

!! UT-LCS Ver.1.0 2017.11.22

!!

ELEMENTS

O H N HE AR

END

SPECIES

NO NH3

H2 O2 H O OH HO2 H2O H2O2

NH2 NH N NNH

NH2OH H2NO HNOH HNO HON NO2 HONO HNO2 NO3 HONO2 N2O

N2H4 N2H3 N2H2 H2NN

AR HE N2

! OH*

END

!

!Most of the data from Song et al. Fuel 2016, 181, 358

THERMO ALL

300.00 1000.00 5000.00

AR REF ELEMENT g 5/97AR 1. 0. 0. 0.G 200.000 6000.000 1000. 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

HE REF ELEMENT g 5/97HE 1. 0. 0. 0.G 200.000 6000.000 1000. 1

2.50000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 2

-7.45375000E+02 9.28723974E-01 2.50000000E+00 0.00000000E+00 0.00000000E+00 3

0.00000000E+00 0.00000000E+00 -7.45375000E+02 9.28723974E-01 0.00000000E+00 4

N2 REF ELEMENT G 8/02N 2. 0. 0. 0.G 200.000 6000.000 1000. 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

H2 REF ELEMENT tpi 5/78H 2. 0. 0. 0.G 200.000 6000.000 1000. 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
O2 REF ELEMENT RUS 89O 2 0 0 OG 200.000 6000.000 1000. 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
O3 L 5/90O 3 0 0 OG 200.000 6000.000 1000. 1
1.23302914E+01-1.19324783E-02 7.98741278E-06-1.77194552E-09 1.26755824E-12 2
1.26755831E+04-4.08823374E+01 3.40738221E+00 2.05379063E-07 8.486052E-05 3
-2.23311542E-08 9.76073226E-12 1.58644979E+04 8.28247580E+00 1.7051228E+04 4
H L 6/94H 1 0 0 OG 200.000 6000.000 1000. 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
O L 1/90O 1 0 0 OG 200.000 6000.000 1000. 1
2.54363697E+00-2.73162486E-05 1.0029520E-07 4.95481845E-12-4.79553694E-16 2
2.92260120E+04 4.9222945E+00 3.1026710E+00-3.27931884E-03 6.64306396E-06 3
-6.12806624E-09 2.1126597E-12 2.0122253E+04 2.05193346E+00 2.99687009E+04 4
OH HYDROXYL RADICAL RU3/03O 1.000 0. 0.G 200.000 6000.000 1000. 1
2.83853033E+00 1.16111289E-03-2.9000209E-07 4.20698729E-11-2.42289890E-15 2
3.69780008E+03 5.8449400E+00 3.99198424E+00-2.40106655E-03 4.61664033E-06 3
-3.00916306E+00 1.36319502E-12 3.36889836E+03-1.03998477E-01 4.48613328E+03 4
HO2 T 1/09H 2O 2. 0. 0.G 200.000 5000.000 1000. 1
1.7228700E+00 1.88117627E-03-3.46277286E-07 1.94657549E-11 1.76256905E-16 2
1.0206839E+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
H2O L 5/89H 2O 1 0 0 OG 200.000 6000.000 1000. 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

