02
4
C3H5-T PD5/98C 3H 5 0 0G 300.000 3000.00 1000.00
1
0.54255528E+01 0.15511072E-01-0.56678350E-05 0.79224388E-09-0.16878034E-13 2
0.27843027E+05-0.33527184E+01 0.17329209E+01 0.22394620E-01-0.51490611E-05 3
-0.67596466E-08 0.38253211E-11 0.29040498E+05 0.16568878E+02
4
C3H5-S PD5/98C 3H 5 0 0G 300.000 3000.00 1000.00
1
0.53725281E+01 0.15780509E-01-0.59922850E-05 0.93089664E-09-0.36550966E-13 2
0.29614760E+05-0.34186478E+01 0.91372931E+00 0.26432343E-01-0.11758950E-04 3
-0.23035678E-08 0.27715488E-11 0.30916867E+05 0.19989269E+02
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
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
HCCCHCCH 0C 5H 3 0 0G 200.000 5000.000 1000.00
0 1
0.10313636E+02 0.10278554E-01-0.37086568E-05 0.60568664E-09-0.36721455E-13 2
0.65859508E+05-0.26380088E+02 0.10442368E+01 0.44574721E-01-0.50980758E-04 3
0.29338989E-07-0.65246891E-11 0.67852460E+05 0.19034765E+02
4
C4H5C2H 0C 6H 6 0 0G 200.000 5000.000 1100.00
0 1
0.13903605E+02 0.17453182E-01-0.63026581E-05 0.10316520E-08-0.63440931E-13 2
0.35975470E+05-0.47671401E+02-0.23220260E+00 0.54092928E-01-0.36134322E-04 3

0.69104632E-08 0.13734168E-11 0.39978520E+05 0.25932864E+02
 4
 FULVENE 0C 6H 6 0 0G 200.000 5000.000 1000.00
 0 1
 0.11103525E+02 0.20600685E-01-0.75302224E-05 0.12388695E-08-0.75415976E-
 13 2
 0.20361843E+05-0.36665197E+02-0.71813191E+00 0.37934312E-01 0.11398837E-
 04 3
 -0.41333503E-07 0.18055927E-10 0.24223825E+05 0.27855714E+02
 4
 CHCCH2CH2CHCH2 C 6H 8 G 298.000 3000.000 1000.00
 1
 6.73656828E+00 3.59801214E-02-1.79442697E-05 4.36251971E-09-4.18063104E-
 13 2
 2.66969542E+04-5.89162957E+00 6.81481260E-01 5.74228263E-02-4.59418624E-
 05 3
 2.02499383E-08-3.69550697E-12 2.80468538E+04 2.40150759E+01
 4
 CH2CCHCH2CHCH2 C 6H 8 G 298.000 3000.000 1000.00
 1
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 13 2
 2.64952935E+04-1.70336741E+00 3.40906598E+00 3.94865090E-02-1.07919414E-
 05 3
 -8.29929939E-09 4.69973999E-12 2.74305565E+04 1.33764700E+01
 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
 C3H3O 1/31/13 C 3H 3O 1 0G 300.000 5000.000
 1539.000 21
 1.53343473E+01 3.37165935E-03-1.47376680E-06 2.68145680E-10-1.73488725E-
 14 2
 2.24265932E+04-6.26451420E+01-1.26339760E+00 9.87046868E-03 3.01369100E-
 05 3
 -3.05869836E-08 7.86111517E-12 3.15351916E+04 3.81681389E+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

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
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
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
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05 3
1.48540053E-08-2.49981756E-12 2.32580844E+02 2.20973041E+01
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1387.000 41
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05 3
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1393.000 41
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05 3
1.53695144E-08-2.81167824E-12-1.80979612E+03 1.69923285E+01
4
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1387.000 41

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 1404.000 51
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 4
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 4.26576768E+03 4
 IC3H7O 9/ 1/12 C 3H 7O 1 OG 300.000 5000.000
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 9.75233898E+03 4
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 1.11564001E+04 4
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 C3KET13 7/19/ 0 THERMC 3H 60 3 OG 300.000 5000.000
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 C3KET21 7/19/ 0 THERMC 3H 60 3 OG 300.000 5000.000
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 C3H51-2-3OOH 8/26/3 THRMC 3H 70 4 0G 300.000 5000.000
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 2.28208029E-08-4.02231508E-12-1.31353414E+04 2.21043799E+01
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 1.45851637E-08-2.29820536E-12-1.22759164E+04 1.48367359E+01
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 C3H6OH1-2 9/ 1/12 C 3H 70 1 0G 300.000 5000.000
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 HOC3H6O2 9/ 1/12 C 3H 70 3 0G 300.000 5000.000
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 4
 CH3CHCO 03/03/95 THERMC 3H 40 1 0G 300.000 5000.000 1400.00
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 4
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 4
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C2H3OOH 4/18/ 8 THERMC 2H 40 2 0G 300.000 5000.000
 1397.000 21
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 SC4H9 9/ 1/12 C 4H 9 0 0G 300.000 5000.000
 1388.000 31
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 3.72842176E+00 4
 C4H8-2 T 5/09C 4 H 8 0 0 G 200.000 6000.00 1000.00
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 1.34523863E+03 4
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 1.42360731E+01 1.81176105E-02-6.46263809E-06 1.03194372E-09-6.10557331E-
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 -2.99478670E+04-5.52081041E+01-3.28505561E+00 5.04800902E-02-2.51998984E-
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3.65743744E-09 3.94863161E-13-2.30067422E+04 4.19349253E+01
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 1384.000 51
 1.58263859E+01 1.64400938E-02-5.80680311E-06 9.21146000E-10-5.42511002E-14 2
 -2.35334573E+04-6.34844562E+01-2.98701197E+00 6.32678880E-02-5.20855777E-05 3
 2.24064364E-08-3.95416618E-12-1.71957196E+04 3.66920390E+01
 4
 PC4H8OH 2/12/ 9 THERMC 4H 90 1 0G 300.000 5000.000
 1503.000 41
 1.40357398E+01 1.94173155E-02-6.50230141E-06 9.95481694E-10-5.72034525E-14 2
 -1.67631276E+04-4.41162528E+01 1.20329680E+00 4.40218297E-02-2.12295754E-05 3
 3.03714993E-09 3.72027554E-13-1.18622440E+04 2.65515175E+01
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 SC4H8OH 2/12/ 9 THERMC 4H 90 1 0G 300.000 5000.000
 1392.000 41
 1.48421985E+01 1.78435665E-02-6.16709050E-06 1.00443458E-09-6.10697983E-14 2
 -1.81714637E+04-4.96976895E+01-1.04565044E+00 5.72423420E-02-4.43109142E-05 3
 1.80944672E-08-3.02843329E-12-1.28718032E+04 3.48383489E+01
 4
 C4H8OH-1O2 6/26/95 THERMC 4H 90 3 0G 300.000 5000.000
 1396.000 51
 1.74383247E+01 2.16778876E-02-7.37772628E-06 1.14128811E-09-6.60391451E-14 2
 -3.55892620E+04-5.71247140E+01 2.88497398E+00 5.63287929E-02-3.98403503E-05 3
 1.53891643E-08-2.51940787E-12-3.05246721E+04 2.09293355E+01
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 C4H8OH-2O2 6/26/95 THERMC 4H 90 3 0G 300.000 5000.000
 1399.000 51
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 -3.80505855E+04-6.29154326E+01 2.10003504E+00 6.17528218E-02-4.77238541E-05 3
 1.99145784E-08-3.44416275E-12-3.26698755E+04 2.30901271E+01
 4
 C4H8OOH1-1 9/ 1/12 C 4H 90 2 0G 300.000 5000.000
 1406.000 51
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 -1.07801268E+04-6.30302177E+01 2.42373919E+00 5.35214167E-02-3.61077604E-05 3
 1.19327599E-08-1.49401799E-12-5.42740641E+03 2.08094850E+01
 4
 C4H8OOH2-2 9/ 1/12 C 4H 90 2 0G 300.000 5000.000
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 -1.33270491E+04-5.71817113E+01 4.37013729E+00 4.69920537E-02-3.01352597E-05 3
 9.97591165E-09-1.33717929E-12-8.82637791E+03 1.13424525E+01
 4

