

Ferenc Kubicsek, Ferenc Hegedűs / Assessment of the Energy Efficiency of Ammonia Production by Microbubbles

!! 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, 358-365.

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 tpi78H 2. 0. 0. 0.G 200.000 6000.000 1000. 1

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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 890 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 5/900 3 0 0 OG 200.000 6000.000 1000. 1  
1.23302914E+01-1.19324783E-02 7.98741278E-06-1.77194552E-09 1.26075824E-13 2  
1.26755831E+04-4.08823374E+01 3.40738221E+00 2.05379063E-03 1.38486052E-05 3  
-2.23311542E-08 9.76073226E-12 1.58644979E+04 8.28247580E+00 1.70545228E+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 1/900 1 0 0 OG 200.000 6000.000 1000. 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  
OH HYDROXYL RADI IU3/03O 1.H 1. 0. 0.G 200.000 6000.000 1000. 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  
HO2 T 1/09H 1.O 2. 0. 0.G 200.000 5000.000 1000. 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  
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

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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+00-5.48041917E+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-10-5.75241187E-15 2  
2.18865421E+04 7.90565351E+00 4.19198016E+00-2.04602827E-03 6.67756134E-06 3  
-5.24907235E-09 1.55589948E-12 2.14991387E+04-9.04785244E-02 2.27072912E+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 7.83494442E-11-5.50451310E-15 2  
4.23461945E+04 5.74084863E+00 3.49295037E+00 3.11795720E-04-1.48906628E-06 3  
2.48167402E-09-1.03570916E-12 4.21059722E+04 1.84834973E+00 4.31525130E+04 4

N L 6/88N 1 0 0 OG 200.000 6000.000 1000. 1  
0.24159429E+01 0.17489065E-03-0.11902369E-06 0.30226244E-10-0.20360983E-14 2  
0.56133775E+05 0.46496095E+01 0.25000000E+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 T 1/06N 2.H 1. 0. 0.G 200.000 6000.000 1000. 1 !  
3.42744423E+00 3.23295234E-03-1.17296299E-06 1.90508356E-10-1.14491506E-14 2  
2.88067740E+04 6.39209233E+00 4.25474632E+00-3.45098298E-03 1.37788699E-05 3  
-1.33263744E-08 4.41023397E-12 2.88323793E+04 3.28551762E+00 3.02815661E+04 4

NH2OH ATcT/AN 1.H 3.O 1. 0.G 200.000 6000.000 1000. 1  
3.88112502E+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

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-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 1.51571801E-05 3  
-1.96181113E-08 7.75279218E-12 1.28164979E+04 5.90835846E+00 1.40705826E+04 4  
HNO ATcT/AH 1.N 1.O 1. 0.G 200.000 6000.000 1000. 1  
3.16598124E+00 2.99958892E-03-3.94376786E-07-3.85344089E-11 7.07602668E-15 2  
1.17726311E+04 7.64511172E+00 4.53525574E+00-5.68543377E-03 1.85198540E-05 3  
-1.71881225E-08 5.55818157E-12 1.16183003E+04 1.74315886E+00 1.28500657E+04 4  
HON T11/11N 1.O 1.H 1. 0.G 200.000 6000.000 1000. 1  
4.00745749E+00 2.41824666E-03-8.13734001E-07 1.25573064E-10-7.28062602E-15 2  
2.43965586E+04 4.01091333E+00 4.30796097E+00-5.01538487E-03 2.27054537E-05 3  
-2.65676371E-08 1.02998699E-11 2.45850141E+04 3.93009562E+00 2.57994759E+04 4  
NO RUS 89N 1O 1 0 OG 200.000 6000.000 1000. 1  
3.26071234E+00 1.19101135E-03-4.29122646E-07 6.94481463E-11-4.03295681E-15 2  
9.92143132E+03 6.36900518E+00 4.21859896E+00-4.63988124E-03 1.10443049E-05 3  
-9.34055507E-09 2.80554874E-12 9.84509964E+03 2.28061001E+00 1.09770882E+04 4  
NO2 L7/88N 1O 2 0 OG 200.000 6000.000 1000. 1  
0.48847540E+01 0.21723955E-02-0.82806909E-06 0.15747510E-09-0.10510895E-13 2  
0.23164982E+04-0.11741695E+00 0.39440312E+01-0.15854290E-02 0.16657812E-04 3  
-0.20475426E-07 0.78350564E-11 0.28966180E+04 0.63119919E+01 0.41124701E+04 4  
HONO 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