H2O2 T 8/03H 2.O 2. 0. 0.G 200.000 6000.000 1000. 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
NH3 RRHO A12/04H 3.N 1. 0. 0.G 200.000 6000.000 1000. 1
2.09566674E+00 6.14750045E-03-2.00328925E-06 3.01334626E-10-1.71227204E-14 2
-6.30945436E+03 9.59574081E+00 4.46075151E+00-5.68781763E-03 2.11411484E-05 3
-2.02849980E-08 6.89500555E-12-6.70753514E+03-1.34450793E+00-5.48041877E+03 4
NH2 AMIDOGEN RAD IU3/03N 1.H 2. 0. 0.G 200.000 3000.000 1000. 1
2.59263049E+00 3.47683597E-03-1.08271624E-06 1.49342558E-10-1.5241187E-15 2
2.18865421E+04 7.90565351E+00 4.19198016E+00-2.04602827E-03 6.6775134E-06 3
-5.24907235E-09 1.55589948E-12 2.14991387E+04-9.04751277E+02 2.27072911E-04 4
NH ATcT/AN 1.H 1. 0. 0.G 200.000 6000.000 1000. 1
2.78372644E+00 1.32985888E-03-4.24785573E-07 7.81194442E-11-5.91451310E-15 2
4.23461945E+04 5.74084863E+00 3.49295115E+00 3.11795102E-03-1.48906628E-06 3
2.48167402E-09-1.03570916E-12 4.21059721E+04 1.11114073E+00 4.31525130E+04 4
N L 6/88N 1 0 0 0.G 200.000 6000.000 1000. 1
0.24159429E+01 0.17489002E-03-0.11102369E-06 0.30226244E-10-0.20360983E-14 2
0.56133775E+05 0.46496051E+01-1.2500681E+01 0.00000000E+00 0.00000000E+00 3
0.00000000E+00 0.00000000E+00-0.56104638E+05 0.41939088E+01 0.56850013E+05 4
NNH A12/06N 1.H 1. 0. 0.G 200.000 6000.000 1000. 1 !
3.4274123E+00 3.2329521E-03-1.17296299E-06 1.90508356E-10-1.14491506E-14 2
2.81067740E+04 6.39209233E+00 4.25474632E+00-3.45098298E-03 1.37788699E-05 3
-1.33153704E-08 4.41123397E-12 2.88323793E+04 3.28551762E+00 3.02815661E+04 4
NH2OH cis T02/12N 1.H 3.O 1. 0.G 200.000 6000.000 1000. 1
2.88112502E+00 8.15708448E-03-2.82615576E-06 4.37930933E-10-2.52724604E-14 2
-6.86018419E+03 3.79156136E+00 3.21016092E+00 6.19671676E-03 1.10594948E-05 3
-1.96668262E-08 8.82516590E-12-6.58148481E+03 7.93293571E+00-5.28593988E+03 4
NH2OH cis T02/12N 1.H 3.O 1. 0.G 200.000 6000.000 1000. 1
4.00743867E+00 7.32310180E-03-2.47602819E-06 3.83254459E-10-2.22649810E-14 2
-4.74292237E+03 2.73458714E+00 3.93981196E+00-1.77979633E-03 2.86748802E-05 3

-3.54484775E-08 1.38290834E-11-4.31981942E+03 5.21025339E+00-3.03445423E+03 4

HNOH trans & Equ T11/11H 2.N 1.O 1. 0.G 200.000 6000.000 1000. 1

3.98321933E+00 4.88846374E-03-1.65086637E-06 2.55371446E-10-1.48308561E-14 2

1.05780106E+04 3.62582838E+00 3.95608248E+00-3.02611020E-03 2.56874396E-05 3

-3.15645120E-08 1.24084574E-11 1.09199790E+04 5.55950983E+00 1.21354115E+04 4

HNOH cis ATcT C T11/11H 2.N 1.O 1. 0.G 200.000 6000.000 1000. 1

4.11664692E+00 4.81707273E-03-1.63507639E-06 2.53797646E-10-1.47744717E-14 2

1.25020921E+04 3.12195287E+00 3.80983976E+00 4.35965662E-04 1.51571812E-05 3

-1.96181113E-08 7.75279218E-12 1.28164979E+04 5.90835846E+00 1.40155826E+04 4

HNO ATcT/AH 1.N 1.O 1. 0.G 200.000 6000.000 1000.