C4H8OOH1-2 8/23/12 C 4H 90 2 0G 300.000 5000.000
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 2.16287651E-09 6.28147736E-13-4.21015542E+03 1.31340908E+01
 4
 C4H8OOH1-3 9/ 1/12 C 4H 90 2 0G 300.000 5000.000
 1407.000 51
 1.75957868E+01 1.78823172E-02-5.84601568E-06 8.80852127E-10-5.00662655E-14 2
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 9.34788901E-09-9.92348731E-13-4.34048889E+03 1.65183354E+01
 4
 C4H8OOH1-4 9/ 1/12 C 4H 90 2 0G 300.000 5000.000
 1400.000 51
 1.85835797E+01 1.74940527E-02-5.81082562E-06 8.85581555E-10-5.07537090E-14 2
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 1.28721497E-08-1.58263019E-12-2.58786910E+03 2.67435065E+01
 4
 C4H8OOH2-1 9/ 1/12 C 4H 90 2 0G 300.000 5000.000
 1399.000 51
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 2.20415677E-08-3.84993017E-12-4.54848974E+03 2.46740872E+01
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 C4H8OOH2-3 9/ 1/12 C 4H 90 2 0G 300.000 5000.000
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 1.62832583E-08-2.56698689E-12-6.13134926E+03 2.42065717E+01
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 C4H8OOH2-4 9/ 1/12 C 4H 90 2 0G 300.000 5000.000
 1399.000 51
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 2.20415677E-08-3.84993017E-12-4.54848974E+03 2.46740872E+01
 4
 C4H8OOH2-2 9/ 1/12 C 4H 90 2 0G 300.000 5000.000
 1386.000 51
 1.70610154E+01 1.84604624E-02-6.07047864E-06 9.18310457E-10-5.23395593E-14 2
 -1.33270491E+04-5.71817113E+01 4.37013729E+00 4.69920537E-02-3.01352597E-05 3
 9.97591165E-09-1.33717929E-12-8.82637791E+03 1.13424525E+01
 4
 C4H8OOH1-2O2 9/ 1/12 C 4H 90 4 0G 300.000 5000.000
 1407.000 61

2.20047701E+01 1.84524759E-02-5.96541861E-06 8.91556992E-10-5.03719127E-
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 2.14022338E-08-3.61837516E-12-2.33785644E+04 9.92185868E+00
 4
 C4H8OOH1-3O2 9/ 1/12 C 4H 90 4 OG 300.000 5000.000
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 2.25294170E+01 1.79966270E-02-5.89860391E-06 8.90459870E-10-5.06832571E-
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 1.94853380E-08-3.10968451E-12-2.32812507E+04 1.19093259E+01
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 C4H8OOH1-4O2 9/ 1/12 C 4H 90 4 OG 300.000 5000.000
 1401.000 61
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 4
 C4H8OOH2-1O2 9/ 1/12 C 4H 90 4 OG 300.000 5000.000
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 2.20047701E+01 1.84524759E-02-5.96541861E-06 8.91556992E-10-5.03719127E-
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 4
 NC4KET12 7/19/ 0 THERMC 4H 80 3 OG 300.000 5000.000
 1388.000 51
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 2.13454896E-08-3.59860255E-12-3.92395961E+04 2.84908472E+01
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 NC4KET13 7/19/ 0 THERMC 4H 80 3 OG 300.000 5000.000
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 1.83200130E-08-3.11765369E-12-4.01065878E+04 1.88072090E+01
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 NC4KET14 7/19/ 0 THERMC 4H 80 3 0G 300.000 5000.000
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 1.36862855E-08-2.13798779E-12-3.77919233E+04 1.65580190E+01
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 NC4KET21 7/19/ 0 THERMC 4H 80 3 0G 300.000 5000.000
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 NC4KET23 7/19/ 0 THERMC 4H 80 3 0G 300.000 5000.000
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 NC4KET24 7/19/ 0 THERMC 4H 80 3 0G 300.000 5000.000
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 1.30880106E-08-1.99245456E-12-4.14118815E+04 1.86567511E+01
 4
 C2H5COCH3 T09/10C 4 H 8 O 1 0 G 200.000 6000.000 1000.00
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 2.88403536E+04 4
 C2H5COCH2 4/ 3/ 0 THERMC 4H 70 1 0G 300.000 5000.000
 1383.000 31
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 CH2CH2COCH3 6/21/95 THERC 4H 70 1 0G 300.000 5000.000 1380.00
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5.07323216E-09-4.99655275E-13-6.15006886E+03 1.93993386E+01
 4
 CH3CHCOCH3 4/ 3/ 0 THERMC 4H 70 1 0G 300.000 5000.000
 1384.000 31
 1.31388032E+01 1.66091073E-02-5.76924215E-06 9.04978165E-10-5.28826527E-
 14 2
 -1.51162098E+04-4.38876580E+01 8.12941079E-01 4.29256944E-02-2.69230252E-
 05 3
 8.59326807E-09-1.13188129E-12-1.05247481E+04 2.32952685E+01
 4
 C2H3COCH3 6/19/95 THERMC 4H 60 1 0G 300.000 5000.000 1386.00
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 14 2
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 1.03478392E-08-1.53551381E-12-1.70305379E+04 2.64430799E+01
 4
 CH3CHOOCH3 6/27/95 C 4H 70 3 0G 300.000 5000.000 1393.00
 41
 1.72170832E+01 1.76740453E-02-6.10387321E-06 9.53711693E-10-5.55757409E-
 14 2
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 05 3
 2.01816805E-08-3.61175600E-12-2.53445178E+04 2.60857480E+01
 4
 CH2CHOOHCOCH3 6/27/95 C 4H 70 3 0G 300.000 5000.000 1394.00
 51
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 14 2
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 2.16347587E-08-3.75674081E-12-1.89563540E+04 2.71011896E+01
 4
 NC3H7CHO T05/09 C 4H 80 1 0G 200.000 6000.000 1000.00
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 14 2
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 05 3
 -1.07815910E-07 4.25781054E-11-2.71198341E+04 4.93592991E+00-
 2.47924787E+04 4
 NC3H7CO 9/27/95 THERMC 4H 70 1 0G 300.000 5000.000 1380.00
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 14 2
 -1.25523385E+04-4.02608515E+01 2.67256826E+00 3.71198825E-02-2.06862859E-
 05 3
 5.48873888E-09-5.35864183E-13-8.58050888E+03 1.64848950E+01
 4
 C3H6CHO-1 9/27/95 THERMC 4H 70 1 0G 300.000 5000.000
 1379.000 31
 1.30322954E+01 1.62418373E-02-5.54388124E-06 8.59723685E-10-4.98459726E-
 14 2
 -6.45915975E+03-3.92399021E+01 2.67672303E+00 3.73064128E-02-2.11281405E-
 05 3
 5.80472681E-09-6.09688236E-13-2.49714183E+03 1.75750933E+01
 4