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-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 0G 200.00 6000.00 1000. 1  
8.03098942E+00 4.46958589E-03-1.72459491E-06 2.91556153E-10-1.80102702E-14 2  
-1.92821685E+04-1.62616720E+01 1.69329154E+00 1.90167702E-02-8.25176697E-06 3  
-6.06113827E-09 4.65236978E-12-1.73882411E+04 1.71839655E+01 4!  
N2O L 7/88N 2O 1 0 0G 200.000 6000.000 1000. 1  
0.48230729E+01 0.26270251E-02-0.95850872E-06 0.16000712E-09-0.97752302E-14 2  
0.80734047E+04-0.22017208E+01 0.22571502E+01 0.11304728E-01-0.13671319E-04 3  
0.96819803E-08-0.29307182E-11 0.87417746E+04 0.10757992E+02 0.98141682E+04 4  
H2NO 1510 H 2N 1O 1 G 298.00 3000.000 1000.0 1  
3.33719385E+00 5.72250531E-03-2.14985397E-06 3.65983461E-10-2.18615301E-14 2  
6.50621112E+03 6.86465421E+00 4.07694692E+00 2.19179940E-04 9.92160372E-06 3  
-1.02259681E-08 3.26220462E-12 6.48547616E+03 3.93185152E+00 4  
H2NN DBOZ00M93/JBPM3 96 N 2H 2 0 0G 300.000 5000.000 1695.000 1  
3.13531032E+00 5.68632569E-03-1.93983467E-06 3.01290501E-10-1.74978144E-14 2  
3.33678346E+04 7.04815840E+00 2.88544262E+00 4.69495999E-03 7.01983230E-07 3  
-1.53359038E-09 3.79345858E-13 3.36030690E+04 8.95096779E+00 4  
N2H2 121286N 2H 2 G 0300.00 5000.00 1000.00 1  
0.03371185E+02 0.06039968E-01-0.02303854E-04 0.04062789E-08-0.02713144E-12 2  
0.02418172E+06 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

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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-06 3

3.18901984E-09-1.35451838E-12 5.07349466E+04 1.73976415E+00 5.17770741E+04 4

END

REACTIONS

!

!\*\*\*\*\*

! H2/O2 subset \*

!\*\*\*\*\*

!

!H+O2=O+OH 1.0E14 0.000 15286 !

!O+H2=OH+H 3.8E12 0.000 7948 !

! DUPLICATE !

!O+H2=OH+H 8.8E14 0.000 19175 !

! DUPLICATE !

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

!OH+OH=O+H2O 1.4E07 1.689 -1167 !

! DUPLICATE

!OH+OH=O+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/

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!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 1.24 -1.31E+03  
! DUPLICATE  
!HO2+HO2=H2O2+O2 1.2E09 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+24 -2.30 4.8749E+04/  
! TROE/0.43 1E-30 1E+30/  
! AR/1.0/ H2O/7.5/ 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 !

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! 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 3.3E06 1.949 -217 !

!NH2+HO2=NH3+O2 1.7E04 1.550 2027 !

!NH2+HO2=H2NO+OH 5.0E13 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=HON+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 !



