```
units(length='cm', time='s', quantity='mol', act_energy='cal/mol')

ideal_gas(name='gas',
          elements="O H C N Ar He",
          species="""O  CO    O2   CO2""",
          reactions='all',
          transport='Mix',
          initial_state=state(temperature=300.0, pressure=OneAtm))

#-------------------------------------------------------------------------------
# Species data
#-------------------------------------------------------------------------------


species(name='H2',
        atoms='H:2',
        thermo=(NASA([200.00, 1000.00],
                     [ 2.34433112E+00,  7.98052075E-03, -1.94781510E-05,
                       2.01572094E-08, -7.37611761E-12, -9.17935173E+02,
                       6.83010238E-01]),
                NASA([1000.00, 3500.00],
                     [ 3.33727920E+00, -4.94024731E-05,  4.99456778E-07,
                      -1.79566394E-10,  2.00255376E-14, -9.50158922E+02,
                      -3.20502331E+00])),
        transport=gas_transport(geom='linear',
                                diam=2.92,
                                well_depth=38.0,
                                polar=0.79,
                                rot_relax=280.0),
        note='TPIS78')

species(name='H',
        atoms='H:1',
        thermo=(NASA([200.00, 1000.00],
                     [ 2.50000000E+00,  7.05332819E-13, -1.99591964E-15,
                       2.30081632E-18, -9.27732332E-22,  2.54736599E+04,
                      -4.46682853E-01]),
                NASA([1000.00, 3500.00],
                     [ 2.50000001E+00, -2.30842973E-11,  1.61561948E-14,
                      -4.73515235E-18,  4.98197357E-22,  2.54736599E+04,
                      -4.46682914E-01])),
        transport=gas_transport(geom='atom',
                                diam=2.05,
                                well_depth=145.0),
        note='L7/88')

species(name='AR',
        atoms='Ar:1',
        thermo=(NASA([300.00, 1000.00],
                     [ 2.50000000E+00,  0.00000000E+00,  0.00000000E+00,
```

```
                      0.00000000E+00,  0.00000000E+00, -7.45375000E+02,
                      4.36600000E+00]),
             NASA([1000.00, 5000.00],
                  [ 2.50000000E+00,  0.00000000E+00,  0.00000000E+00,
                      0.00000000E+00,  0.00000000E+00, -7.45375000E+02,
                      4.36600000E+00])),
        transport=gas_transport(geom='atom',
                                diam=3.33,
                                well_depth=136.5),
        note='120186')

species(name='N2',
        atoms='N:2',
        thermo=(NASA([300.00, 1000.00],
                  [ 3.29867700E+00,  1.40824040E-03, -3.96322200E-06,
                    5.64151500E-09, -2.44485400E-12, -1.02089990E+03,
                    3.95037200E+00]),
                NASA([1000.00, 5000.00],
                  [ 2.92664000E+00,  1.48797680E-03, -5.68476000E-07,
                    1.00970380E-10, -6.75335100E-15, -9.22797700E+02,
                    5.98052800E+00])),
        transport=gas_transport(geom='linear',
                                diam=3.621,
                                well_depth=97.53,
                                polar=1.76,
                                rot_relax=4.0),
        note='121286')

species(name='HE',
        atoms='He:1',
        thermo=(NASA([200.00, 1000.00],
                  [ 2.50000000E+00,  0.00000000E+00,  0.00000000E+00,
                    0.00000000E+00,  0.00000000E+00, -7.45375000E+02,
                    9.28723974E-01]),
                NASA([1000.00, 6000.00],
                  [ 2.50000000E+00,  0.00000000E+00,  0.00000000E+00,
                    0.00000000E+00,  0.00000000E+00, -7.45375000E+02,
                    9.28723974E-01])),
        transport=gas_transport(geom='atom',
                                diam=2.576,
                                well_depth=10.2),
        note='L10/90')

species(name='O',
        atoms='O:1',
        thermo=(NASA([200.00, 1000.00],
                  [ 3.16826710E+00, -3.27931884E-03,  6.64306396E-06,
                   -6.12806624E-09,  2.11265971E-12,  2.91222592E+04,
                    2.05193346E+00]),
                NASA([1000.00, 3500.00],
```

```
                    [ 2.56942078E+00, -8.59741137E-05,  4.19484589E-08,
                     -1.00177799E-11,  1.22833691E-15,  2.92175791E+04,
                      4.78433864E+00])),
        transport=gas_transport(geom='atom',
                                diam=2.75,
                                well_depth=80.0),
        note='L1/90')

species(name='OH',
        atoms='H:1 O:1',
        thermo=(NASA([200.00, 1000.00],
                    [ 4.12530561E+00, -3.22544939E-03,  6.52764691E-06,
                     -5.79853643E-09,  2.06237379E-12,  3.38153812E+03,
                     -6.90432960E-01]),
                NASA([1000.00, 6000.00],
                    [ 2.86472886E+00,  1.05650448E-03, -2.59082758E-07,
                      3.05218674E-11, -1.33195876E-15,  3.71885774E+03,
                      5.70164073E+00])),
        transport=gas_transport(geom='linear',
                                diam=2.75,
                                well_depth=80.0),
        note='S9/01')

species(name='HCO',
        atoms='H:1 C:1 O:1',
        thermo=(NASA([200.00, 1000.00],
                    [ 4.22118584E+00, -3.24392532E-03,  1.37799446E-05,
                     -1.33144093E-08,  4.33768865E-12,  3.83956496E+03,