C3H6CHO-2 11/15/95 THERMC 4H 70 1 0G 300.000 5000.000
 1682.000 31
 1.11942816E+01 1.81806772E-02-6.35916662E-06 1.00727333E-09-5.93943618E-
 14 2
 -6.86826460E+03-2.80298956E+01 2.95067531E+00 3.34223079E-02-1.45356815E-
 05 3
 1.67282048E-09 2.62011555E-13-3.79034324E+03 1.74324072E+01
 4
 C3H6CHO-3 11/15/95 THERMC 4H 70 1 0G 300.000 5000.000
 1387.000 31
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 14 2
 -1.13561098E+04-4.47371262E+01 1.35168659E+00 4.23714083E-02-2.69123192E-
 05 3
 8.70132567E-09-1.15287455E-12-6.91166610E+03 2.09381509E+01
 4
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 14 2
 -1.83790837E+04-4.45295352E+01 2.76600655E-01 4.82966593E-02-4.02376928E-
 05 3
 1.76564254E-08-3.14365357E-12-1.41717351E+04 2.47118671E+01
 4
 SC3H5CHO 11/15/95 THERC 4H 60 1 0G 300.000 5000.000
 1390.000 21
 1.31695904E+01 1.42484434E-02-4.90843998E-06 7.65789041E-10-4.45834896E-
 14 2
 -2.04032613E+04-4.43673205E+01 4.35795171E-01 4.48719314E-02-3.36582931E-
 05 3
 1.33066870E-08-2.17839128E-12-1.60394651E+04 2.37597452E+01
 4
 SC3H5CO 11/15/95 THERMC 4H 50 1 0G 300.000 5000.000
 1392.000 21
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 14 2
 -4.25349795E+03-4.02864145E+01 1.74191343E+00 3.97229536E-02-3.20061901E-
 05 3
 1.38227925E-08-2.46272017E-12-6.64428100E+02 1.70762023E+01
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 05 3
 -1.14647616E-07 4.64569994E-11-1.84593929E+04 4.92740653E+00-
 1.62354727E+04 4
 IC4H9 T 6/04C 4 H 9 0 0 G 200.000 6000.00 1000.00
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 14 2
 4.15218608E+03-2.66485099E+01 3.34476784E+00 2.31869650E-02 3.28261040E-
 05 3
 -5.96398514E-08 2.58980820E-11 6.66201200E+03 9.68860372E+00
 8.87422590E+03 4
 TC4H9 T 6/04C 4 H 9 0 0 G 200.000 6000.00 1000.00
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6.72557390E+00 2.53649194E-02-9.05306262E-06 1.45474620E-09-8.67934112E-
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 04 3
 -1.25717030E-07 4.75543216E-11 4.43420391E+03 1.30648608E+00
 6.61981524E+03 4
 IC4H8 T05/09C 4 H 8 0 0 G 200.000 6000.00 1000.00
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 05 3
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 2.11365432E+03 4
 IC4H7 T05/04C 4 H 7 0 0 G 200.000 6000.00 1000.00
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 7.82602559E+03 4
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 IC3H6CHO 2/22/96 THERMC 4H 70 1 0G 300.000 5000.000
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 8.93548675E-09-1.11327422E-12-9.07755468E+03 2.61991461E+01
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 7.79536931E-09-6.21665008E-13-2.22782534E+04 1.52623111E+01
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IC4H8OOH-TO2 9/ 1/12 C 4H 90 4 0G 300.000 5000.000
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 2.46040165E-08-4.32848680E-12-2.51137558E+04 1.65767339E+01
 4
 TC4H8OOH-IO2 9/ 1/12 C 4H 90 4 0G 300.000 5000.000
 1385.000 61
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 -3.16533132E+04-8.88301710E+01 3.36413530E+00 6.93742776E-02-5.70416393E-05 3
 2.46040165E-08-4.32848680E-12-2.51137558E+04 1.65767339E+01
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 IC4KETII 7/19/ 0 THERMC 4H 80 3 0G 300.000 5000.000
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 1.70514654E-08-2.65948602E-12-3.82747956E+04 2.69612235E+01
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 IC4KETIT 7/19/ 0 THERMC 4H 80 3 0G 300.000 5000.000
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 1.77145373E-08-2.67265475E-12-4.09366796E+04 2.34844867E+01
 4
 IC4H7OH 4/ 8/97 THERMC 4H 80 1 0G 300.000 5000.000
 1384.000 31
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 7.00961522E-09-7.23262828E-13-2.14512334E+04 1.99500833E+01
 4
 IC4H6OH 8/19/95 THERMC 4H 70 1 0G 300.000 5000.000
 1390.000 31
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 1.33031052E-08-2.13914975E-12-3.14948305E+03 2.29075523E+01
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 IC3H5CHO 7/19/95 THERMC 4H 60 1 0G 300.000 5000.000
 1396.000 21
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 IC3H5CO 4/ 3/ 0 THERMC 4H 50 1 0G 300.000 5000.000
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 IC4H7OOH 7/19/95 THERMC 4H 80 2 OG 300.000 5000.000 1392.00
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 IC3H6CO 03/03/95 THERMC 4H 60 1 OG 300.000 5000.000 1397.00
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 C3H6OH2-1 8/ 9/ 4 THERMC 3H 70 1 OG 300.000 5000.000
 1392.000 31
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 CH2CCH2OH 9/ 8/95 THERMC 3H 50 1 0G 300.000 5000.000 1372.00
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 4
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 C3H5OH T06/10C 3 H 6 O 1 0 G 200.000 6000.00 1000.00
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 1.48710589E+04 4
 TIC4H7Q2-I 5/ 6/96 THERMC 4H 90 4 0G 300.000 5000.000
 1400.000 71
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 1394.000 71
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 1377.000 71
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 1377.000 71
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 C5H11-1 8/26/12 C 5H 11 0 0G 300.000 5000.000
 1388.000 41
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 C5H11-2 8/26/12 C 5H 11 0 0G 300.000 5000.000
 1389.000 41
 1.49269509E+01 2.45505750E-02-8.44033262E-06 1.31477729E-09-7.64544033E-
 14 2
 -2.25446647E+03-5.23093796E+01-7.43804386E-01 5.63967863E-02-3.17173658E-
 05 3
 8.41850668E-09-7.99507437E-13 3.72139256E+03 3.36368332E+01
 4
 C5H11-3 8/26/12 C 5H 11 0 0G 300.000 5000.000
 1389.000 41
 1.49269509E+01 2.45505750E-02-8.44033262E-06 1.31477729E-09-7.64544033E-
 14 2
 -2.25446647E+03-5.29988612E+01-7.43804386E-01 5.63967863E-02-3.17173658E-
 05 3
 8.41850668E-09-7.99507437E-13 3.72139256E+03 3.29473516E+01
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C5H81-3 3/27/97 THERMC 5H 8 0 0G 300.000 5000.000
 1396.000 21
 1.45574490E+01 1.80939266E-02-6.21671892E-06 9.67920254E-10-5.62629326E-14 2
 1.22365462E+03-5.43889766E+01-2.32617433E+00 6.38696042E-02-5.57052591E-05 3
 2.58049480E-08-4.83405924E-12 6.55183321E+03 3.42036513E+01
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 -1.00010574E+04-5.15399538E+01-9.44396392E-01 5.68704795E-02-3.67439266E-05 3
 1.23594281E-08-1.71986028E-12-4.47154633E+03 3.15526141E+01
 4
 C5H10-2 9/ 1/12 C 5H 10 0 0G 300.000 5000.000
 1381.000 31
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 1C5H91-3 9/ 1/12 C 5H 9 0 0G 300.000 5000.000
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 -3.32164559E+04-5.06056620E+01-1.23771006E+00 5.51220954E-02-3.61914162E-05 3
 1.22436788E-08-1.69512209E-12-2.77634901E+04 3.18040307E+01
 4
 C5H91-4 9/ 1/12 C 5H 9 0 0G 300.000 5000.000
 1397.000 31
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 1.37969452E+04-4.07010872E+01 4.34968883E-02 4.89527215E-02-2.92918964E-05 3
 8.84634229E-09-1.06552108E-12 1.85915504E+04 3.00013194E+01
 4
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 31
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 1.53444932E+04-4.46188067E+01-1.94334279E-01 5.36496542E-02-3.77721740E-05 3
 1.43750586E-08-2.29911391E-12 2.01539066E+04 2.99493171E+01
 4
 C5H92-4 9/ 1/12 C 5H 9 0 0G 300.000 5000.000
 1378.000 21
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 8.36378780E-09-7.70804084E-13-2.91241940E+04 2.94748899E+01
 4
 C5H92-5 9/ 1/12 C 5H 9 0 0G 300.000 5000.000
 1384.000 31

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 14 2
 1.38021278E+04-4.79074581E+01 2.10752536E-01 5.05823175E-02-3.24762808E-
 05 3
 1.06441294E-08-1.40196726E-12 1.88009879E+04 2.78735182E+01
 4
 C5H901-3 4/ 7/97 THERMC 5H 90 1 0G 300.000 5000.000
 1393.000 31
 1.86270165E+01 1.85189638E-02-6.21111137E-06 9.52916260E-10-5.48704082E-
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 05 3
 2.13591167E-08-3.36511599E-12 1.91826163E+03 3.99711270E+01
 4
 C5H902-4 4/ 7/97 THERMC 5H 90 1 0G 300.000 5000.000
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 C5H110-1 4/ 7/97 THERMC 5H 110 1 0G 300.000 5000.000
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 14 2
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 05 3
 1.36982820E-08-1.89646466E-12-1.20333690E+04 3.05672313E+01
 4
 C5H110-2 4/ 7/97 THERMC 5H 110 1 0G 300.000 5000.000
 1396.000 41
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 05 3
 1.75936532E-08-2.73651943E-12-1.42372243E+04 3.16370708E+01
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 C5H110-3 4/ 7/97 THERMC 5H 110 1 0G 300.000 5000.000
 1396.000 41
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 -2.06350810E+04-6.74510029E+01-4.94527725E-01 6.73149844E-02-4.72324734E-
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 1.75936532E-08-2.73651943E-12-1.42372243E+04 3.09475892E+01
 4
 C5H1102H-1 7/19/ 0 THERMC 5H 120 2 0G 300.000 5000.000
 1387.000 61
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 -3.80401323E+04-8.39746734E+01 4.74596161E-01 7.38808098E-02-5.12216645E-
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 1.87797149E-08-2.90291870E-12-3.05323779E+04 2.91362231E+01
 4
 C5H1102H-2 7/19/ 0 THERMC 5H 120 2 0G 300.000 5000.000
 1390.000 61
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 14 2

