

Ferenc KUBICSEK, Ferenc HEGEDŰS, Péter CSIZMADIA / Optimization of sonochemical ammonia synthesis in non-Newtonian fluids

!! 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

!

THERMO ALL

300.0000 1000.00 5000.0000

! Refitting species AR:

! max difference Cp/R = 1.7764e-15 at T = 200.0000 K

! max difference H/RT = 8.8818e-16 at T = 208.7044 K

! max difference S/R = 7.1054e-15 at T = 249.3247 K

! T_match = 1000.000000 jump

! Delta(Cp/R, H/RT, S/R) = (4.441e-16, 0.000e+00, 0.000e+00)

AR REF ELEMENT g 5/97AR 1. 0. 0. 0.G 200.0000 6000.0000 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 -1.21434192e-16 3.14642268e-19 3

-3.30872200e-22 1.21191563e-25-7.45375000e+02 4.37967491e+00 4

! Refitting species HE:

! max difference Cp/R = 1.7764e-15 at T = 200.0000 K

! max difference H/RT = 8.8818e-16 at T = 208.7044 K

! max difference S/R = 3.5527e-15 at T = 437.9190 K

! T_match = 1000.000000 jump

! Delta(Cp/R, H/RT, S/R) = (4.441e-16, 0.000e+00, 0.000e+00)

HE REF ELEMENT g 5/97HE 1. 0. 0. 0.G 200.0000 6000.0000 1000.00 1

2.50000000e+00 0.00000000e+00 0.00000000e+00 0.00000000e+00 0.00000000e+00 2

-7.45375000e+02 9.28723974e-01 2.50000000e+00-1.21434192e-16 3.14642268e-19 3

-3.30872200e-22 1.21191563e-25-7.45375000e+02 9.28723974e-01 4

! Refitting species N2:

! max difference Cp/R = 4.5555e-03 at T = 200.0000 K

! max difference H/RT = 8.2895e-04 at T = 200.0000 K

! max difference S/R = 7.3491e-04 at T = 200.0000 K

! T_match = 1000.000000 jump

! Delta(Cp/R, H/RT, S/R) = (8.882e-16, 0.000e+00, 0.000e+00)

N2 REF ELEMENT G 8/02N 2. 0. 0. 0.G 200.0000 6000.0000 1000.00 1

2.95257637e+00 1.39690040e-03-4.92631603e-07 7.86010195e-11-4.60755204e-15 2

-9.24423063e+02 5.87156477e+00 3.58256851e+00-5.58781407e-04 7.83391479e-07 3

8.73631719e-10-7.49971666e-13-1.05160018e+03 2.75873431e+00 4

! Refitting species H2:

! max difference Cp/R = 3.0330e-02 at T = 200.0000 K

! max difference H/RT = 5.5191e-03 at T = 200.0000 K

! max difference S/R = 4.8930e-03 at T = 200.0000 K

! T_match = 1000.000000 jump

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! Delta(Cp/R, H/RT, S/R) = (2.220e-15, 0.000e+00, 0.000e+00)

H2 REF ELEMENT tpis78H 2. 0. 0. 0.G 200.0000 6000.0000 1000.00 1
2.93286575e+00 8.26608026e-04-1.46402364e-07 1.54100414e-11-6.88804800e-16 2
-8.16223900e+02-1.02647801e+00 2.68763434e+00 5.08352924e-03-1.09134795e-05 3
9.75972638e-09-2.98961778e-12-9.48720664e+02-7.06735279e-01 4

! Refitting species O2:

! max difference Cp/R = 1.0265e-02 at T = 200.0000 K

! max difference H/RT = 1.8678e-03 at T = 200.0000 K

! max difference S/R = 1.6560e-03 at T = 200.0000 K

! T_match = 1000.000000 jump

! Delta(Cp/R, H/RT, S/R) = (8.882e-16, 4.441e-16, 0.000e+00)

O2 REF ELEMENT RUS 89O 2 0 0 OG 200.0000 6000.0000 1000.00 1
3.66096065e+00 6.56365811e-04-1.41149627e-07 2.05797935e-11-1.29913436e-15 2
-1.21490829e+03 3.41609021e+00 3.66627111e+00-2.01629566e-03 6.94873168e-06 3
-6.16244023e-09 1.75919060e-12-1.05352472e+03 4.12801194e+00 4

! Refitting species H:

! max difference Cp/R = 1.7764e-15 at T = 200.0000 K

! max difference H/RT = 2.8422e-14 at T = 200.0000 K

! max difference S/R = 3.5527e-15 at T = 664.2321 K

! T_match = 1000.000000 jump

! Delta(Cp/R, H/RT, S/R) = (4.441e-16, 0.000e+00, 0.000e+00)

H L 6/94H 1 0 0 OG 200.0000 6000.0000 1000.00 1
2.50000000e+00 0.00000000e+00 0.00000000e+00 0.00000000e+00 0.00000000e+00 2
2.54736600e+04-4.46682850e-01 2.50000000e+00-1.21434192e-16 3.14642268e-19 3
-3.30872200e-22 1.21191563e-25 2.54736600e+04-4.46682850e-01 4

! Refitting species O:

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! max difference Cp/R = 4.9696e-03 at T = 200.0000 K

! max difference H/RT = 9.0429e-04 at T = 200.0000 K

! max difference S/R = 8.0172e-04 at T = 200.0000 K

! T_match = 1000.000000 jump

! Delta(Cp/R, H/RT, S/R) = (-4.441e-16, 3.553e-15, -3.553e-15)

O L 1/900 1 0 0 0G 200.0000 6000.0000 1000.00 1

2.54363697e+00-2.73162486e-05-4.19029520e-09 4.95481845e-12-4.79553694e-16 2

2.92265295e+04 4.92264671e+00 3.11201699e+00-2.80464778e-03 5.23974549e-06 3

-4.42444222e-09 1.39393321e-12 2.91273034e+04 2.27964278e+00 4

! Refitting species OH:

! max difference Cp/R = 5.9918e-04 at T = 200.0000 K

! max difference H/RT = 1.0903e-04 at T = 200.0000 K

! max difference S/R = 9.6662e-05 at T = 200.0000 K

! T_match = 1000.000000 jump

! Delta(Cp/R, H/RT, S/R) = (-4.441e-16, 0.000e+00, 0.000e+00)

OH HYDROXYL RAD I U3/03O 1.H 1. 0. 0.G 200.0000 6000.0000 1000.00 1

2.83853033e+00 1.10741289e-03-2.94000209e-07 4.20698729e-11-2.42289890e-15 2

3.69787047e+03 5.84498899e+00 3.98520224e+00-2.34383614e-03 4.44744427e-06 3

-3.67375964e-09 1.27653925e-12 3.36950653e+03-7.65438871e-02 4

! Refitting species HO2:

! max difference Cp/R = 3.4144e-02 at T = 200.0000 K

! max difference H/RT = 6.2130e-03 at T = 200.0000 K

! max difference S/R = 5.5082e-03 at T = 200.0000 K

! T_match = 1000.000000 jump

! Delta(Cp/R, H/RT, S/R) = (-8.882e-16, 8.882e-16, 0.000e+00)

HO2 T 1/09H 1.O 2. 0. 0.G 200.0000 5000.0000 1000.00 1

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4.17228741e+00 1.88117627e-03-3.46277286e-07 1.94657549e-11 1.76256905e-16 2
3.45761323e+01 2.96009637e+00 3.91532945e+00-1.48787475e-03 1.15167354e-05 3
-1.25715747e-08 4.35421300e-12 2.98674804e+02 5.28114803e+00 4

! Refitting species H2O:

! max difference Cp/R = 3.2870e-03 at T = 200.0000 K

! max difference H/RT = 5.9812e-04 at T = 200.0000 K

! max difference S/R = 5.3027e-04 at T = 200.0000 K

! T_match = 1000.000000 jump

! Delta(Cp/R, H/RT, S/R) = (0.000e+00, 0.000e+00, 0.000e+00)

H2O L 5/89H 2O 1 0 OG 200.0000 6000.0000 1000.00 1
2.67703890e+00 2.97318160e-03-7.73768890e-07 9.44335140e-11-4.26899910e-15 2
-2.98862362e+04 6.88231731e+00 4.23584018e+00-2.35035878e-03 7.44852451e-06 3
-6.61473728e-09 2.24734749e-12-3.02970623e+04-9.99620648e-01 4

! Refitting species H2O2:

! max difference Cp/R = 3.9197e-02 at T = 200.0000 K

! max difference H/RT = 7.1325e-03 at T = 200.0000 K

! max difference S/R = 6.3234e-03 at T = 200.0000 K

! T_match = 1000.000000 jump

! Delta(Cp/R, H/RT, S/R) = (0.000e+00, 0.000e+00, 0.000e+00)

