!! 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

! 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 0G 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 0G 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:

! 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 1/90O 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 RADI IU3/03O 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

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 0G 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

! 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

! 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 & 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:

! 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 0G 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 0G 200.0000 6000.0000 1000.00 1

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

! 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 0G 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 0G 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 0 0G 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

! 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
```

!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

```
!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 !

!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 5.0E14 -0.4 0 !

!NH+NO=N2+OH 2.7E12 -0.0721 -512 !

!NH+HONO=NH2+NO2 1.0E13 0.000 0 !

!NH+NO2=N2O+OH 4.1E12 0.000 0 !

!NH+NO2=HNO+NO 5.9E12 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 !

NNH=N2+H 1.0E09 0.000 0 !

NNH+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 -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 !

!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 !

!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 !

!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/                          !
 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 !

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 !
```

```
!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
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