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2.33029166E-08-3.83794655E-12-3.28329870E+04 3.17836191E+01
4
C5H1102H-3 7/19/ 0 THERMC 5H 120 2 0G 300.000 5000.000
1390.000 61
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2.33029166E-08-3.83794655E-12-3.28329870E+04 3.17836191E+01
4
C5H1102-1 7/19/ 0 THERMC 5H 110 2 0G 300.000 5000.000
1386.000 51
1.89702536E+01 2.60355552E-02-9.00706834E-06 1.40888868E-09-8.21618381E-14 2
-2.01253683E+04-6.97477616E+01 1.39788038E+00 6.52788893E-02-4.34224032E-05 3
1.57151743E-08-2.46631324E-12-1.36791222E+04 2.55411824E+01
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C5H1102-2 7/19/ 0 THERMC 5H 110 2 0G 300.000 5000.000
1389.000 51
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-2.26521255E+04-7.38934310E+01 7.10786402E-01 7.03521821E-02-5.11565299E-05 3
2.03005197E-08-3.42470585E-12-1.59903126E+04 2.79113132E+01
4
C5H1102-3 7/19/ 0 THERMC 5H 110 2 0G 300.000 5000.000
1389.000 51
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-2.26521255E+04-7.38934310E+01 7.10786402E-01 7.03521821E-02-5.11565299E-05 3
2.03005197E-08-3.42470585E-12-1.59903126E+04 2.79113132E+01
4
C5H100OH1-2 7/19/ 0 THRMC 5H 110 2 0G 300.000 5000.000
1379.000 61
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-1.43245680E+04-7.79152904E+01 1.66304681E+00 6.42511734E-02-3.94124754E-05 3
1.15348101E-08-1.25128422E-12-7.22288006E+03 2.70063739E+01
4
C5H100OH1-3 7/19/ 0 THRMC 5H 110 2 0G 300.000 5000.000
1379.000 61
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-1.43245680E+04-7.79152904E+01 1.66304681E+00 6.42511734E-02-3.94124754E-05 3
1.15348101E-08-1.25128422E-12-7.22288006E+03 2.70063739E+01
4
C5H100OH1-4 7/19/ 0 THRMC 5H 110 2 0G 300.000 5000.000
1379.000 61
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-1.43245680E+04-7.79152904E+01 1.66304681E+00 6.42511734E-02-3.94124754E-05 3

1.15348101E-08-1.25128422E-12-7.22288006E+03 2.70063739E+01
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C5H10OOH1-5 7/19/ 0 THRMC 5H 110 2 OG 300.000 5000.000
1387.000 61
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14 2
-1.29757849E+04-7.89329903E+01 1.26957212E+00 6.92172253E-02-4.85626715E-
05 3
1.80144791E-08-2.81415382E-12-5.92384799E+03 2.76017751E+01
4
C5H10OOH2-1 7/19/ 0 THRMC 5H 110 2 OG 300.000 5000.000
1390.000 61
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14 2
-1.55260698E+04-8.33092449E+01 5.18861756E-01 7.44934918E-02-5.64622871E-
05 3
2.26488673E-08-3.77612026E-12-8.22372586E+03 3.02858118E+01
4
C5H10OOH2-3 7/19/ 0 THRMC 5H 110 2 OG 300.000 5000.000
1388.000 61
2.10899451E+01 2.37168023E-02-8.19006128E-06 1.27986065E-09-7.45974063E-
14 2
-1.66702092E+04-7.91383677E+01 1.27092209E+00 6.82958985E-02-4.63421243E-
05 3
1.61403755E-08-2.30884220E-12-9.58339948E+03 2.79668173E+01
4
C5H10OOH2-4 7/19/ 0 THRMC 5H 110 2 OG 300.000 5000.000
1388.000 61
2.10899451E+01 2.37168023E-02-8.19006128E-06 1.27986065E-09-7.45974063E-
14 2
-1.66702092E+04-7.91383677E+01 1.27092209E+00 6.82958985E-02-4.63421243E-
05 3
1.61403755E-08-2.30884220E-12-9.58339948E+03 2.79668173E+01
4
C5H10OOH2-5 7/19/ 0 THRMC 5H 110 2 OG 300.000 5000.000
1390.000 61
2.17441074E+01 2.33958311E-02-8.13002591E-06 1.27566943E-09-7.45598238E-
14 2
-1.55260698E+04-8.33092449E+01 5.18861756E-01 7.44934918E-02-5.64622871E-
05 3
2.26488673E-08-3.77612026E-12-8.22372586E+03 3.02858118E+01
4
C5H10OOH3-1 7/19/ 0 THRMC 5H 110 2 OG 300.000 5000.000
1390.000 61
2.17441074E+01 2.33958311E-02-8.13002591E-06 1.27566943E-09-7.45598238E-
14 2
-1.55260698E+04-8.33092449E+01 5.18861756E-01 7.44934918E-02-5.64622871E-
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4
C5H10OOH3-2 7/19/ 0 THRMC 5H 110 2 OG 300.000 5000.000
1388.000 61
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14 2
-1.66702092E+04-7.91383677E+01 1.27092209E+00 6.82958985E-02-4.63421243E-
05 3
1.61403755E-08-2.30884220E-12-9.58339948E+03 2.79668173E+01
4

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 2.05330738E-08-3.37999472E-12-1.79263879E+04 3.83402738E+01
 4
 C5H1001-3 1/22/95 THERMC 5H 100 1 0G 300.000 5000.000
 1370.000 61
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 05 3
 1.12983558E-08-1.18141056E-12-1.81611984E+04 3.87589334E+01
 4
 C5H1001-4 1/22/95 THERMC 5H 100 1 0G 300.000 5000.000
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 4
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 05 3
 1.76515898E-08-2.56653255E-12-2.03198734E+04 4.22612571E+01
 4
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 1387.000 71
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 14 2
 -3.46345151E+04-9.91022020E+01 2.53072834E+00 8.12167401E-02-6.33054798E-
 05 3
 2.63900700E-08-4.58739612E-12-2.67337637E+04 2.39105049E+01
 4
 C5H100OH1-3O2 7/19/ 0 TMC 5H 110 4 0G 300.000 5000.000
 1387.000 71

2.55478814E+01 2.50385111E-02-8.74243938E-06 1.37611416E-09-8.06073182E-14 2
-3.46345151E+04-9.91022020E+01 2.53072834E+00 8.12167401E-02-6.33054798E-05 3
2.63900700E-08-4.58739612E-12-2.67337637E+04 2.39105049E+01
4
C5H10OOH1-4O2 7/19/ 0 TMC 5H 110 4 OG 300.000 5000.000
1387.000 71
2.55478814E+01 2.50385111E-02-8.74243938E-06 1.37611416E-09-8.06073182E-14 2
-3.46345151E+04-9.91022020E+01 2.53072834E+00 8.12167401E-02-6.33054798E-05 3
2.63900700E-08-4.58739612E-12-2.67337637E+04 2.39105049E+01
4
C5H10OOH1-5O2 7/19/ 0 TMC 5H 110 4 OG 300.000 5000.000
1385.000 71
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2.23236523E-08-3.71501383E-12-2.43447483E+04 2.35135259E+01
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1387.000 71
2.55478814E+01 2.50385111E-02-8.74243938E-06 1.37611416E-09-8.06073182E-14 2
-3.46345151E+04-9.91022020E+01 2.53072834E+00 8.12167401E-02-6.33054798E-05 3
2.63900700E-08-4.58739612E-12-2.67337637E+04 2.39105049E+01
4
C5H10OOH2-3O2 7/19/ 0 TMC 5H 110 4 OG 300.000 5000.000
1389.000 71
2.62850175E+01 2.43678422E-02-8.50101950E-06 1.33736519E-09-7.83075048E-14 2
-3.71537284E+04-1.03435286E+02 2.08935173E+00 8.57156954E-02-7.04986902E-05 3
3.07497216E-08-5.51132533E-12-2.90970365E+04 2.50297599E+01
4
C5H10OOH2-4O2 7/19/ 0 TMC 5H 110 4 OG 300.000 5000.000
1389.000 71
2.62850175E+01 2.43678422E-02-8.50101950E-06 1.33736519E-09-7.83075048E-14 2
-3.71537284E+04-1.03435286E+02 2.08935173E+00 8.57156954E-02-7.04986902E-05 3
3.07497216E-08-5.51132533E-12-2.90970365E+04 2.50297599E+01
4
C5H10OOH2-5O2 7/19/ 0 TMC 5H 110 4 OG 300.000 5000.000
1387.000 71
2.55478814E+01 2.50385111E-02-8.74243938E-06 1.37611416E-09-8.06073182E-14 2
-3.46345151E+04-9.91022020E+01 2.53072834E+00 8.12167401E-02-6.33054798E-05 3
2.63900700E-08-4.58739612E-12-2.67337637E+04 2.39105049E+01
4
C5H10OOH3-1O2 7/19/ 0 TMC 5H 110 4 OG 300.000 5000.000
1387.000 71
2.55478814E+01 2.50385111E-02-8.74243938E-06 1.37611416E-09-8.06073182E-14 2