H2O2 T 8/03H 2.O 2. 0. 0.G 200.0000 6000.0000 1000.00 1
4.57977305e+00 4.05326003e-03-1.29844730e-06 1.98211400e-10-1.13968792e-14 2
-1.80030958e+04 6.67748430e-01 3.87148687e+00 2.89650863e-03 6.57196077e-06 3
-9.23920581e-09 3.42064984e-12-1.76669584e+04 5.06975745e+00 4

! Refitting species NH3:

! max difference Cp/R = 1.7760e-02 at T = 200.0000 K

! max difference H/RT = 3.2317e-03 at T = 200.0000 K

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! max difference S/R = 2.8651e-03 at T = 200.0000 K

! T_match = 1000.000000 jump

! Delta(Cp/R, H/RT, S/R) = (3.553e-15,-8.882e-16, 3.553e-15)

NH3 RRHO A12/04H 3.N 1. 0. 0.G 200.0000 6000.0000 1000.00 1
2.09566674e+00 6.14750045e-03-2.00328925e-06 3.01334626e-10-1.71227204e-14 2
-6.30760502e+03 9.59699937e+00 4.25973162e+00-3.99149530e-03 1.61261377e-05 3
-1.41967916e-08 4.32650740e-12-6.68950881e+03-5.30747736e-01 4

! Refitting species NH2:

! max difference Cp/R = 2.5394e-03 at T = 200.0000 K

! max difference H/RT = 4.6208e-04 at T = 200.0000 K

! max difference S/R = 4.0966e-04 at T = 200.0000 K

! T_match = 1000.000000 jump

! Delta(Cp/R, H/RT, S/R) = (0.000e+00, 0.000e+00, 0.000e+00)

NH2 AMIDOGEN RAD IU3/03N 1.H 2. 0. 0.G 200.0000 3000.0000 1000.00 1
2.59263049e+00 3.47683597e-03-1.08271624e-06 1.49342558e-10-5.75241187e-15 2
2.18868065e+04 7.90583344e+00 4.16323757e+00-1.80348166e-03 5.96049610e-06 3
-4.37855755e-09 1.18864591e-12 2.15017162e+04 2.58760010e-02 4

! Refitting species NH:

! max difference Cp/R = 2.9750e-03 at T = 200.0000 K

! max difference H/RT = 5.4135e-04 at T = 200.0000 K

! max difference S/R = 4.7994e-04 at T = 200.0000 K

! T_match = 1000.000000 jump

! Delta(Cp/R, H/RT, S/R) = (8.882e-16, 0.000e+00,-3.553e-15)

NH ATcT/AN 1.H 1. 0. 0.G 200.0000 6000.0000 1000.00 1
2.78372644e+00 1.32985888e-03-4.24785573e-07 7.83494442e-11-5.50451310e-15 2
4.23458847e+04 5.74063777e+00 3.52662396e+00 2.76384425e-05-6.48983088e-07 3

1.46181571e-09-6.05450344e-13 4.21029525e+04 1.71203374e+00 4

! Refitting species N:

! max difference Cp/R = 1.0031e-03 at T = 200.0000 K

! max difference H/RT = 1.8253e-04 at T = 200.0000 K

! max difference S/R = 1.6183e-04 at T = 200.0000 K

! T_match = 1000.000000 jump

! Delta(Cp/R, H/RT, S/R) = (0.000e+00, 0.000e+00, 0.000e+00)

N L 6/88N 1 0 0 0G 200.0000 6000.0000 1000.00 1

2.41594290e+00 1.74890650e-04-1.19023690e-07 3.02262440e-11-2.03609830e-15 2

5.61336705e+04 4.64953840e+00 2.51135408e+00-9.58123439e-05 2.83259838e-07 3

-3.43876564e-10 1.45074992e-13 5.61036198e+04 4.14794568e+00 4

! Refitting species NNH:

! max difference Cp/R = 1.8419e-02 at T = 200.0000 K

! max difference H/RT = 3.3517e-03 at T = 200.0000 K

! max difference S/R = 2.9715e-03 at T = 200.0000 K

! T_match = 1000.000000 jump

! Delta(Cp/R, H/RT, S/R) = (8.882e-16, 0.000e+00, 0.000e+00)

