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Ignition by moving hot spheres in H_2-O_2-N_2 environments: Supplementary Materials Proc. Combust. Inst. 37, 2017

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1 Additional Schematics

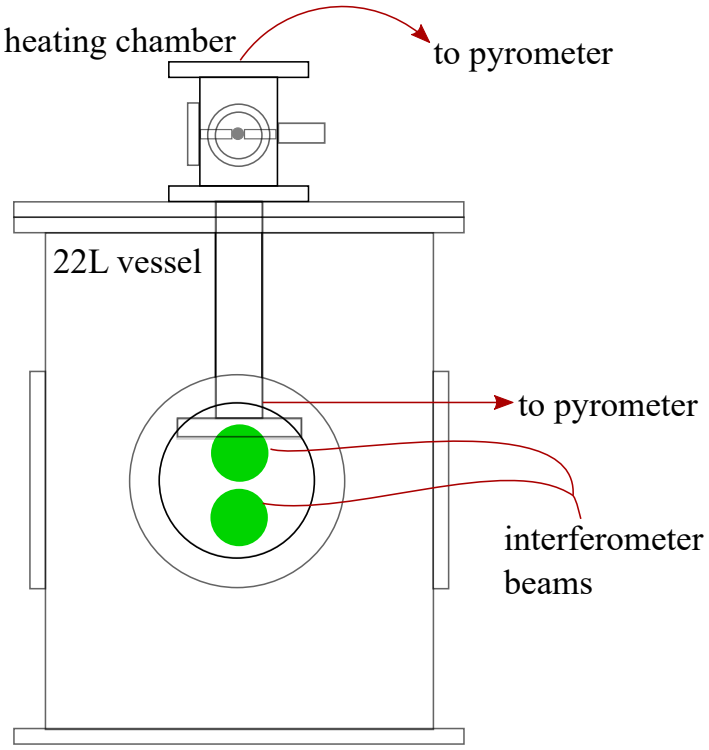

Figure S1: Combustion vessel showing heating chamber and location of pyrometer temperature readings as described in Section 2 of the manuscript.

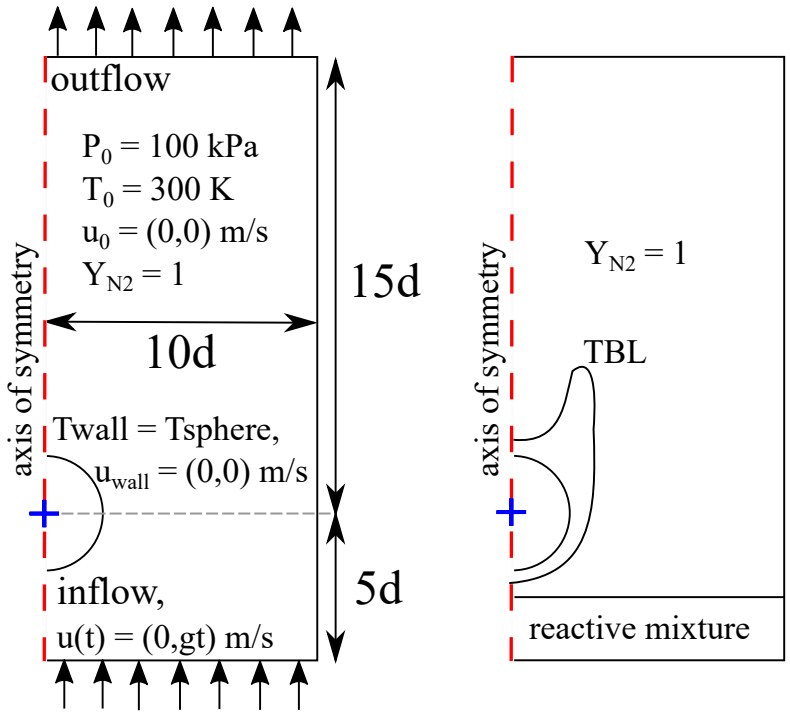

Figure S2: Schematic of the computational setup including the initial and boundary conditions described in Section 3 of the manuscript.