3.16598124E+00 2.99958892E-03-3.94376786E-07-3.85344089E-11 7.07615568E-15 2

1.17726311E+04 7.64511172E+00 4.53525574E+00-5.68513371E-03 1.85198541E-05 3

-1.71881225E-08 5.55818157E-12 1.16183003E+04 1.71315886E+00 1.23500657E+04 4

HON T11/11N 1.O 1.H 1. 0.G 200.000 6000.000 1000. 1

4.00745749E+00 2.41824666E-03-8.13734115E-07 1.25573115E-10-1.28062602E-15 2

2.43965586E+04 4.01091333E+00 4.30796011E+00-5.11108487E-03 2.27054537E-05 3

-2.65676371E-08 1.02998699E-11 1.15850141E+04 3.93009562E+00 2.57994759E+04 4

NO RUS 89N 1O 1.H 0.G 200.000 6000.000 1000. 1

3.26071234E+00 1.19101151E-03-1.29122611E-07 6.94481463E-11-4.03295681E-15 2

9.92143132E+03 1.36900518E+00 4.21859896E+00-4.63988124E-03 1.10443049E-05 3

-9.34055507E-09 2.80114874E-12 9.81309964E+03 2.28061001E+00 1.09770882E+04 4

NO2 L7/88N 1O 1.H 0.G 200.000 6000.000 1000. 1

0.13647540E+02 0.21723955E-02-0.82806909E-06 0.15747510E-09-0.10510895E-13 2

0.23114912E+04-0.111141695E+00 0.39440312E+01-0.15854290E-02 0.16657812E-04 3

1.20475411E-07-1.78350564E-11 0.28966180E+04 0.63119919E+01 0.41124701E+04 4

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

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

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

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

HNO2 103190H 1N 1O 2 G 0300.00 4000.00 1500.00 1

6.47963000E+00 1.99527400E-03-1.74038700E-07-9.69587200E-11 1.70148000E-14 2

-7.80950291E+03-1.06771518E+01 1.93483800E+00 1.01003600E-02-4.96461600E-06 3

8.70112000E-10-2.32413500E-15-5.91571591E+03 1.47282082E+01 4

NO3 ATcT/AN 1.O 3. 0. 0.G 200.000 6000.000 1000. 1

7.48347702E+00 2.57772064E-03-1.00945831E-06 1.72314063E-10-1.07154008E-14 2

6.12990474E+03-1.41618136E+01 2.17359330E+00 1.04902685E-02 1.10472669E-05 3

-2.81561867E-08 1.36583960E-11 7.81290905E+03 1.46022090E+01 8.97563416E+03 4

HONO2 T 8/03H 1N 1O 3 OG 200.00 6000.00 1000. 1

8.03098942E+00 4.46958589E-03-1.72459491E-06 2.91556153E-10-1.80102700E-14 2

-1.92821685E+04-1.62616720E+01 1.69329154E+00 1.90167702E-02-8.20076690E-06 3

-6.06113827E-09 4.65236978E-12-1.73882411E+04 1.71839655E+01 4!