NNH T 1/06N 2.H 1. 0. 0.G 200.0000 6000.0000 1000.00 1

3.42744423e+00 3.23295234e-03-1.17296299e-06 1.90508356e-10-1.14491506e-14 2

2.88086920e+04 6.39339762e+00 4.04626045e+00-1.69165832e-03 8.57759881e-06 3

-7.01204812e-09 1.74633997e-12 2.88510751e+04 4.12950127e+00 4

! Refitting species NH2OH:

! max difference Cp/R = 4.6508e-02 at T = 200.0000 K

! max difference H/RT = 8.4629e-03 at T = 200.0000 K

! max difference S/R = 7.5029e-03 at T = 200.0000 K

! T_match = 1000.000000 jump

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! Delta(Cp/R, H/RT, S/R) = (1.776e-15,-4.441e-16, 0.000e+00)

NH2OH ATcT/AN 1.H 3.O 1. 0.G 200.0000 6000.0000 1000.00 1

3.88112502e+00 8.15708448e-03-2.82615576e-06 4.37930933e-10-2.52724604e-14 2

-6.85534125e+03 3.79485718e+00 2.68374332e+00 1.06389335e-02-2.07348345e-06 3

-3.72343389e-09 2.09895275e-12-6.53427866e+03 1.00639571e+01 4

! Refitting species HNOH:

! max difference Cp/R = 5.1536e-02 at T = 200.0000 K

! max difference H/RT = 9.3778e-03 at T = 200.0000 K

! max difference S/R = 8.3140e-03 at T = 200.0000 K

! T_match = 1000.000000 jump

! Delta(Cp/R, H/RT, S/R) = (8.882e-16, 0.000e+00, 0.000e+00)

HNOH trans s Equ T11/11H 2.N 1.O 1. 0.G 200.0000 6000.0000 1000.00 1

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

1.05833771e+04 3.62948054e+00 3.37275545e+00 1.89634132e-03 1.11346941e-05 3

-1.38975267e-08 4.95509312e-12 1.09722885e+04 7.92090954e+00 4

! Refitting species HNO:

! max difference Cp/R = 5.2235e-03 at T = 200.0000 K

! max difference H/RT = 9.5049e-04 at T = 200.0000 K

! max difference S/R = 8.4267e-04 at T = 200.0000 K

! T_match = 1000.000000 jump

! Delta(Cp/R, H/RT, S/R) = (-8.882e-16, 3.553e-15, 0.000e+00)

HNO ATcT/AH 1.N 1.O 1. 0.G 200.0000 6000.0000 1000.00 1

3.16598124e+00 2.99958892e-03-3.94376786e-07-3.85344089e-11 7.07602668e-15 2

1.17720872e+04 7.64474157e+00 4.59437921e+00-6.18435183e-03 1.99948561e-05 3

-1.89787698e-08 6.31362132e-12 1.16129984e+04 1.50381772e+00 4

! Refitting species HON:

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! max difference Cp/R = 3.9017e-02 at T = 200.0000 K

! max difference H/RT = 7.0998e-03 at T = 200.0000 K

! max difference S/R = 6.2944e-03 at T = 200.0000 K

! T_match = 1000.000000 jump

! Delta(Cp/R, H/RT, S/R) = (2.665e-15, 0.000e+00, 0.000e+00)

HON T11/11N 1.O 1.H 1. 0.G 200.0000 6000.0000 1000.00 1

4.00745749e+00 2.41824666e-03-8.13734001e-07 1.25573064e-10-7.28062602e-15 2

2.44006215e+04 4.01367835e+00 3.86632909e+00-1.28863909e-03 1.16876949e-05 3

-1.31921139e-08 4.65699158e-12 2.46246171e+04 5.71789104e+00 4

! Refitting species NO:

! max difference Cp/R = 6.4335e-03 at T = 200.0000 K

! max difference H/RT = 1.1707e-03 at T = 200.0000 K

! max difference S/R = 1.0379e-03 at T = 200.0000 K

! T_match = 1000.000000 jump

! Delta(Cp/R, H/RT, S/R) = (0.000e+00,-1.776e-15, 0.000e+00)

NO RUS 89N 1O 1 0 OG 200.0000 6000.0000 1000.00 1

3.26071234e+00 1.19101135e-03-4.29122646e-07 6.94481463e-11-4.03295681e-15 2

9.92210128e+03 6.36946115e+00 4.14577886e+00-4.02538298e-03 9.22760068e-06 3

-7.13508162e-09 1.87510129e-12 9.85162973e+03 2.57539722e+00 4

! Refitting species NO2:

! max difference Cp/R = 3.6108e-02 at T = 200.0000 K

! max difference H/RT = 6.5703e-03 at T = 200.0000 K

! max difference S/R = 5.8250e-03 at T = 200.0000 K

! T_match = 1000.000000 jump

! Delta(Cp/R, H/RT, S/R) = (0.000e+00, 0.000e+00, 0.000e+00)

NO2 L 7/88N 1O 2 0 OG 200.0000 6000.0000 1000.00 1

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4.88475400e+00 2.17239550e-03-8.28069090e-07 1.57475100e-10-1.05108950e-14 2

2.32025808e+03-1.14858031e-01 3.53533598e+00 1.86337812e-03 6.46175178e-06 3

-8.09744241e-09 2.61302115e-12 2.93326748e+03 7.96645454e+00 4

! Refitting species HONO:

! max difference Cp/R = 3.6827e-02 at T = 200.0000 K

! max difference H/RT = 6.7012e-03 at T = 200.0000 K

! max difference S/R = 5.9411e-03 at T = 200.0000 K

! T_match = 1000.000000 jump

! Delta(Cp/R, H/RT, S/R) = (-1.776e-15, 8.882e-16, 0.000e+00)

HONO equil ATcT T 9/11H 1.N 1.O 2. 0.G 200.0000 6000.0000 1000.00 1

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

-1.15915547e+04-4.05277876e+00 2.79732125e+00 1.16453005e-02-8.73921345e-06 3

3.09645082e-09-4.54762949e-13-1.07456930e+04 1.15094261e+01 4

! Refitting species HNO2:

! max difference Cp/R = 1.8131e-06 at T = 1423.5118 K

! max difference H/RT = 3.1425e-07 at T = 1499.3997 K

! max difference S/R = 3.2152e-06 at T = 1501.2506 K

! T_match = 1500.000000 jump

! Delta(Cp/R, H/RT, S/R) = (-1.776e-15, 0.000e+00, 7.105e-15)

HNO2 103190H 1N 1O 2 G 300.0000 4000.0000 1500.00 1

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

-7.80950328e+03-1.06771486e+01 1.93482897e+00 1.01004186e-02-4.96473863e-06 3

8.70212516e-10-2.35191805e-15-5.91571493e+03 1.47282468e+01 4

! Refitting species NO3:

! max difference Cp/R = 8.8881e-02 at T = 200.0000 K

! max difference H/RT = 1.6173e-02 at T = 200.0000 K

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! max difference S/R = 1.4339e-02 at T = 200.0000 K

! T_match = 1000.000000 jump

! Delta(Cp/R, H/RT, S/R) = (1.776e-15, 0.000e+00, 0.000e+00)

NO3 ATcT/AN 1.O 3. 0. 0.G 200.0000 6000.0000 1000.00 1

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

6.13915999e+03-1.41555150e+01 1.16756871e+00 1.89796870e-02-1.40508671e-05 3

2.31286562e-09 8.04083704e-13 7.90312364e+03 1.86747550e+01 4

! Refitting species HONO2:

! max difference Cp/R = 5.7786e-02 at T = 200.0000 K

! max difference H/RT = 1.0515e-02 at T = 200.0000 K

! max difference S/R = 9.3223e-03 at T = 200.0000 K

! T_match = 1000.000000 jump

! Delta(Cp/R, H/RT, S/R) = (0.000e+00, 3.553e-15,-7.105e-15)

HONO2 T 8/03H 1N 1O 3 OG 200.0000 6000.0000 1000.00 1

8.03098942e+00 4.46958589e-03-1.72459491e-06 2.91556153e-10-1.80102702e-14 2

-1.92761511e+04-1.62575769e+01 1.03922026e+00 2.45362027e-02-2.45694284e-05 3

1.37484493e-08-3.70491756e-12-1.73295877e+04 1.98317491e+01 4

! Refitting species N2O:

! max difference Cp/R = 6.9486e-03 at T = 200.0000 K

! max difference H/RT = 1.2644e-03 at T = 200.0000 K

! max difference S/R = 1.1210e-03 at T = 200.0000 K

! T_match = 1000.000000 jump

! Delta(Cp/R, H/RT, S/R) = (-1.776e-15, 0.000e+00, 0.000e+00)