2 Temperature Fields

2.1 Lean Mixture

The ignition sequence in Figure S3 is taken from shot 21, $\Phi = 0.39$, $\beta = 2.97$, $T_{sphere} = 987$ K. Before ignition, the experimental and numerical temperature fields are in good agreement. At $t = t_{ign}$, the experimental ignition kernel appears to originate at a slightly larger θ than seen in the simulation, and this slight discrepancy in ignition location is a possible cause of the larger error seen in the boundary layer profiles at $\theta = \pi/2$ in Figure S3b. At $t=t_{ign} + 0.2$ ms, the flame has begun to propagate away from the sphere, and it can be observed despite the noise from processing a single frame that the flame temperature measured experimentally is similar to that predicted numerically, with the average temperature in the flame region reaching 1737 K in the experiments and a flame temperature of 1918 K in the simulations.

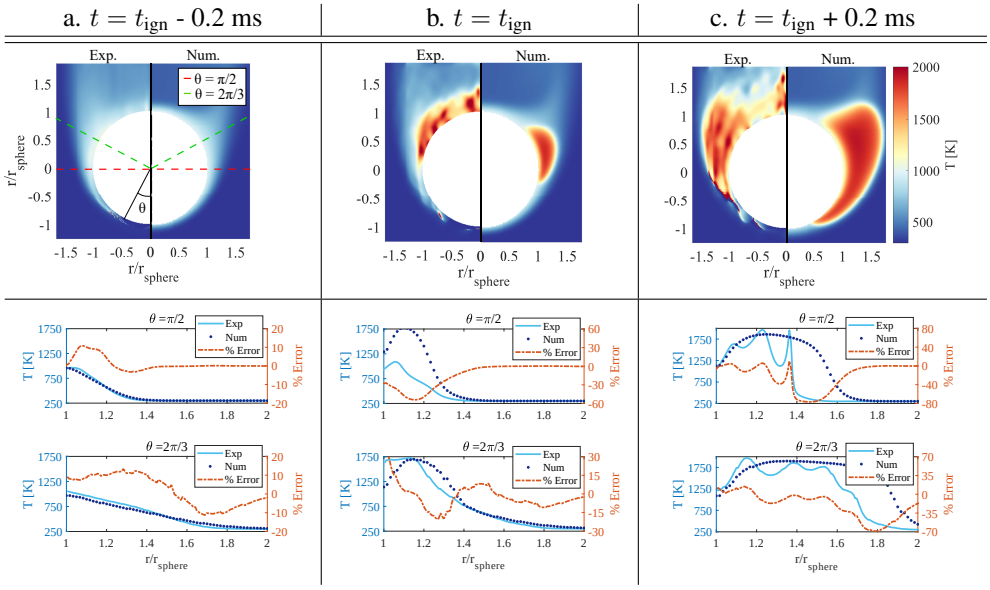

Figure S3: Ignition dynamics for $\Phi = 0.39$, $\beta = 2.97$: a. shortly before ignition, t = t_{ign} - 0.2 ms; b. at ignition, t = t_{ign}; and c. during early stages of flame propagation, t = t_{ign} + 0.2 ms. Length scale, $r_{sphere} = 3$ mm. Top row: experimental ($T_{sphere} = 987 \pm 30$ K) and numerically predicted ($T_{sphere} = 980$ K) gas temperature fields. All temperature fields share a common colorbar, shown in Fig. 2c (top row). Bottom row: comparison of experimental and numerical thermal boundary layer and error profiles at $\theta = \pi/2$ (top) and $2\pi/3$ (bottom).

2.2 Rich Mixture

The ignition sequence in Figure S4 is taken from shot 23, $\Phi = 1.35$, $\beta = 11.84$, $T_{sphere} = 1014$ K. Before ignition, there is good agreement in the profiles of the thermal boundary layer around the sphere at angles $\pi/2$ and $2\pi/3$ from the front stagnation point. At t = t_{ign}, the agreement continues to be excellent. Finally, at t = t_{ign} + 0.2 ms, the average flame temperature as measured by the experiments is 1275 K and the max flame temperature predicted in the simulations was 1394 K. Note that the front stagnation point of the sphere is cut off in Figure S4. This is because the sphere ignited close to the bottom of the field of view, and therefore to keep the sphere placement uniform in the images the very front of the sphere is not shown. The region of where ignition takes place (near flow separation) is far from the front stagnation point.