-3.46345151E+04-9.91022020E+01 2.53072834E+00 8.12167401E-02-6.33054798E-05 3
2.63900700E-08-4.58739612E-12-2.67337637E+04 2.39105049E+01
4
C5H10OOH3-2O2 7/19/ 0 TMC 5H 110 4 0G 300.000 5000.000
1389.000 71
2.62850175E+01 2.43678422E-02-8.50101950E-06 1.33736519E-09-7.83075048E-14 2
-3.71537284E+04-1.03435286E+02 2.08935173E+00 8.57156954E-02-7.04986902E-05 3
3.07497216E-08-5.51132533E-12-2.90970365E+04 2.50297599E+01
4
NC5KET12 7/19/ 0 THERMC 5H 100 3 0G 300.000 5000.000
1389.000 61
2.34427049E+01 2.21540692E-02-7.74817880E-06 1.22107095E-09-7.15883644E-14 2
-4.99350593E+04-9.09970812E+01 5.64845658E-01 7.74889690E-02-6.00818427E-05 3
2.42432817E-08-4.02329880E-12-4.21262314E+04 3.12910774E+01
4
NC5KET13 7/19/ 0 THERMC 5H 100 3 0G 300.000 5000.000
1387.000 61
2.27897549E+01 2.26387719E-02-7.89832354E-06 1.24260309E-09-7.27609759E-14 2
-5.00526193E+04-8.71676166E+01 2.53945153E+00 7.08645319E-02-5.32266350E-05 3
2.12906293E-08-3.56676536E-12-4.29988725E+04 2.14543054E+01
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-5.00526193E+04-8.71676166E+01 2.53945153E+00 7.08645319E-02-5.32266350E-05 3
2.12906293E-08-3.56676536E-12-4.29988725E+04 2.14543054E+01
4
NC5KET15 7/19/ 0 THERMC 5H 100 3 0G 300.000 5000.000
1383.000 61
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-4.75611599E+04-8.35091033E+01 3.22565144E+00 6.57620962E-02-4.52752542E-05 3
1.64810866E-08-2.54467139E-12-4.06876266E+04 1.90851234E+01
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NC5KET21 7/19/ 0 THERMC 5H 100 3 0G 300.000 5000.000
1379.000 61
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-5.12815467E+04-8.09340957E+01 4.56687437E+00 6.01978739E-02-3.82935508E-05 3
1.29220662E-08-1.89791227E-12-4.47703435E+04 1.29580830E+01
4
NC5KET23 7/19/ 0 THERMC 5H 100 3 0G 300.000 5000.000
1387.000 61
2.31409808E+01 2.24801534E-02-7.87662916E-06 1.24282516E-09-7.29252729E-14 2
-5.36784029E+04-9.00538236E+01 1.09304151E-01 7.75997760E-02-5.94124810E-05 3

2.36744270E-08-3.89094338E-12-4.57495597E+04 3.32799795E+01
 4
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 2.25126387E+01 2.29495597E-02-8.02286486E-06 1.26389975E-09-7.40777420E-
 14 2
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 05 3
 2.00741570E-08-3.28568948E-12-4.66368524E+04 2.29520202E+01
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 1.58213340E-08-2.38800145E-12-4.43093682E+04 2.11180678E+01
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 14 2
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 05 3
 1.85573234E-08-3.11995924E-12-4.46228757E+04 1.89760116E+01
 4
 NC5KET32 7/19/ 0 THERMC 5H 100 3 OG 300.000 5000.000
 1387.000 61
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 14 2
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 05 3
 2.55909432E-08-4.44696298E-12-4.60989830E+04 3.00522534E+01
 4
 C5H10OH-1 1/14/99 THERMC 5H 110 1 OG 300.000 5000.000
 1371.000 51
 1.75642279E+01 2.33577469E-02-7.81503517E-06 1.19674654E-09-6.88114207E-
 14 2
 -2.11605652E+04-6.19821034E+01 9.51873649E-01 5.58286144E-02-2.87750953E-
 05 3
 5.54684921E-09 1.10578801E-14-1.48168651E+04 2.93877119E+01
 4
 C5H10OH-2 1/14/99 THERMC 5H 110 1 OG 300.000 5000.000
 1390.000 51
 1.72742775E+01 2.39409708E-02-8.07388576E-06 1.24188426E-09-7.15926603E-
 14 2
 -2.31054055E+04-6.11106423E+01 4.68530877E-01 6.05595171E-02-3.75900684E-
 05 3
 1.16488887E-08-1.41506375E-12-1.70158316E+04 3.00652481E+01
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 O2C5H10OH-1 1/14/99 THRMC 5H 110 3 OG 300.000 5000.000
 1395.000 61
 2.06059936E+01 2.61750874E-02-8.92270421E-06 1.38184638E-09-8.00235870E-
 14 2
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 05 3
 1.81238720E-08-2.90871344E-12-3.44822614E+04 2.22673007E+01
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O2C5H10OH-2 1/14/99 THRCM 5H 110 3 OG 300.000 5000.000
 1398.000 61
 2.15259930E+01 2.54039694E-02-8.65952886E-06 1.34110440E-09-7.76663740E-
 14 2
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 05 3
 2.24979959E-08-3.79045894E-12-3.66230283E+04 2.45460172E+01
 4
 C6H10 4/12/13 THERMC 6H 10 0 OG 300.000 5000.000
 1413.000 21
 1.60456030E+01 2.34774145E-02-7.85797929E-06 1.20200542E-09-6.90100029E-
 14 2
 2.11899382E+03-5.88452460E+01-1.01375402E+00 6.38242808E-02-4.40653860E-
 05 3
 1.58295163E-08-2.30830701E-12 7.94033696E+03 3.25056094E+01
 4
 C6H9-T 12/ 5/12 THERMC 6H 9 0 OG 300.000 5000.000
 1399.000 21
 1.54942945E+01 2.20330442E-02-7.49571333E-06 1.15926130E-09-6.70685889E-
 14 2
 3.08542766E+04-5.24245446E+01-4.64746975E-01 6.09216456E-02-4.47292952E-
 05 3
 1.77756829E-08-2.95693412E-12 3.62924888E+04 3.28081912E+01
 4
 C6H9-S 12/ 5/12 THERMC 6H 9 0 OG 300.000 5000.000
 1396.000 31
 1.62958005E+01 2.11783659E-02-7.25674435E-06 1.12780699E-09-6.54746480E-
 14 2
 3.20417675E+04-5.73406449E+01-6.12878674E-01 6.32013662E-02-4.85579869E-
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 2.01072289E-08-3.46242218E-12 3.77343371E+04 3.26952798E+01
 4
 C6H9-A 12/ 5/12 THERMC 6H 9 0 OG 300.000 5000.000
 1400.000 21
 1.70842767E+01 2.08842788E-02-7.14529004E-06 1.10943563E-09-6.43676989E-
 14 2
 2.01040204E+04-6.39326012E+01-2.66715213E+00 7.26196475E-02-6.05323920E-
 05 3
 2.66000571E-08-4.74613408E-12 2.64415017E+04 4.02220332E+01
 4
 C6H9O-2 12/ 5/12 THERMC 6H 90 1 OG 300.000 5000.000
 1381.000 41
 1.99353187E+01 2.10902650E-02-7.42714919E-06 1.17580440E-09-6.91504434E-
 14 2
 7.67409302E+03-7.62069031E+01-7.85602487E-02 6.81070170E-02-5.11911414E-
 05 3
 2.04828658E-08-3.45141659E-12 1.47423639E+04 3.14323712E+01
 4
 C6H6 G 6/01C 6H 6 0 OG 200.000 6000.000
 1000.000 1
 1.10809576E+01 2.07176746E-02-7.52145991E-06 1.22320984E-09-7.36091279E-
 14 2
 4.30641035E+03-4.00413310E+01 5.04818632E-01 1.85020642E-02 7.38345881E-
 05 3
 -1.18135741E-07 5.07210429E-11 8.55247913E+03 2.16412893E+01
 9.96811598E+03 4
 C6H5CH3 L 6/87C 7H 8 0 OG 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
 C6H5CH2 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
 C*CCJC*C 3/1/95 Z&B C 5H 7 0 0G 300.000 5000.000
 1388.000 21
 1.40879309E+01 1.62398907E-02-5.64768950E-06 8.86857524E-10-5.18698993E-
 14 2
 1.76798698E+04-5.13735038E+01-2.94595603E+00 5.68783623E-02-4.31336497E-
 05 3
 1.68169537E-08-2.67926433E-12 2.35156925E+04 3.98188778E+01
 4
 CC3H4 T12/81C 3H 4 0 0G 300.000 5000.00 1000.00
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 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
 C4H4 H6W/94C 4H 4 0 0G 300.000 3000.00 1000.00
 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
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 C4H3-I AB1/93C 4H 3 0 0G 300.000 3000.00 1000.00
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 0.90978165E+01 0.92207119E-02-0.33878441E-05 0.49160498E-09-0.14529780E-
 13 2
 0.56600574E+05-0.19802597E+02 0.20830412E+01 0.40834274E-01-0.62159685E-
 04 3
 0.51679358E-07-0.17029184E-10 0.58005129E+05 0.13617462E+02
 4
 C4H612 A 8/83C 4H 6 0 0G 300. 3000. 1000.0
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 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
 0.1950807E+05 4
 C6H5 T04/02C 6H 5 0 0G 200.000 6000.000 1000.
 1
 1.08444762E+01 1.73212473E-02-6.29233249E-06 1.02369961E-09-6.16216828E-
 14 2