N2O L 7/88N 2O 1 0 OG 200.0000 6000.0000 1000.00 1

4.82307290e+00 2.62702510e-03-9.58508720e-07 1.60007120e-10-9.77523020e-15 2

8.07412818e+03-2.20122859e+00 2.17850018e+00 1.19684226e-02-1.56334679e-05 3

1.20640237e-08-3.93565749e-12 8.74882749e+03 1.10763796e+01 4

! Refitting species H2NO:

! max difference Cp/R = 2.0865e-08 at T = 999.5198 K

! max difference H/RT = 2.9661e-09 at T = 1000.8714 K

! max difference S/R = 2.0586e-08 at T = 1007.6298 K

! T_match = 1000.000000 jump

! Delta(Cp/R, H/RT, S/R) = (2.665e-15, 0.000e+00, 0.000e+00)

H2NO 1510 H 2N 1O 1 G 298.0000 3000.0000 1000.00 1

3.33719385e+00 5.72250531e-03-2.14985397e-06 3.65983461e-10-2.18615301e-14 2

6.50621112e+03 6.86465419e+00 4.07694678e+00 2.19180991e-04 9.92160103e-06 3

-1.02259653e-08 3.26220362e-12 6.48547617e+03 3.93185210e+00 4

! Refitting species H2NN:

! max difference Cp/R = 1.0320e-02 at T = 1496.7484 K

! max difference H/RT = 1.8528e-03 at T = 1677.7889 K

! max difference S/R = 3.3002e-03 at T = 1696.5983 K

! T_match = 1695.000000 jump

! Delta(Cp/R, H/RT, S/R) = (1.776e-15,-3.553e-15, 0.000e+00)

H2NN DBOZ00M93/JBPM3 96 N 2H 2 O OG 300.0000 5000.0000 1695.00 1

3.13531032e+00 5.68632569e-03-1.93983467e-06 3.01290501e-10-1.74978144e-14 2

3.33647095e+04 7.04485820e+00 2.94840788e+00 4.29905889e-03 1.48887782e-06 3

-2.14228978e-09 5.38242847e-13 3.35960682e+04 8.68034385e+00 4

! Refitting species N2H2:

! max difference Cp/R = 6.4476e-06 at T = 998.2991 K

! max difference H/RT = 9.0970e-06 at T = 1000.6503 K

! max difference S/R = 1.3605e-06 at T = 1007.7039 K

! T_match = 1000.000000 jump

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! Delta(Cp/R, H/RT, S/R) = (0.000e+00, 0.000e+00, 0.000e+00)

N2H2 121286N 2H 2 G 300.0000 5000.0000 1000.00 1
3.37118500e+00 6.03996800e-03-2.30385400e-06 4.06278900e-10-2.71314400e-14 2
2.41817109e+04 4.98058364e+00 1.61793839e+00 1.30635784e-02-1.71583135e-05 3
1.60573529e-08-6.09410984e-12 2.46752659e+04 1.37949214e+01 4

! Refitting species N2H3:

! max difference Cp/R = 2.0102e-02 at T = 899.5498 K

! max difference H/RT = 3.0706e-03 at T = 993.5968 K

! max difference S/R = 4.4470e-03 at T = 1024.1621 K

! T_match = 1000.000000 jump

! Delta(Cp/R, H/RT, S/R) = (1.776e-15, 7.105e-15, 0.000e+00)

N2H3 120186N 2H 3 G 300.0000 5000.0000 1000.00 1
4.44184600e+00 7.21427100e-03-2.49568400e-06 3.92056500e-10-2.29895000e-14 2
1.66452716e+04-4.23073470e-01 2.65784686e+00 8.72895665e-03 2.48636948e-06 3
-6.98011085e-09 2.63643786e-12 1.73223998e+04 9.68717587e+00 4

! Refitting species N2H4:

! max difference Cp/R = 5.0874e-06 at T = 998.2991 K

! max difference H/RT = 5.3548e-06 at T = 1000.6503 K

! max difference S/R = 3.8025e-06 at T = 1000.6503 K

! T_match = 1000.000000 jump

! Delta(Cp/R, H/RT, S/R) = (-1.776e-15, 0.000e+00, 0.000e+00)

N2H4 121286N 2H 4 G 300.0000 5000.0000 1000.00 1
4.97731700e+00 9.59551900e-03-3.54763900e-06 6.12429900e-10-4.02979500e-14 2
9.34122436e+03-2.96298620e+00 6.44655703e-02 2.74970029e-02-2.89937434e-05 3
1.74515927e-08-4.42198880e-12 1.04519161e+04 2.12777259e+01 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/

!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

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!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 !