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$\text{!NH}_2+\text{NO}=\text{N}_2+\text{H}_2\text{O}$	1.3E16	-1.25	0 !
! DUP			
$\text{!NH}_2+\text{NO}=\text{N}_2+\text{H}_2\text{O}$	-3.1E13	-0.48	1180 !
! DUP			
$\text{!NH}_2+\text{NO}=\text{NNH}+\text{OH}$	4.29E10	0.29	-870 !
$\text{!NH}_2+\text{HONO}=\text{NH}_3+\text{NO}_2$	7.1E01	3.020	-4940 !
$\text{!NH}_2+\text{NO}_2=\text{N}_2\text{O}+\text{H}_2\text{O}$	2.6E18	-2.191	455 !
$\text{!NH}_2+\text{NO}_2=\text{H}_2\text{NO}+\text{NO}$	9.1E11	0.0321	-1512 !
$\text{NH}+\text{H}=\text{N}+\text{H}_2$	1.0E14	0.0	0 !
$\text{!NH}+\text{O}=\text{NO}+\text{H}$	9.2E13	0.000	0 !
$\text{!NH}+\text{OH}=\text{HNO}+\text{H}$	3.2E14	-0.376	-46 !
$\text{!NH}+\text{OH}=\text{N}+\text{H}_2\text{O}$	1.6E07	1.733	-576 !
$\text{!NH}+\text{O}_2=\text{HNO}+\text{O}$	4.6E05	2.000	6500 !
$\text{!NH}+\text{O}_2=\text{NO}+\text{OH}$	1.3E06	1.500	100 !
$\text{NH}+\text{NH}=\text{NH}_2+\text{N}$	5.7E-1	3.880	342 !
$\text{NH}+\text{N}=\text{N}_2+\text{H}$	3.0E13	0.000	0 !
$\text{!NH}+\text{NO}=\text{N}_2\text{O}+\text{H}$	5.0E14	-0.4	0 !
$\text{!NH}+\text{NO}=\text{N}_2+\text{OH}$	2.7E12	-0.0721	-512 !
$\text{!NH}+\text{HONO}=\text{NH}_2+\text{NO}_2$	1.0E13	0.000	0 !
$\text{!NH}+\text{NO}_2=\text{N}_2\text{O}+\text{OH}$	4.1E12	0.000	0 !
$\text{!NH}+\text{NO}_2=\text{HNO}+\text{NO}$	5.9E12	0.000	0 !
$\text{!N}+\text{OH}=\text{NO}+\text{H}$	3.8E13	0.000	0 !
$\text{!N}+\text{O}_2=\text{NO}+\text{O}$	6.4E09	1.000	6280 !
$\text{!N}+\text{NO}=\text{N}_2+\text{O}$	9.4E12	0.140	0 !
$\text{NNH}=\text{N}_2+\text{H}$	1.0E09	0.000	0 !
$\text{NNH}+\text{H}=\text{N}_2+\text{H}_2$	1.0E14	0.000	0 !
$\text{!NNH}+\text{O}=\text{N}_2\text{O}+\text{H}$	1.9E14	-0.274	-22 !
$\text{!NNH}+\text{O}=\text{N}_2+\text{OH}$	1.2E13	0.145	-217 !
$\text{!NNH}+\text{O}=\text{NH}+\text{NO}$	5.2E11	0.381	-409 !
$\text{!NNH}+\text{OH}=\text{N}_2+\text{H}_2\text{O}$	5.0E13	0.000	0 !
$\text{!NNH}+\text{O}_2=\text{N}_2+\text{HO}_2$	5.6E14	-0.385	-13 !

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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	-97 !
!NH2OH+NH2=H2NO+NH3	9.5E00	3.42	-1013 !
!NH2OH+NH=HNOH+NH2	2.9E-3	4.40	1564 !
!NH2OH+NH=H2NO+NH2	1.5E-3	4.60	2424 !
!NH2OH+HO2=HNOH+H2O2	2.9E04	2.69	9557 !
!NH2OH+HO2=H2NO+H2O2	1.4E04	2.69	6418 !
!H2NO+M=HNO+H+M	2.8E24	-2.830	64915 !
! H2O/10/			
!H2NO+M=HNOH+M	1.1E29	-4.000	44000 !
! H2O/10/			
!H2NO+M=H2+NO+M	3.83E27	-4.29	60300 !
!H2NO+H=HNO+H2	3.0E07	2.000	2000 !
!H2NO+H=NH2+OH	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 !