N2O L 7/88N 2O 1 0 OG 200.000 6000.000 1000. 1

0.48230729E+01 0.26270251E-02-0.95850872E-06 0.16000000E-09-0.97752300E-14 2

0.80734047E+04-0.22017208E+01 0.22571502E+01 0.000304728E-01-0.003671319E-04 3

0.96819803E-08-0.29307182E-11 0.87417746E+04 0.10057992E+02 0.000141682E+04 4

H2NO 1510 H 2N 1O 1 G 298.15 2000.000 1000. 1

3.33719385E+00 5.72250531E-03-2.14985300E-06 3.00000000E-10-2.18615301E-14 2

6.50621112E+03 6.86465421E+00 0.0007694692E+00 2.19179940E-04 9.92160372E-06 3

-1.02259681E-08 3.26220460E-12 6.48007616E+00 3.93185152E+00 4

H2NN DBOZ00M93/JBPM3 2000.00 5000.000 1695.000 1

3.13531032E+00 0.0008632569E-01 0.93983467E-06 3.01290501E-10-1.74978144E-14 2

3.33678346E+04 7.00005840E+00 2.000544262E+00 4.69495999E-03 7.01983230E-07 3

-1.53350000E-09 3.79345000E-13 3.36030690E+04 8.95096779E+00 4

N2H2 121286N 2H 2 G 0300.00 5000.00 1000.00 1

0.03000000E+02 0.00000000E-01-0.02303854E-04 0.04062789E-08-0.02713144E-12 2

0.02418000E+00 0.04980585E+02 0.01617999E+02 0.01306312E+00-0.01715712E-03 3

0.01605608E-06-0.06093639E-10 0.02467526E+06 0.01379467E+03 4

N2H3 120186N 2H 3 G 0300.00 5000.00 1000.00 1

0.04441846E+02 0.07214271E-01-0.02495684E-04 0.03920565E-08-0.02298950E-12 2

0.01664221E+06-0.04275205E+01 0.03174204E+02 0.04715907E-01 0.01334867E-03 3

-0.01919685E-06 0.07487564E-10 0.01727270E+06 0.07557224E+02 4

N2H4 121286N 2H 4 G 0300.00 5000.00 1000.00 1

0.04977317E+02 0.09595519E-01-0.03547639E-04 0.06124299E-08-0.04029795E-12 2

0.09341219E+05-0.02962990E+02 0.06442606E+00 0.02749730E+00-0.02899451E-03 3

0.01745240E-06-0.04422282E-10 0.01045192E+06 0.02127789E+03 4

!***** OH* from Burcat *****

OH* A 2Sigma+ ATcT AO 1.H 1. 0. 0.G 200.000 6000.000 1000. 1

2.75582920E+00 1.39848756E-03-4.19428493E-07 6.33453282E-11-3.56042218E-15 2

5.09751756E+04 5.62581429E+00 3.46084428E+00 5.01872172E-04-2.00254474E- 3

3.18901984E-09-1.35451838E-12 5.07349466E+04 1.73976415E+00 5.177707E+04 4

END

REACTIONS

!

! *****

! H2/O2 subset *

! *****

!

!H+O2=O+OH 1.0E+00 0.000 15.0 !

!O+H2=OH+H 1.8E12 0.000 794.0 !

! DUPLICATE !

!O+H2=OH+H 8.8E+00 0.000 19175 !

! DUPLICATE !

!OH+H2=H+H2O 2.2E08 1.510 3430 !

!OH+OH=O+H2 1.4E07 1.689 -1167 !

! DUPLICATE

!H+OH=H+H2O -2.7E10 0.567 0 !

! DUPLICATE

H2+M=H+H+M 4.6E19 -1.400 104380 !

H2/2.5/ H2O/12/ AR/0.0/

H2+AR=H+H+AR 5.8E18 -1.100 104380 !

!H+O+M=OH+M 4.7E18 -1.000 0 !

! H2/2.5/ H2O/12/ AR/0.75/

!O+O+M=O2+M 1.9E13 0.000 -1788 !

! H2/2.5/ H2O/12/ AR/0.0/

!H2O+M = H+OH+M 6.1E27 -3.322 120790 !

! H2/3.0/ H2O/0.0/ N2/2.0/ O2/1.5/

!H2O+H2O = H+OH+H2O 1.006E+26 -2.44 1.2018E+05

!H+O2(+M)=HO2(+M) 4.7E12 0.440 0 !

! LOW/6.366E+20 -1.72 5.248E+02/

! TROE/0.5 1E-30 1E+30/

! H2/2.0/ H2O/14/ O2/0.78/ AR/0.67/

!HO2+H=H2+O2 2.8E06 2.090 -1451 !

!HO2+H=OH+OH 7.1E13 0.000 295 !

!HO2+H=H2O+O 1.4E12 0.000 0 !

!HO2+O=O2+OH 2.9E10 1.000 -724 !

!HO2+OH = H2O+O2 1.93E20 -2.49 5.84E+02

! DUPLICATE

!HO2+OH = H2O+O2 1.21E+09 -24 -1.7E+02

! DUPLICATE

!HO2+HO2=H2O2+O2 1.2E12 0.7712 -1825 !

! DUPLICATE

!HO2+HO2=H2O2+O2 1.3E12 0.295 7397 !

! DUPLICATE

!H2O2(+M) = OH+OH(+M) 2.00E+12 0.90 4.8749E+04

! LOW/2.49E+20 -2.30 4.8749E+04/

! TROE/0.5 1E-30 1E+30/

! AR/1.0/ H2O/7/ N2/1.5/ O2/1.2/ H2O2/7.7/ H2/3.7/

!H2O2+H=H2O+OH 2.4E13 0.000 3970 !

!H2O2+H=HO2+H2 4.8E13 0.000 7950 !

! Tsang and Hampson, J. Phys. Chem. Ref. Data, 15:1087 (1986)

!

!H2O2+O=HO2+OH 9.6E06 2.000 3970 !

!H2O2+OH=HO2+H2O 1.7E12 0.000 318 !

! DUPLICATE

!H2O2+OH=HO2+H2O 7.6E13 0.000 7270 !

! DUPLICATE

! *****

! NH3 subset *

! *****

NH3+M=NH2+H+M 2.2E16 0.000 93470 !

NH3+H=NH2+H2 6.4E05 2.390 10171 !

!NH3+O=NH2+OH 9.4E06 1.940 6460 !

!NH3+OH=NH2+H2O 2.0E06 2.040 566 !

!NH3+HO2=NH2+H2O2 3.0E11 0.000 22000 !

