```
! NASA-parameter thermodynamic parameters used in PSR simulations
! of the following work:
!
! A. Andersen and E. A. Carter,
! First-Principles-Derived Kinetics of the Reactions Involved
! in Low-Temperature Dimethyl Ether Oxidation,
! Molecular Physics, 106, 367-396 (2008).
!
! Parameters were generating using the KHIMERA kinetics package (see above
! text for KHIMERA reference details).
!
!
! The following parmeters were adjusted to the heats of formation estimated
! by Curran et al. (see above text for reference detail).
!
! Hf = 1.0 kcal/mol
CH3OCH2          021004C   2H   5O   1     G    300.00  2000.00  1000.00      1
 1.94398179E+00 2.34198261E-02-1.25712830E-05 3.39817347E-09-3.74528375E-13    2
-4.87656761E+07 1.28275684E+01 3.04818446E+00 1.36757444E-02 1.28836242E-05    3
-2.31398424E-08 9.35688557E-12-1.10028905E+03 8.62978653E+00                   4
! Hf = -34.6 kcal/mol
CH3OCH2O2        021004C   2O   3H   5     G    300.00  2000.00  1000.00      1
 2.88836614E+00 3.21733342E-02-1.89859873E-05 5.62471175E-09-6.75165218E-13    2
-9.62878954E+07 1.05877223E+01 3.24440522E+00 2.13135199E-02 1.56136731E-05    3
-3.31249265E-08 1.39910614E-11-1.94239713E+04 1.09382650E+01                   4
! Hf = -24.0 kcal/mol
CH2OCH2O2H       021004C   2H   5O   3     G    300.00  2000.00  1000.00      1
 5.85692625E+00 2.67889880E-02-1.51612112E-05 4.36609250E-09-5.14762674E-13    2
-9.62822829E+07-5.22153035E+00 1.67865805E+00 3.84223065E-02-2.28342740E-05    3
 1.08749911E-09 2.98958809E-12-1.41079478E+04 1.60609136E+01                   4
! Hf = -59.6 kcal/mol
O2CH2OCH2O2H     021004C   2O   5H   5     G    300.00  2000.00  1000.00      1
 6.38918487E+00 3.62730429E-02-2.20713791E-05 6.74741729E-09-8.34114762E-13    2
-1.43804696E+08-6.59682996E+00 1.42111949E+00 4.74537279E-02-2.25734452E-05    3
-6.58110008E-09 6.79494713E-12-3.23402815E+04 1.93272717E+01                   4
! Hf = -109.4 kcal/mol
HO2CH2OCHO       021004C   2O   4H   4     G    300.00   2000.00 1000.00      1
 5.04783124E+00 3.00907219E-02-1.82599779E-05 5.56605885E-09-6.86151497E-13    2
-1.19891649E+08-7.23528959E-01 1.53678231E+00 3.74145426E-02-1.67458330E-05    3
-5.88629621E-09 5.44746774E-12-5.70366076E+04 1.77330915E+01                   4
!Hf = -75.5
OCH2OCHO         021004C   2H   3O   3     G    300.00   2000.00 1000.00      1
 3.76329090E+00 2.51185020E-02-1.57269656E-05 4.88357447E-09-6.08189494E-13    2
-9.59381100E+07 6.34960258E+00 2.20926999E+00 2.57436425E-02-6.11730137E-06    3
-1.04220636E-08 6.02388745E-12-3.97830798E+04 1.50982863E+01                   4
! Hf(HOCHO...CH2OO) = -80.4 kcal/mol adjusted to -109.4 kcal/mol for hpmf
HOCHOCH2OO       020404C   2H   4O   4     G   300.00   2000.00  1000.00      1
 5.90231974E+00 2.88659477E-02-1.73449785E-05 5.22108310E-09-6.35260823E-13    2
-1.19877178E+08 1.07386719E-01 4.54890428E+00 2.77826817E-02-3.37982183E-06    3
-1.45292466E-08 7.59482341E-12-4.30259175E+04 8.08305945E+00                   4
!
!
! The following parmeters were adjusted to reflect heats of formation of
```

! known experimental heat of formation. See text (above) for more details.
!
!
CH2OO 020404C 1H 2O 2 G 300.00 2000.00 1000.00 1
3.33183473E+00 1.21205869E-02-7.06434563E-06 2.08191546E-09-2.49797106E-13 2
-5.99062273E+07 5.50074749E+00 1.25882136E+00 1.82326151E-02-1.20405963E-05 3
1.79353776E-09 9.79316356E-13 1.13355951E+04 1.59855612E+01 4
dioxirane 020404C 1O 2H 2 G 300.00 2000.00 1000.00 1
1.96563081E+00 1.46331532E-02-8.93008823E-06 2.72742032E-09-3.36175158E-13 2
-5.99168083E+07 1.15701662E+01 1.52543866E+00 1.10054716E-02 6.96906318E-06 3
-1.68465640E-08 7.41403711E-12 4.40920986E+02 1.48761201E+01 4
mbisoxy 020404H 2C 1O 2 G 300.00 2000.00 1000.00 1
3.73775802E+00 1.26117906E-02-7.81325206E-06 2.40451798E-09-2.97266695E-13 2
-5.99167342E+07 2.75805584E+00 5.68828844E-01 2.50057445E-02-2.59093297E-05 3
1.40023246E-08-3.02244243E-12 1.05147343E+03 1.81176863E+01 4
HOCOCOH 012604C 2H 2O 3 G 300.00 2000.00 1000.00 1
3.87501487E+00 2.09095444E-02-1.31461138E-05 4.09818860E-09-5.12127087E-13 2
-9.57740101E+07 6.24928008E+00 3.31348868E+00 1.82852873E-02-1.92291125E-07 3
-1.20207117E-08 5.84403211E-12-6.02105653E+04 1.00594383E+01 4
SOZ 021004H 4C 2O 3 G 300.00 2000.00 1000.00 1
1.73935726E+00 3.15357272E-02-1.95915039E-05 6.06696460E-09-7.55726019E-13 2
-9.61092379E+07 1.32729994E+01-7.60704056E-01 3.18689652E-02-1.57084467E-06 3
-2.17297920E-08 1.12004298E-11-2.60219570E+04 2.74757901E+01 4
dirad-SOZ 021004H 4O 3C 2 G 300.00 2000.00 1000.00 1
3.87509958E+00 2.88808742E-02-1.79916703E-05 5.56888616E-09-6.92200018E-13 2
-9.61025317E+07 4.80472926E+00 5.15232520E-01 3.61699578E-02-1.71522412E-05 3
-5.06380738E-09 5.18108258E-12-1.91690956E+04 2.23809810E+01 4
HMF 021004C 2O 3H 4 G 300.00 2000.00 1000.00 1
3.37092584E+00 2.76975354E-02-1.65107130E-05 4.96743710E-09-6.06595298E-13 2
-9.61486861E+07 6.81209540E+00 1.77193583E+00 2.62730252E-02 4.13467954E-07 3
-1.87739558E-08 9.24364157E-12-6.56017847E+04 1.62711853E+01 4
HMHP 021004C 1H 4O 3 G 300.00 2000.00 1000.00 1
5.10022967E+00 1.95899134E-02-1.08102381E-05 3.07951820E-09-3.62775584E-13 2
-8.40757735E+07-1.80063715E+00 2.16590365E+00 2.55854121E-02-8.84774133E-06 3
-7.53887434E-09 5.23970547E-12-4.04661598E+04 1.36310658E+01 4