3.55598475E+04-3.53735134E+01 2.10306633E-01 2.04745507E-02 5.89743006E-
 05 3
 -1.01534255E-07 4.47105660E-11 3.95468722E+04 2.52910455E+01
 4.08610970E+04 4
 C4H2 D11/99C 4H 2 0 0G 300.000 3000.000
 1
 0.91576328E+01 0.55430518E-02-0.13591604E-05 0.18780075E-10 0.23189536E-
 13 2
 0.52588039E+05-0.23711460E+02 0.10543978E+01 0.41626960E-01-0.65871784E-
 04 3
 0.53257075E-07-0.16683162E-10 0.54185211E+05 0.14866591E+02
 4
 C4H3-N H6W/94C 4H 3 0 0G 300.000 3000.00 1000.00
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 0.54328279E+01 0.16860981E-01-0.94313109E-05 0.25703895E-08-0.27456309E-
 12 2
 0.61600680E+05-0.15673981E+01-0.31684113E+00 0.46912100E-01-0.68093810E-
 04 3
 0.53179921E-07-0.16523005E-10 0.62476199E+05 0.24622559E+02
 4
 C4H5-N H6W/94C 4H 5 0 0G 300.000 3000.00 1000.00
 1
 0.98501978E+01 0.10779008E-01-0.13672125E-05-0.77200535E-09 0.18366314E-
 12 2
 0.38840301E+05-0.26001846E+02 0.16305321E+00 0.39830137E-01-0.34000128E-
 04 3
 0.15147233E-07-0.24665825E-11 0.41429766E+05 0.23536163E+02
 4
 C4H5-I H6W/94C 4H 5 0 0G 300.000 3000.00 1000.00
 1
 0.10229092E+02 0.94850138E-02-0.90406445E-07-0.12596100E-08 0.24781468E-
 12 2
 0.34642812E+05-0.28564529E+02-0.19932900E-01 0.38005672E-01-0.27559450E-
 04 3
 0.77835551E-08 0.40209383E-12 0.37496223E+05 0.24394241E+02
 4
 CH3CHCHCO 12/ 6/13 THERMC 4H 50 1 0G 300.000 5000.000
 1396.000 11
 1.21043198E+01 1.28210886E-02-4.36704943E-06 6.75949572E-10-3.91295106E-
 14 2
 -1.86544623E+03-3.77298604E+01 1.78215470E+00 3.99251915E-02-3.27534130E-
 05 3
 1.45472667E-08-2.65454288E-12 1.47887943E+03 1.67433588E+01
 4
 CH2CHCHCHO T03/97C 4H 50 1 0G 200.000 6000.000 1000.0
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 8.90967920E+00 1.34364140E-02-7.62977390E-07-1.69114810E-09 2.95540440E-
 13 2
 1.48898740E+03-1.79662460E+01-1.08199860E+00 3.64929760E-02-1.52255950E-
 05 3
 -5.62607170E-18 2.16113750E-21 3.56713230E+03 3.27142550E+01
 4.73074990E+03 4
 C4H6O25 T 3/97C 4H 60 1 0G 200.000 5000.000 1000.0
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 13 2
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 05 3

-1.26219194E-07 5.23991321E-11-1.46572472E+04 1.45722395E+01-
 1.30831522E+04 4
 C2H3CHOCH2 A 8/83C 4H 60 1 0G 300. 3000. 1000.0
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 1.75352252E+03 5.17190420E+01 7.97985440E-01 3.44034320E-02-1.24598510E-
 05 3
 -5.18062790E-18 1.99359540E-21-6.48927540E+02 2.18896980E+01
 1.00654250E+03 4
 C4H5-2 12/ 6/13 THERMC 4H 5 0 0G 300.000 5000.000
 2021.000 21
 8.67673333E+00 1.42789766E-02-5.26476298E-06 8.62021059E-10-5.19571720E-
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 3.21729573E+04-2.14573334E+01 2.74016965E+00 2.31992086E-02-7.25585511E-
 06 3
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 4
 C4H6-2 12/ 6/13 THERMC 4H 6 0 0G 300.000 5000.000
 1525.000 21
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 4
 C4H6O23 T 3/97C 4H 60 1 0G 200.000 5000.000 1000.0
 1
 8.60658242E+00 2.08310051E-02-8.42229481E-06 1.56717640E-09-1.09391202E-
 13 2
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 05 3
 -1.26219194E-07 5.23991321E-11-1.02787872E+04 1.45722395E+01-
 1.30831522E+04 4
 CH3CHCHCHO T 5/92C 4H 60 1 0G 298.150 3000.0 1000.0
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 1.98794540E+01-2.09130550E-02 4.45360508E-05-2.60374870E-08 4.86836120E-
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 05 3
 -6.00928140E-18 2.31368530E-21-1.41394920E+04 3.74707580E+01-
 1.29340710E+04 4
 C4H4O T03/97C 4H 40 1 0G 200.000 6000.0 1000.0
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 4.17166616E+03 4
 H2CC L12/89H 2C 2 0 0G 200.000 6000.000
 1000.000 1
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 13 2
 0.48316688E+05 0.64023701E+00 0.32815483E+01 0.69764791E-02-0.23855244E-
 05 3
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 0.49887266E+05 4

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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
C6H2 P 1/93C 6H 2 0 OG 300.000 3000.00 1000.00
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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 OG 300.000 3000.00 1000.00
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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
L-C6H4 H6W/94C 6H 4 0 OG 300.000 3000.00 1000.00
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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
C-C6H4 H6W/94C 6H 4 0 OG 300.000 3000.00 1000.00
1
0.13849209E+02 0.78807920E-02 0.18243836E-05-0.21169166E-08 0.37459977E-
12 2
0.47446340E+05-0.50404953E+02-0.30991268E+01 0.54030564E-01-0.40839004E-
04 3
0.10738837E-07 0.98078490E-12 0.52205711E+05 0.37415207E+02
4
C6H5OH L 4/84C 6H 60 1 OG 300.000 5000.000 1000.
1
0.14912073E+02 0.18378135E-01-0.61983128E-05 0.91983221E-09-0.49209565E-
13 2
-0.18375199E+05-0.55924103E+02-0.16956539E+01 0.52271299E-01-0.72024050E-
05 3
-0.35859603E-07 0.20449073E-10-0.13284121E+05 0.32542160E+02-
0.11594207E+05 4
C6H5O T05/02C 6H 50 1 OG 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
P-C6H4O2 AK0405C 6H 40 2 OG 270.000 3000.000 1370.00
1