NH2+H=NH+H2 1.0E06 2.32 799 !

!NH2+O=HNO+H 6.6E13 0.000 0 !

!NH2+O=NH+OH 7.0E12 0.000 0 !

! DUP

!NH2+O=NH+OH 8.6E-1 4.010 1673 !

! DUP

!NH2+OH=NH+H2O 3.3E0 1.949 17 !

!NH2+HO2=NH3+O2 1.1E04 1.5 2027 !

!NH2+HO2=H2NO+H 1.0E13 0.000 0 !

!NH2+HO2=HNO+H2O 1.6E07 0.550 525 !

! DUP

!NH2+HO2=HNO+H2O 5.7E15 -1.120 707 !

! DUP

!NH2+HO2=HNO+H2O 2.1E07 0.640 811 !

!NH2+O2=H2NO+O 2.6E11 0.4872 29050 !

!NH2+O2=HNO+OH 2.9E-2 3.764 18185 !

!NH2+NH2=NH3+NH 5.6E00 3.530 552 !

!NH2+NH=NH3+N 9.6E03 2.460 107 !

!NH2+N=N2+H+H 7.0E13 0.000 0 !

!NH2+HNO=NH3+NO 3.6E06 1.630 -1250 !

!NH₂+NO=N₂+H₂O 1.3E16 -1.25 0 !

! DUP

!NH₂+NO=N₂+H₂O -3.1E13 -0.48 1180 !

! DUP

!NH₂+NO=NNH+OH 4.29E10 0.29 -870 !

!NH₂+HONO=NH₃+NO₂ 7.1E01 3.020 -4940 !

!NH₂+NO₂=N₂O+H₂O 2.6E18 -2.191 455 !

!NH₂+NO₂=H₂NO+NO 9.1E11 0.0321 -1512 !

NH+H=N+H₂ 1.0E14 0.0 0 !

!NH+O=NO+H 9.2E13 0.000 0 !

!NH+OH=HNO+H 3.2E14 -0.376 -46 !

!NH+OH=N+H₂O 1.6E07 1.733 -576 !

!NH+O₂=HNO+O 4.6E05 2.000 6500 !

!NH+O₂=NO+OH 1.3E06 1.500 100 !

NH+NH=NH₂+N 5.7E-1 3.880 -342 !

NH+N=N₂+H 3.0E13 0.000 0 !

!NH+NO=N₂O+H 5.8E-1 -0.4

!NH+NO=N₂+OH 2.7E12 0.0721 -12 !

!NH+HONO=NH₂+NO₂ 9.1E15 0 0 !

!NH+NO₂=N₂O+O 1E12 0.000 0 !

!NH+NO₂=HNO+NO 5.9E-2 0.000 0 !

!N+OH=NO+H 3.8E13 0.000 0 !

!N+O₂=NO+O 6.4E09 1.000 6280 !

!N+NO=N₂+O 9.4E12 0.140 0 !

!NH=N₂+H 1.0E09 0.000 0 !

!NH+H=N₂+H₂ 1.0E14 0.000 0 !

!NNH+O=N₂O+H 1.9E14 -0.274 -22 !

!NNH+O=N₂+OH 1.2E13 0.145 -217 !

!NNH+O=NH+NO 5.2E11 0.381 -409 !

!NNH+OH=N₂+H₂O 5.0E13 0.000 0 !

!NNH+O₂=N₂+HO₂ 5.6E14 -0.385 -13 !