!

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

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

! DUPLICATE

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!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 !

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$\text{NH}_2 + \text{NH}_2 = \text{NH}_3 + \text{NH}$	5.6E00	3.530	552 !
$\text{NH}_2 + \text{NH} = \text{NH}_3 + \text{N}$	9.6E03	2.460	107 !
$\text{NH}_2 + \text{N} = \text{N}_2 + \text{H} + \text{H}$	7.0E13	0.000	0 !
$!\text{NH}_2 + \text{HNO} = \text{NH}_3 + \text{NO}$	3.6E06	1.630	-1250 !
$!\text{NH}_2 + \text{NO} = \text{N}_2 + \text{H}_2\text{O}$	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 !

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$\text{!N+O}_2=\text{NO+O}$	6.4E09	1.000	6280 !
$\text{!N+NO=N}_2\text{+O}$	9.4E12	0.140	0 !
$\text{NNH=N}_2\text{+H}$	1.0E09	0.000	0 !
$\text{NNH+H=N}_2\text{+H}_2$	1.0E14	0.000	0 !
$\text{!NNH+O=N}_2\text{O+H}$	1.9E14	-0.274	-22 !
$\text{!NNH+O=N}_2\text{+OH}$	1.2E13	0.145	-217 !
!NNH+O=NH+NO	5.2E11	0.381	-409 !
$\text{!NNH+OH=N}_2\text{+H}_2\text{O}$	5.0E13	0.000	0 !
$\text{!NNH+O}_2=\text{N}_2\text{+HO}_2$	5.6E14	-0.385	-13 !
$\text{NNH+NH}=\text{N}_2\text{+NH}_2$	5.0E13	0.000	0 !
$\text{NNH+NH}_2=\text{N}_2\text{+NH}_3$	5.0E13	0.000	0 !
$\text{!NNH+NO=N}_2\text{+HNO}$	5.0E13	0.000	0 !
$\text{!NH}_2\text{OH(+M)=NH}_2\text{+OH(+M)}$	1.4E20	-1.310	64080 !
$\text{! LOW /5.4E37 -5.96 66783/}$!
$\text{! TROE /0.31 1E-30 1E30 1E30/}$!
$\text{!NH}_2\text{OH+H=HNOH+H}_2$	4.8E08	1.50	6249 !
$\text{!NH}_2\text{OH+H=H}_2\text{NO+H}_2$	2.4E08	1.50	5067 !
$\text{!NH}_2\text{OH+O=HNOH+OH}$	3.3E08	1.50	3865 !
$\text{!NH}_2\text{OH+O=H}_2\text{NO+OH}$	1.7E08	1.50	3010 !
$\text{!NH}_2\text{OH+OH=HNOH+H}_2\text{O}$	1.5E04	2.61	-3537 !
$\text{!NH}_2\text{OH+OH=H}_2\text{NO+H}_2\text{O}$	1.5E05	2.28	-1296 !
$\text{!NH}_2\text{OH+NH}_2=\text{HNOH+NH}_3$	1.1E-1	4.00	-97 !
$\text{!NH}_2\text{OH+NH}_2=\text{H}_2\text{NO+NH}_3$	9.5E00	3.42	-1013 !
$\text{!NH}_2\text{OH+NH=HNOH+NH}_2$	2.9E-3	4.40	1564 !
$\text{!NH}_2\text{OH+NH=H}_2\text{NO+NH}_2$	1.5E-3	4.60	2424 !
$\text{!NH}_2\text{OH+HO}_2=\text{HNOH+H}_2\text{O}_2$	2.9E04	2.69	9557 !

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!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 !

!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 !

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!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 !
!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 !

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! 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 !
!NO2+OH(+M)=HONO2(+M) 3.0E13  0.000   0 !
! LOW /2.938E25 -3.0 0/
!

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! 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 !

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$\text{!HNOH}+\text{NH}_2=\text{H}_2\text{NN}+\text{H}_2\text{O}$ 8.8E16 -1.080 1113 !