1.23423732E+01 2.40612690E-02-1.16565184E-05 2.71393504E-09-2.47643065E-
 13 2
 -2.06185312E+04-4.08244024E+01-2.43170113E+00 6.87937608E-02-6.41382837E-
 05 3
 3.08126855E-08-5.99832072E-12-1.65696994E+04 3.48309430E+01
 4
 P-C6H3O2 AK0505C 6H 30 2 OG 270.000 3000.000 1290.00
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 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
 O-C6H4O2 AK0405C 6H 40 2 OG 270.000 3000.000 1370.00
 1
 1.23614349E+01 2.40491397E-02-1.16529057E-05 2.71332785E-09-2.47593219E-
 13 2
 -1.67079717E+04-4.00310857E+01-2.36179712E+00 6.86058343E-02-6.39129516E-
 05 3
 3.06903009E-08-5.97357785E-12-1.26704431E+04 3.53724482E+01
 4
 C5H5 TAK0505C 5H 5 0 OG 298.150 3500.000 969.35
 1
 1.33675715E+00 3.24793912E-02-1.67587774E-05 4.03514137E-09-3.70739036E-
 13 2
 3.00730524E+04 1.60315806E+01-3.97555452E+00 7.41370991E-02-1.11803345E-
 04 3
 9.04628776E-08-2.80999747E-11 3.01769405E+04 3.67153636E+01
 4
 C5H6 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
 C5H5OH 5/ 2/91 THE.MC 5H 60 1 OG 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
 C5H4O T 8/99C 5H 40 1 OG 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
 C5H5O 5/16/90 THERMC 5H 50 1 OG 300.000 5000.000
 1392.000 01
 1.48322894E+01 1.40483376E-02-4.92302051E-06 7.77041219E-10-4.56103939E-
 14 2

1.45523665E+04-5.73228191E+01-2.83112840E+00 5.67277287E-02-4.44757303E-
 05 3
 1.74924447E-08-2.76004847E-12 2.04992154E+04 3.69634411E+01
 4
 C5H4OH T 8/99C 5H 50 1 0G 200.000 6000.000 1000.
 1
 1.33741248E+01 1.51996469E-02-5.45685046E-06 8.80944866E-10-5.27493258E-
 14 2
 2.20358027E+03-4.59569069E+01-1.28398054E+00 4.90298511E-02-1.35844414E-
 05 3
 -2.92983743E-08 1.90820619E-11 6.37364803E+03 3.08073591E+01
 8.00114499E+03 4
 C6H5OO 3/26/ 9 THERMC 6H 50 2 0G 300.000 5000.000
 1403.000 11
 1.67078262E+01 1.62326229E-02-5.47969630E-06 8.43510060E-10-4.86562431E-
 14 2
 8.14242915E+03-6.08346973E+01-2.99164672E+00 7.03857150E-02-6.34400574E-
 05 3
 2.91548920E-08-5.30706938E-12 1.41320240E+04 4.20142955E+01
 4
 C6H5OOH 3/26/ 9 THERMC 6H 60 2 0G 300.000 5000.000
 1404.000 21
 1.92317474E+01 1.63154699E-02-5.53448904E-06 8.55059974E-10-4.94583790E-
 14 2
 -1.01971012E+04-7.61674471E+01-4.03105975E+00 7.96101888E-02-7.21655013E-
 05 3
 3.27610696E-08-5.85584239E-12-3.10973017E+03 4.54324978E+01
 4
 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
 HOC6H4OH 4/ 9/ 9 THERMC 6H 60 2 0G 300.000 5000.000
 1405.000 21
 2.31394847E+01 1.31873680E-02-4.49072464E-06 6.95268891E-10-4.02643108E-
 14 2
 -4.25885990E+04-1.02692352E+02-8.68529064E+00 1.17282933E-01-1.33754802E-
 04 3
 7.16697462E-08-1.44385730E-11-3.44903827E+04 5.77087257E+01
 4
 OC6H4OH 4/ 9/ 9 THERMC 6H 50 2 0G 300.000 5000.000
 1403.000 11
 2.22718210E+01 1.21038561E-02-4.18429526E-06 6.54475399E-10-3.81746504E-
 14 2
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 04 3
 6.56286805E-08-1.31527870E-11-1.55949156E+04 5.72175202E+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
 CTCC*CCJ GLAR C 5H 5 0 0G 300.000 5000.000
 1396.000 11
 1.41230912E+01 1.14233190E-02-3.95851276E-06 6.20128961E-10-3.62097887E-
 14 2
 4.25158384E+04-5.02942871E+01-6.16143558E-01 5.06466579E-02-4.48561743E-
 05 3
 2.02459419E-08-3.64542145E-12 4.71532377E+04 2.71623299E+01
 4
 C5H6-L 2/ 5/ 9 THERMC 5H 6 0 0G 300.000 5000.000
 1372.000 21
 1.29600892E+01 1.48953758E-02-5.23622902E-06 8.27916389E-10-4.86464523E-
 14 2
 2.38180800E+04-4.25312093E+01 3.58448213E+00 3.24459626E-02-1.70150991E-
 05 3
 4.22715914E-09-4.18452556E-13 2.76514681E+04 9.60644208E+00
 4
 CJ*CC*CC*O 2/ 5/ 9 THERMC 5H 50 1 0G 300.000 5000.000
 1396.000 21
 1.62360823E+01 1.18297101E-02-4.11454219E-06 6.46026823E-10-3.77767639E-
 14 2
 1.93499885E+04-5.83498817E+01-5.06628841E-01 6.04671965E-02-5.97396749E-
 05 3
 2.96804228E-08-5.76240010E-12 2.42765544E+04 2.82994148E+01
 4
 C*CC*CCJ*O 2/ 5/ 9 THERMC 5H 50 1 0G 300.000 5000.000
 1399.000 11
 1.53178248E+01 1.27352911E-02-4.35882964E-06 6.76912763E-10-3.92771371E-
 14 2
 7.60582726E+03-5.43599625E+01-2.18492198E-01 5.92100223E-02-5.89241174E-
 05 3
 2.97411920E-08-5.85244770E-12 1.20600764E+04 2.55968530E+01
 4
 CJ*CC*O 4/ 8/94 THERMC 3H 30 1 0G 300.000 5000.000
 1402.000 11
 1.07482537E+01 6.19822688E-03-2.06130981E-06 3.14418872E-10-1.80309517E-
 14 2
 1.51410162E+04-3.01266033E+01 1.46654466E+00 3.23390476E-02-3.05588208E-
 05 3
 1.44081861E-08-2.65600505E-12 1.78850058E+04 1.80850321E+01
 4
 C5H3O TAK0905C 5H 30 1 0G 300.000 3500.000 1500.00
 1
 1.19961781E+01 1.34287065E-02-5.90045309E-06 1.22553862E-09-9.86114716E-
 14 2
 2.89592010E+04-4.07548249E+01-3.03242604E+00 5.43937201E-02-4.95018348E-
 05 3
 2.25523751E-08-4.10727920E-12 3.35644081E+04 3.78374823E+01
 4

C5H7 1/22/ 9 WKM C 5H 7 0 OG 300.000 5000.000
1377.000 31
1.36630213E+01 1.68061358E-02-5.98746539E-06 9.55341072E-10-5.64951981E-14 2
1.27238941E+04-5.46331286E+01-6.75118368E+00 6.06461693E-02-4.01260152E-05 3
1.22051562E-08-1.33459844E-12 2.01365277E+04 5.62694938E+01
4
OC5H7O 1/22/ 9 WKM C 5H 7O 2 OG 300.000 5000.000
1375.000 31
1.65416953E+01 1.86677673E-02-6.44836048E-06 1.00787611E-09-5.87521858E-14 2
-2.82017168E+04-5.47258181E+01 4.88394767E+00 4.03401300E-02-1.97774150E-05 3
3.68903501E-09-3.40202384E-14-2.35295942E+04 9.97070337E+00
4
C*CCJC*COH 10/6/95 Z&B C 5H 7O 1 OG 300.000 5000.000
1397.000 31
1.67465815E+01 1.58357240E-02-5.44954706E-06 8.49881387E-10-4.94743246E-14 2
-4.30972870E+03-6.19378748E+01-2.91175436E+00 6.69362484E-02-5.71603047E-05 3
2.48753749E-08-4.33243894E-12 1.96441523E+03 4.17454344E+01
4
C*CC*CCJ Z&B C 5H 7 0 OG 300.000 5000.000
1386.000 21
1.47302883E+01 1.59030900E-02-5.57729508E-06 8.80604825E-10-5.16963733E-14 2
1.74050791E+04-5.42670706E+01-1.60087476E+00 5.38764703E-02-3.96302225E-05 3
1.49599474E-08-2.31995284E-12 2.31199746E+04 3.35492960E+01
4
C*CC*CC 3/1/95 Z&B C 5H 8 0 OG 300.000 5000.000
1395.000 21
1.41303131E+01 1.81877961E-02-6.19208788E-06 9.58333792E-10-5.54785472E-14 2
2.25907168E+03-5.11705577E+01-1.19376866E+00 5.65474329E-02-4.39472481E-05 3
1.82341266E-08-3.12226566E-12 7.36084709E+03 3.02808980E+01
4
C*CC*CCOH 1/23/ 9 WKM C 5H 8O 1 OG 300.000 5000.000
1396.000 31
1.63079670E+01 1.79957763E-02-6.03115896E-06 9.23992259E-10-5.31254053E-14 2
-1.58204603E+04-5.84137244E+01-5.31488384E-01 6.06983915E-02-4.81499862E-05 3
2.00308244E-08-3.38987282E-12-1.03301302E+04 3.07961436E+01
4
C*CCJC*O Z&B C 4H 5O 1 OG 300.000 5000.000
1385.000 11
1.22833215E+01 1.26428506E-02-4.31034879E-06 6.68415867E-10-3.87693974E-14 2
1.86818728E+03-3.84807909E+01-4.83886977E-01 4.23431670E-02-3.05389089E-05 3
1.11441978E-08-1.63863920E-12 6.28635090E+03 3.00860103E+01
4
OC4H6O 1/23/ 9 WKM C 4H 6O 2 OG 300.000 5000.000
1382.000 31