NNH+NH =N2+NH2	5.0E13	0.000	0 !
NNH+NH2=N2+NH3	5.0E13	0.000	0 !
!NNH+NO=N2+HNO	5.0E13	0.000	0 !
!NH2OH(+M)=NH2+OH(+M)	1.4E20	-1.310	64080 !
! LOW /5.4E37 -5.96 66783/			!
! TROE /0.31 1E-30 1E30 1E30/			!
!NH2OH+H=HNOH+H2	4.8E08	1.50	6249 !
!NH2OH+H=H2NO+H2	2.4E08	1.50	5067 !
!NH2OH+O=HNOH+OH	3.3E08	1.50	3865 !
!NH2OH+O=H2NO+OH	1.7E08	1.50	3010 !
!NH2OH+OH=HNOH+H2O	1.5E04	2.61	-3537 !
!NH2OH+OH=H2NO+H2O	1.5E05	2.28	-1296 !
!NH2OH+NH2=HNOH+NH3	1.1E-1	4.00	-9 !
!NH2OH+NH2=H2NO+NH3	9.5E00	3.42	-10 !
!NH2OH+NH=HNOH+NH2	2.9E-3	4.00	1564 !
!NH2OH+NH=H2NO+NH2	1.5E-3	4.00	25 !
!NH2OH+HO2=HNOH+H2O2	2.9E04	2.61	9557 !
!NH2OH+HO2=H2NO+H2O2	2.9E04	2.61	6418 !
!H2NO+M=HNO+H+M	3.8E24	-4.29	64915 !
! H2O/10/			
!H2NO+M=H2NOH+M	1.1E29	-4.000	44000 !
! H2O/1			
!H2NO+M=H2NO+M	3.83E27	-4.29	60300 !
!H2NO+H=HNO+H2	3.0E07	2.000	2000 !
!H2NO+H=H2+H2O	5.0E13	0.000	0 !
!H2NO+O=HNO+OH	3.0E07	2.000	2000 !
!H2NO+OH=HNO+H2O	1.0E14	0.000	0 !
!H2NO+HO2=HNO+H2O2	2.9E04	2.690	-1600 !
!H2NO+O2=HNO+HO2	2.3E02	2.994	18900 !
!H2NO+NH2=HNO+NH3	3.0E12	0.000	1000 !
!H2NO+NO=HNO+HNO	2.0E04	2.000	13000 !

!H₂NO+NO₂=HONO+HNO 6.0E11 0.000 2000 !

!HNOH+M=HNO+H+M 2.0E24 -2.840 58934 !

! H₂O/10/

!HNOH+H=NH₂+OH 4.0E13 0.000 0 !

!HNOH+H=HNO+H₂ 4.8E08 1.500 378 !

!HNOH+O=HNO+OH 7.0E13 0.000 0 !

! DUP

!HNOH+O=HNO+OH 3.3E08 1.500 -358 !

! DUP

!HNOH+OH=HNO+H₂O 2.4E06 2.000 -1192 !

!HNOH+HO₂=HNO+H₂O₂ 2.9E04 2.690 -1600 !

!HNOH+HO₂=NH₂OH+O₂ 2.9E04 2.690 -1600 !

!HNOH+O₂=HNO+HO₂ 3.0E12 0.000 2500 !

!HNOH+NH₂=NH₃+HNO 1.8E06 1.940 -1111 !

!HNOH+NO₂=HONO+HNO 6.0E11 0.000 2000 !

!NO+H(+M)=HNO(+M) 1.5E15 -0.750 0 !

! LOW /2.4E14 0.206 -1550/

! TROE /0.82 1E-30 1E30 1E30/

! N₂/1.6/

!HNO+H=NO+H₂ 9.1E11 0.620 356 !

!HNO+O=NO+OH 1.0E13 0.0 0 !

!HNO+O₂=NO+H₂O 3.6E13 0.000 0 !

!HNO+HO₂=HO₂+NO 2.0E13 0.000 16000 !

!HNO+HNO=H₂N₂O+H₂O 3.95E12 0.0 5000 !

!HNO+NO=HONO+HNO 4.4E04 2.640 4040 !

!HNO+HO₂=NO₂+OH 2.1E12 0.000 -497 !

!NO+O(+M)=NO₂(+M) 1.3E15 -0.750 0 !

! LOW /4.72E24 -2.87 1550/

! TROE /0.750 1E03 1E05 1E30/

!NO+HO₂+M=HONO₂+M 2.23E12 -3.5 2200 !

!NO₂+H=NO+OH 1.3E14 0.000 362 !