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!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	25000 !
!HNOH+NH2=NH3+HNO	1.8E06	1.940	-1152 !
!HNOH+NO2=HONO+HNO	6.0E11	0.000	2000 !
!NO+H(+M)=HNO(+M)	1.5E15	-0.410	0 !
! LOW /2.4E14 0.206 -1550/			
! TROE /0.82 1E-30 1E30 1E30/			
! N2/1.6/			
!HNO+H=NO+H2	9.68E11	0.620	356 !
!HNO+O=NO+OH	1.0E13	0.0	0 !
!HNO+OH=NO+H2O	3.6E13	0.000	0 !
!HNO+O2=HO2+NO	2.0E13	0.000	16000 !
!HNO+HNO=N2O+H2O	3.95E12	0.0	5000 !
!HNO+NO2=HONO+NO	4.4E04	2.640	4040 !
!NO+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 !

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!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	1.0	135 !
!HONO+NO2=HONO2+NO	2.0E11	0.000	32700 !
!HONO+HONO=NO+NO2+H2O	3.5E-01	3.640	12140 !
!HNO2(+M)=HONO(+M)	2.5E14	0.000	32300 !
! LOW /3.1E18 0.0 31500/			!
! TROE /1.149 1E-30 3125 1E30/			!
!HNO2+H=NO2+H2	2.4E08	1.5	5087 !
!HNO2+O=NO2+OH	1.7E08	1.5	3020 !
!HNO2+OH=NO2+H2O	1.2E06	2.0	-596 !
!NO2+O(+M)=NO3(+M)	3.5E12	0.240	0 !
! LOW /2.5E20 -1.50 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 !

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!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  0.000  27679 !
!N2O+O=N2+O2               3.7E12  0.000  15936 !
!N2O+OH=N2+HO2             2.0E12  0.0    40000 !
!HNO+NO=N2O+OH             2.0E12  0.0    26000 !
!HNO+N=NO+NH               1.0E13  0.0    1990 !
!N2O+NO=NO2+N2            5.3E05  2.230  46280 !
!N2O+N=N2+NO               1.0E13  0.0   19870 !
! *****
! N2 amine subset          *
! *****
NH2+NH2=N2H2+H2            1.7E08  1.02  11783 !
NH2+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/     !

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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 2.000 -1192 !

!N2H3+OH=H2NN+H2O 3.0E13 0.000 0 !

!N2H3+OH=NH3+HNO 1.0E12 0.000 15000 !

!N2H3+HO2=N2H2+H2O2 1.4E04 2.690 -1600 !

!N2H3+HO2=N2H4+O2 9.2E05 1.940 2126 !

N2H3+NH2=N2H2+NH3 9.2E05 1.940 -1152 !

N2H3+NH2=H2NN+NH3 3.0E13 0.000 0 !

N2H3+NH=N2H2+NH2 2.0E13 0.000 0 !

N2H2=NNH+H 1.8E40 -8.41 73320 !

PLOGMX / 0.1 5.6E36 -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 !

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$N_2H_2+NH=NNH+NH_2$  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 !

$!H_2NN+OH=NNH+H_2O$  2.4E06 2.000 -1192 !

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

$!H_2NN+HO_2=>NH_2+NO+OH$  9.0E12 0.000 0 !

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

$!H_2NN+O_2=NH_2+NO_2$  1.5E12 0.000 5961 !

$H_2NN+NH_2=NNH+NH_3$  1.8E06 1.940 -1152 !

!

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

$!N+O+M=NO+M$  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
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