1.41894774E+01 1.53345510E-02-5.24594862E-06 8.14655154E-10-4.72759368E-
14 2
-4.10001835E+04-4.43771751E+01 4.21628848E+00 3.57422725E-02-2.04226185E-
05 3
5.63821367E-09-5.88888993E-13-3.72055911E+04 1.02814620E+01
4
OC4H5O 1/23/ 9 WKM C 4H 50 2 OG 300.000 5000.000
1388.000 21
1.32138775E+01 1.37339051E-02-4.62639517E-06 7.10941370E-10-4.09538499E-
14 2
-2.16535271E+04-3.64185255E+01 4.60550978E+00 3.30498712E-02-2.13102363E-
05 3
7.37021089E-09-1.08289438E-12-1.85460831E+04 1.01599453E+01
4
HOC*CC*O 1/26/ 9 WKM C 3H 40 2 OG 300.000 5000.000
1413.000 21
1.66505478E+01 6.11745137E-03-2.09080785E-06 3.24985683E-10-1.88875073E-
14 2
-3.82179939E+04-6.36794754E+01-2.01837189E+00 6.26539783E-02-6.73359280E-
05 3
3.39430425E-08-6.48917648E-12-3.31367523E+04 3.18162860E+01
4
HOC*CCJ*O 1/26/ 9 WKM C 3H 30 2 OG 300.000 5000.000
1414.000 11
1.52720985E+01 5.02586331E-03-1.68408578E-06 2.58390706E-10-1.48849424E-
14 2
-1.98506828E+04-5.54641734E+01 6.07270082E-01 4.96011303E-02-5.32300885E-
05 3
2.68392951E-08-5.13094510E-12-1.58814562E+04 1.94817133E+01
4
C2H2OH H 3C 20 1 OG 300.00 5000.00 1000.00
1
6.81339897E+00 8.05827723E-03-3.11728612E-06 5.54590896E-10-3.71804255E-
14 2
1.31583034E+04-1.09863525E+01 5.62397968E-01 2.64598620E-02-2.28453705E-
05 3
9.14478695E-09-1.06711936E-12 1.48374643E+04 2.10439544E+01
4
O2CCHOOJ Z&B C 2H 10 4 OG 300.000 5000.000
1682.000 01
1.09910849E+01 7.46985861E-03-2.75568271E-06 4.51353051E-10-2.72108652E-
14 2
-3.51335323E+04-2.11652231E+01 8.91497688E+00 8.60571847E-03 5.24416766E-
07 3
-2.79301331E-09 7.62963051E-13-3.40867754E+04-8.72978273E+00
4
HCOH MAR94 C 1H 20 1 OG 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
C2H3OH 2/ 3/ 9 THERMC 2H 40 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
 O2CH2CHO BOZ_03C 2H 30 3 0G 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 30 3 0G 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
 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
 CH3CHCHO 12/ 1/99 THERMC 3H 50 1 0G 300.000 5000.000
 1385.000 21
 1.02647528E+01 1.17295061E-02-4.06267561E-06 6.36086751E-10-3.71220190E-
 14 2
 -7.25910488E+03-2.91646638E+01 1.54196914E+00 3.03297391E-02-1.88922690E-
 05 3
 5.92263358E-09-7.53762316E-13-4.01761098E+03 1.83707011E+01
 4
 CH2CH2CHO 06/09/10 C 3H 50 10 0G 300.00 4000.00 1000.00
 1
 0.38802774E+01 0.19560963E-01-0.65248419E-05 0.10275587E-08-0.62784000E-
 13 2
 0.26971973E+03 0.10725105E+02 0.30829394E+00 0.42721864E-01-0.48484926E-
 04 3
 0.31577844E-07-0.82415281E-11 0.24612408E+03 0.25079893E+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-1 4/ 2/13 THERMC 3H 50 1 0G 300.000 5000.000
 1410.000 21
 1.25628085E+01 8.58651176E-03-2.72582845E-06 4.01908549E-10-2.24787697E-
 14 2
 3.96526183E+03-4.16107625E+01 2.55744565E-01 4.74882684E-02-4.94984843E-
 05 3

2.53799319E-08-4.97487174E-12 7.19097870E+03 2.08288803E+01
 4
 IC3H5O 4/ 2/13 THERMC 3H 50 1 0G 300.000 5000.000
 1397.000 21
 1.23529178E+01 9.83087082E-03-3.37836468E-06 5.26074995E-10-3.05827836E-
 14 2
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 05 3
 2.23584078E-08-4.41548328E-12 4.43070338E+03 1.77897863E+01
 4
 SC3H5OH 2/ 3/ 9 C 3H 60 1 0G 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-
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 1.70906074E-08-3.13775054E-12-2.02502608E+04 2.41528201E+01
 4
 C6H11 4/23/13 THERMC 6H 11 0 0G 300.000 5000.000
 1395.000 41
 1.62895169E+01 2.56916506E-02-8.77728796E-06 1.36135999E-09-7.89198907E-
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 05 3
 1.65326066E-08-2.57560053E-12 1.58086438E+04 3.67347517E+01
 4
 H2COCOCH3 7/ 6/13 THERMC 3H 50 2 0G 300.000 5000.000
 1412.000 21
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 14 2
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 08 3
 -1.14125528E-12-3.30331004E-15-2.24026434E+04-1.59157172E+02
 4
 CCYCOO 7/ 6/13 THERMC 3H 50 2 0G 300.000 5000.000
 1398.000 21
 1.52842170E+01 9.91133864E-03-3.41434716E-06 5.32813858E-10-3.10289585E-
 14 2
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 05 3
 1.69947150E-08-3.01394020E-12 5.41657441E+03 1.44748296E+01
 4
 TC3H5OO 6/ 6/13 THERMC 3H 50 2 0G 300.000 5000.000
 1398.000 21
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 14 2
 -2.14964368E+03-4.82072152E+01 2.32747386E+00 4.28458215E-02-3.71917675E-
 05 3
 1.66530071E-08-2.99207781E-12 1.69979772E+03 1.57682500E+01
 4
 C*CCOC*O 1/17/17 THERMC 4H 60 2 0G 300.000 5000.000
 2018.000 31
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 14 2
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 05 3
 4.25682525E-09-5.12421095E-14-3.60076138E+04 2.39279461E+01
 4

C*CCJOC*O 1/17/17 THERMC 4H 50 2 0G 300.000 5000.000
1488.000 31
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14 2
-2.51390612E+04-6.17195855E+01 6.41757084E-01 4.02826072E-02-1.83524299E-
05 3
3.46272149E-10 1.14439565E-12-1.89824077E+04 2.54305179E+01
4
CYC*CCOHC O 1/19/17 THERMC 4H 60 2 0G 300.000 5000.000
1399.000 11
1.47451744E+01 1.61967071E-02-5.65378715E-06 8.90078141E-10-5.21518902E-
14 2
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05 3
1.72569541E-08-2.49430373E-12-2.78297107E+04 5.22778297E+01
4
CYC*CCOJCO 1/19/17 THERMC 4H 50 2 0G 300.000 5000.000
1683.000 11
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14 2
-6.91217839E+03-4.57309522E+01-2.95279971E+00 5.38570560E-02-3.71914760E-
05 3
1.19365458E-08-1.43382960E-12-1.54491961E+03 4.18839855E+01
4
HOC4H6 23/05/11 THERGASC 4H 70 1 0G 300.000 5000.000
1000.000 1
0.10610399E+02 0.17761393E-01-0.51479733E-05 0.73525375E-09-0.42104077E-
13 2
-0.70508848E+04-0.25888687E+02 0.58910817E+00 0.44971436E-01-0.32455209E-
04 3
0.13392720E-07-0.25772255E-11-0.41895469E+04 0.26194138E+02
4
END