!NO2+O=NO+O2	1.1E14	-0.520	0 !
!NO2+HO2=HONO+O2	1.9E00	3.320	3044 !
!NO2+HO2=HNO2+O2	1.9E01	3.260	4983 !
!NO2+NO2=NO+NO+O2	2.0E12	0.0	26825 !
!NO2+NO2=NO3+NO	9.6E09	0.730	20900 !
!NO2+NO=N2O+O2	1.0E12	0.0	60000 !
!NO+OH(+M)=HONO(+M)	1.1E14	-0.300	0 !
! LOW /3.392E23 -2.5 0/			!
! TROE /0.75 1E-30 1E30 1E30/			!
!NO2+H2=HONO+H	1.3E04	2.760	29770 !
!N+NO2=N2O+O	1.8E12	0.0	0 !
!HONO+H=HNO+OH	5.6E10	0.860	5000 !
!HONO+H=NO+H2O	8.1E06	1.890	3850 !
!HONO+O=NO2+OH	1.2E13	0.000	5960 !
!HONO+OH=NO2+H2O	1.3E10		135 !
!HONO+NO2=HONO2+NO	2.0E11	0.000	11 !
!HONO+HONO=NO+NO2+H2O	3.5E-01	0.040	12140 !
!HNO2(+M)=HONO(+M)	2.5E14	0.000	22300 !
! LOW /3.1E18 0.0 31500/			!
! TROE /1.149 1E-30 3125 1E30/			!
!HNO2+H=NO+H2	2.4E07	1.5	5087 !
!HNO2+H=NO2+OH	1.7E08	1.5	3020 !
!HNO2+OH=NO+H2O	1.2E06	2.0	-596 !
!NO2+O(+M)=NO3(+M)	3.5E12	0.240	0 !
! LOW /2.1E20 -2.5 0/			!
! TROE /0.71 1E-30 1700 1E30/			!
!NO3+H=NO2+OH	6.0E13	0.000	0 !
!NO3+O=NO2+O2	1.0E13	0.000	0 !
!NO3+OH=NO2+HO2	1.4E13	0.000	0 !
!NO3+HO2=NO2+O2+OH	1.5E12	0.000	0 !
!NO3+NO2=NO+NO2+O2	5.0E10	0.000	2940 !

!NO2+OH(+M)=HONO2(+M) 3.0E13 0.000 0 !

! LOW /2.938E25 -3.0 0/ !

! TROE /0.4 1E-30 1E30 1E30/ !

!HONO2+H=H2+NO3 5.6E08 1.500 16400 !

!HONO2+H=H2O+NO2 6.1E01 3.300 6285 !

!HONO2+H=OH+HONO 3.8E05 2.300 6976 !

!HONO2+OH=H2O+NO3 1.0E10 0.000 -1240 !

!N2O(+M)=N2+O(+M) 9.9E10 0.0 57960 !

! LOW /6.62E14 0.0 57500./ !

! N2/1.7/ O2/1.4/ H2O/12/ !

!N2O+H=N2+OH 3.31E10 0.0 5090 !

! DUP !

!N2O+H=N2+OH 7.83E14 0.0 19390 !

! DUP !

!N2O+O=NO+NO 9.2E13 0.0 27679 !

!N2O+O=N2+O2 3.7E12 0.000 15936 !

!N2O+OH=N2+HO2 2.0E13 0.0 1000 !

!HNO+NO=N2O+OH 2.0E13 0.0 2000 !

!HNO+N=NO+NH 1.0E13 0.0 100 !

!N2O+NO=NO2+N 1.0E05 2.230 46280 !

!N2O+N=N2+O 1.0E13 0.0 19870 !

! *****

! Methylamine subset *

! *****

!N2+NH2=N2H2+N2 1.7E08 1.02 11783 !

!N2+NH2=H2NN+H2 7.2E04 1.880 8802 !

!NH2+NH=N2H2+H 1.5E15 -0.5 0 !

!HNOH+NH2=N2H3+OH 1.0E01 3.460 -467 !

!HNOH+NH2=H2NN+H2O 8.8E16 -1.080 1113 !

!NH2+NH2(+M)=N2H4(+M) 5.6E14 -0.414 66 !

! LOW /1.6E34 -5.49 1987/ !