$\text{NH}_2+\text{NH}_2(+\text{M})=\text{N}_2\text{H}_4(+\text{M})$ 5.6E14 -0.414 66 !

LOW /1.6E34 -5.49 1987/ !

TROE /0.31 1E-30 1E30 1E30/ !

$\text{N}_2\text{H}_4+\text{H}=\text{N}_2\text{H}_3+\text{H}_2$ 7.0E12 0.000 2500 !

$\text{!N}_2\text{H}_4+\text{O}=\text{NH}_2\text{OH}+\text{NH}$ 2.9E11 0.000 -1270 !

$\text{!N}_2\text{H}_4+\text{O}=\text{N}_2\text{H}_3+\text{OH}$ 1.5E11 0.000 -1270 !

$\text{!N}_2\text{H}_4+\text{OH}=\text{N}_2\text{H}_3+\text{H}_2\text{O}$ 1.3E13 0.000 -318 !

$\text{N}_2\text{H}_4+\text{NH}_2=\text{N}_2\text{H}_3+\text{NH}_3$ 3.9E12 0.000 1500 !

$\text{N}_2\text{H}_3=\text{N}_2\text{H}_2+\text{H}$ 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/

$\text{N}_2\text{H}_3+\text{H}=\text{N}_2\text{H}_2+\text{H}_2$ 2.4E08 1.500 -10 !

$\text{!N}_2\text{H}_3+\text{O}=\text{N}_2\text{H}_2+\text{OH}$ 1.7E08 1.500 -646 !

$\text{!N}_2\text{H}_3+\text{O}=\text{NH}_2+\text{HNO}$ 3.0E13 0.000 0 !

$\text{!N}_2\text{H}_3+\text{O}=>\text{NH}_2+\text{NO}+\text{H}$ 3.0E13 0.000 0 !

$\text{!N}_2\text{H}_3+\text{OH}=\text{N}_2\text{H}_2+\text{H}_2\text{O}$ 1.2E06 2.000 -1192 !

$\text{!N}_2\text{H}_3+\text{OH}=\text{H}_2\text{NN}+\text{H}_2\text{O}$ 3.0E13 0.000 0 !

$\text{!N}_2\text{H}_3+\text{OH}=\text{NH}_3+\text{HNO}$ 1.0E12 0.000 15000 !

$\text{!N}_2\text{H}_3+\text{HO}_2=\text{N}_2\text{H}_2+\text{H}_2\text{O}_2$ 1.4E04 2.690 -1600 !

$\text{!N}_2\text{H}_3+\text{HO}_2=\text{N}_2\text{H}_4+\text{O}_2$ 9.2E05 1.940 2126 !

$\text{N}_2\text{H}_3+\text{NH}_2=\text{N}_2\text{H}_2+\text{NH}_3$ 9.2E05 1.940 -1152 !

$\text{N}_2\text{H}_3+\text{NH}_2=\text{H}_2\text{NN}+\text{NH}_3$ 3.0E13 0.000 0 !

$\text{N}_2\text{H}_3+\text{NH}=\text{N}_2\text{H}_2+\text{NH}_2$ 2.0E13 0.000 0 !

$\text{N}_2\text{H}_2=\text{NNH}+\text{H}$ 1.8E40 -8.41 73320 !

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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 !

N2H2+NH=NNH+NH2 2.4E06 2.000 -1192 !

!N2H2+NO=N2O+NH2 4.0E12 0.000 11922 !

H2NN=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/

H2NN=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/

H2NN+H=NNH+H2 4.8E08 1.500 -894 !

H2NN+H=N2H2+H 7.0E13 0.000 0 !

!H2NN+O=NNH+OH 3.3E08 1.500 -894 !

!H2NN+O=NH2+NO 7.0E13 0.000 0 !

!H2NN+OH=NNH+H2O 2.4E06 2.000 -1192 !

!H2NN+OH=>NH2+NO+H 2.0E12 0.000 0 !

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!H2NN+HO2=>NH2+NO+OH 9.0E12 0.000 0 !

!H2NN+HO2=NNH+H2O2 2.9E04 2.690 -1600 !

!H2NN+O2=NH2+NO2 1.5E12 0.000 5961 !

H2NN+NH2=NNH+NH3 1.8E06 1.940 -1152 !

!

N2+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*+H2=OH+H2 2.95E12 0.5 -444 !

!OH*+O2=OH+O2 2.10E12 0.5 -482 !

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

!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