                      3.39437243E+00]),
                NASA([1000.00, 3500.00],
                    [ 2.77217438E+00,  4.95695526E-03, -2.48445613E-06,
                      5.89161778E-10, -5.33508711E-14,  4.01191815E+03,
                      9.79834492E+00])),
        transport=gas_transport(geom='nonlinear',
                                diam=3.59,
                                well_depth=498.0),
        note='L12/89')

species(name='HO2',
        atoms='H:1 O:2',
        thermo=(NASA([200.00, 1000.00],
                    [ 4.30179801E+00, -4.74912051E-03,  2.11582891E-05,
                     -2.42763894E-08,  9.29225124E-12,  2.94808040E+02,
                      3.71666245E+00]),
                NASA([1000.00, 3500.00],
                    [ 4.01721090E+00,  2.23982013E-03, -6.33658150E-07,
                      1.14246370E-10, -1.07908535E-14,  1.11856713E+02,
                      3.78510215E+00])),
        transport=gas_transport(geom='nonlinear',
                                diam=3.458,
```

```
                               well_depth=107.4,
                               rot_relax=1.0),
        note='L5/89')

species(name='H2O',
        atoms='H:2 O:1',
        thermo=(NASA([200.00, 1000.00],
                     [ 4.19864056E+00, -2.03643410E-03,  6.52040211E-06,
                      -5.48797062E-09,  1.77197817E-12, -3.02937267E+04,
                      -8.49032208E-01]),
                NASA([1000.00, 3500.00],
                     [ 3.03399249E+00,  2.17691804E-03, -1.64072518E-07,
                      -9.70419870E-11,  1.68200992E-14, -3.00042971E+04,
                       4.96677010E+00])),
        transport=gas_transport(geom='nonlinear',
                               diam=2.605,
                               well_depth=572.4,
                               dipole=1.844,
                               rot_relax=4.0),
        note='L8/89')

species(name='CO',
        atoms='C:1 O:1',
        thermo=(NASA([200.00, 1000.00],
                     [ 3.57953347E+00, -6.10353680E-04,  1.01681433E-06,
                       9.07005884E-10, -9.04424499E-13, -1.43440860E+04,
                       3.50840928E+00]),
                NASA([1000.00, 3500.00],
                     [ 2.71518561E+00,  2.06252743E-03, -9.98825771E-07,
                       2.30053008E-10, -2.03647716E-14, -1.41518724E+04,
                       7.81868772E+00])),
        transport=gas_transport(geom='linear',
                               diam=3.65,
                               well_depth=98.1,
                               polar=1.95,
                               rot_relax=1.8),
        note='TPIS79')

species(name='O2',
        atoms='O:2',
        thermo=(NASA([200.00, 1000.00],
                     [ 3.78245636E+00, -2.99673416E-03,  9.84730201E-06,
                      -9.68129509E-09,  3.24372837E-12, -1.06394356E+03,
                       3.65767573E+00]),
                NASA([1000.00, 3500.00],
                     [ 3.28253784E+00,  1.48308754E-03, -7.57966669E-07,
                       2.09470555E-10, -2.16717794E-14, -1.08845772E+03,
                       5.45323129E+00])),
        transport=gas_transport(geom='linear',
                               diam=3.458,
```

```
                               well_depth=107.4,
                               polar=1.6,
                               rot_relax=3.8),
        note='TPIS89')

species(name='H2O2',
        atoms='H:2 O:2',
        thermo=(NASA([200.00, 1000.00],
                     [ 4.27611269E+00, -5.42822417E-04,  1.67335701E-05,
                      -2.15770813E-08,  8.62454363E-12, -1.77025821E+04,
                       3.43505074E+00]),
                NASA([1000.00, 3500.00],
                     [ 4.16500285E+00,  4.90831694E-03, -1.90139225E-06,
                       3.71185986E-10, -2.87908305E-14, -1.78617877E+04,
                       2.91615662E+00])),
        transport=gas_transport(geom='nonlinear',
                               diam=3.458,
                               well_depth=107.4,
                               rot_relax=3.8),
        note='L7/88')

species(name='CO2',
        atoms='C:1 O:2',
        thermo=(NASA([200.00, 1000.00],
                     [ 2.35677352E+00,  8.98459677E-03, -7.12356269E-06,
                       2.45919022E-09, -1.43699548E-13, -4.83719697E+04,
                       9.90105222E+00]),
                NASA([1000.00, 3500.00],
                     [ 3.85746029E+00,  4.41437026E-03, -2.21481404E-06,
                       5.23490188E-10, -4.72084164E-14, -4.87591660E+04,
                       2.27163806E+00])),
        transport=gas_transport(geom='linear',
                               diam=3.763,
                               well_depth=244.0,
                               polar=2.65,
                               rot_relax=2.1),
        note='L7/88')


#-----------------------------------------------------------------------------
# Reaction data
#-----------------------------------------------------------------------------

falloff_reaction('CO + O (+ M) <=> CO2 (+ M)',
                 kf=[1.362000e+10, 0.0, 2384.0],
                 kf0=[1.173000e+24, -2.79, 4191.0],
                 efficiencies='CO2:3.6 CO:1.75')
# 99MUE/KIM * 0.76

reaction('CO + O2 <=> CO2 + O', [1.119000e+12, 0.0, 47700.0])
```

```
# 86TSA/HAM * 0.44

three_body_reaction('O + O + M <=> O2 + M', [1.200000e+17, -1.0, 0.0],
                    efficiencies='CO2:3.6 CO:1.75')
```