TROE /0.31 1E-30 1E30 1E30/			!
N2H4+H=N2H3+H2	7.0E12	0.000	2500 !
!N2H4+O=NH2OH+NH	2.9E11	0.000	-1270 !
!N2H4+O=N2H3+OH	1.5E11	0.000	-1270 !
!N2H4+OH=N2H3+H2O	1.3E13	0.000	-318 !
N2H4+NH2=N2H3+NH3	3.9E12	0.000	1500 !
N2H3=N2H2+H	3.6E47	-10.380	69009 !
PLOG / 0.1 2.3E43 -9.55 64468.0/			
PLOG / 1.0 3.6E47 -10.38 69009.0/			
PLOG /10.0 1.8E45 -9.39 70141.0/			
N2H3+H=N2H2+H2	2.4E08	1.500	-10 !
!N2H3+O=N2H2+OH	1.7E08	1.500	-646 !
!N2H3+O=NH2+HNO	3.0E13	0.000	0 !
!N2H3+O=>NH2+NO+H	3.0E13	0.000	0 !
!N2H3+OH=N2H2+H2O	1.2E06	1.500	-1192 !
!N2H3+OH=H2NN+H2O	3.0E13	0.000	0 !
!N2H3+OH=NH3+HNO	1.5E12	0.000	-15000 !
!N2H3+HO2=N2H2+H2O2	1.4E04	2.690	-1600 !
!N2H3+HO2=N2H4+O2	1.2E05	1.940	-2126 !
N2H3+NH2=N2H2+NH3	1.2E05	1.940	-1152 !
N2H3+NH2=H2NN+NH3	3.0E13	0.000	0 !
N2H3+NH2=N2H2+NH2	2.0E13	0.000	0 !
N2H2=NNH+H	1.8E40	-8.41	73320 !
PLOGMX /0.1 5.6E37 -7.75 70340./			!*
PLOGMX /1.0 1.8E40 -8.41 73320./			!*
PLOGMX /10.0 3.1E41 -8.42 76102./			!*
N2H2+H=NNH+H2	8.5E04	2.630	230 !
!N2H2+O=NNH+OH	3.3E08	1.500	497 !
!N2H2+O=NH2+NO	1.0E13	0.000	0 !
!N2H2+OH=NNH+H2O	5.9E01	3.400	1360 !
N2H2+NH2=NNH+NH3	8.8E-2	4.050	1610 !

$N_2H_2+NH=NNH+NH_2$ 2.4E06 2.000 -1192 !

$!N_2H_2+NO=N_2O+NH_2$ 4.0E12 0.000 11922 !

$H_2NN=NNH+H$ 3.4E26 -4.830 46228 !

DUP

PLOG / 0.1 5.9E32 -6.99 51791.0/

PLOG / 1.0 9.6E35 -7.57 54841.0/

PLOG /10.0 5.0E36 -7.43 57295.0/

$H_2NN=NNH+H$ 3.4E26 -4.830 46228 !

DUP

PLOG / 0.1 7.2E28 -7.77 50758.0/

PLOG / 1.0 3.2E31 -6.22 52318.0/

PLOG /10.0 5.1E33 -6.52 54215.0/

$H_2NN+H=NNH+H_2$ 4.8E08 1.500 -894 !

$H_2NN+H=N_2H_2+H$ 7.0E13 0.000 0 !

$!H_2NN+O=NNH+OH$ 3.3E08 1.500 -894 !

$!H_2NN+O=NH_2+NO$ 7.0E13 0.000 0 !

$!H_2NN+OH=NNH+H_2O$ 5.06 2.000 -1192 !

$!H_2NN+OH=>NH_2+NO+H$ 2.0E12 0.000 0 !

$!H_2NN+HO_2=>NH_2+NO+OH$ 9.0E13 0.000 0 !

$!H_2NN+HO_2=NNH+H_2O_2$ 2.9E04 2.690 -1600 !

$!H_2NN+O_2=N_2+NO_2$ 1.5E12 0.000 5961 !

$H_2NN+N_2=NNH+NH_3$ 1.8E06 1.940 -1152 !

!

$N_2+M=N_2+M$ 1.89E18 -0.85 224950 !

$!H+O+M=H_2O+M$ 7.60E14 -0.1 -1770 !

*** OH* reactions *****

$!H+O+M=OH^*+M$ 3.1E14 0.0 10000 !

$!OH^*+AR=OH+AR$ 2.17E10 0.5 2060 !

$!OH^*+H_2=OH+H_2$ 2.95E12 0.5 -444 !

$!OH^*+O_2=OH+O_2$ 2.10E12 0.5 -482 !

$!OH^*+OH=OH+OH$ 1.50E12 0.5 0 !

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!OH*+H=OH+H	1.50E12	0.5	0 !
!OH*+O=OH+O	1.50E12	0.5	0 !
!N2O+H=N2+OH*	1.60E14	0.0	50300 !
!OH*=OH	1.40E06	0.0	0 !
!			
END			

RETRACTED