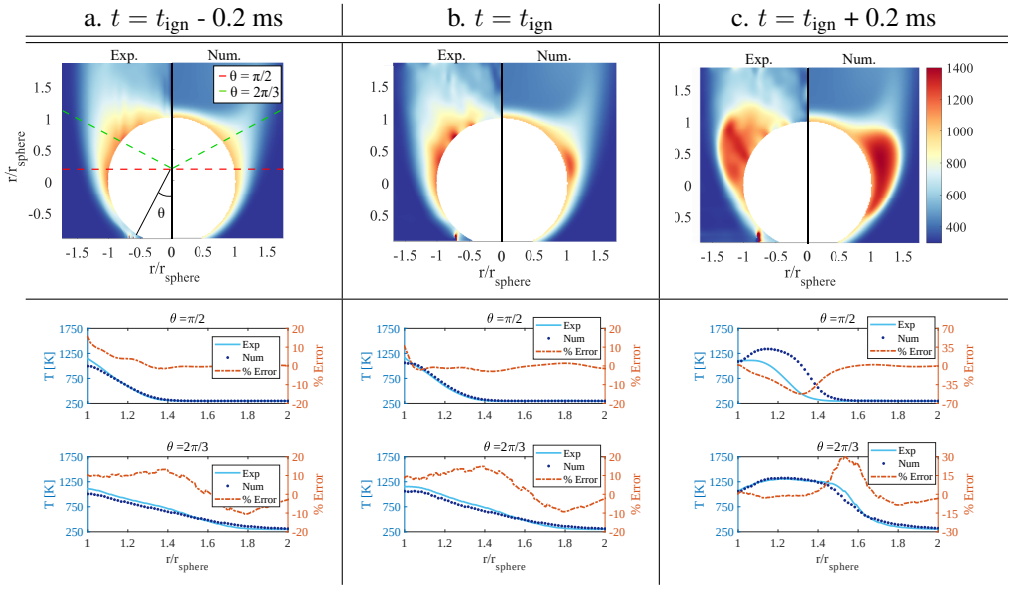

Figure S4: Ignition dynamics for $\Phi = 1.35$, $\beta = 11.84$: a. shortly before ignition, t = t_{ign} - 0.2 ms; b. at ignition, t = t_{ign}; and c. during early stages of flame propagation, t = t_{ign} + 0.2 ms. Length scale, $r_{sphere} = 3$ mm. Top row: experimental ($T_{sphere} = 1014 \pm 30$ K) and numerically predicted ($T_{sphere} = 1020$ K) gas temperature fields. All temperature fields share a common colorbar, shown in Fig. 2c (top row). Bottom row: comparison of experimental and numerical thermal boundary layer and error profiles at $\theta = \pi/2$ (top) and $2\pi/3$ (bottom).

3 Kinetic Mechanisms

Enclosed are the Mével and Konnov kinetic mechanisms used in the numerical work. GRI-Mech 3.0 is readily accessible and can be found at http://combustion.berkeley.edu/gri-mech/version30/text30.html.

3.1 Mével

H2chemMevel:

```
ELEMENTS
H O N AR
END
SPECIES
H2 O2 O H2O H OH HO2 H2O2 N2
END
REACTIONS
! H2 REACTIONS
```

```
H2+M=H+H+M                4.57E+19  -1.40   105100
H2/2.5/ H2O/12/
! O REACTIONS
O+H2=H+OH                 5.08E+04   2.67   6.290E+03
O+O+M=O2+M                6.17E+15  -0.50   0.000E+00
H2/2.5/ H2O/12/
! H REACTIONS
H+O2=O+OH                 1.91E+14  0.00   1.6439E+04
H+O2(+M)=HO2(+M)          1.48E+12  0.60  0.00E+00
LOW/3.482E+16  -0.411  -1.12E+03/
TROE/0.5  1E-30  1E30  1E100/
H2/1.3/ H2O/14/
H+O+M=OH+M                4.72E+18  -1.00   0.000E+00
H2/2.5/ H2O/12/
! OH REACTIONS
OH+H2=H2O+H               2.16E+08   1.51   3.430E+03
H2O+O=OH+OH               2.97E6     2.02   1.340E+04
H2O2(+M)=OH+OH(+M)        2.95E+14   0.00   48.4E+03
LOW/1.27E+17 0.00 45.5E+03/
TROE/0.5 1E-30 1E+30 1E100/
H2/2.5/ H2O/12/
OH+H+M=H2O+M              4.5E+22  -2.00   0.000E+00
H2/0.73/ H2O/12/
! HO2 REACTIONS
HO2+O=O2+OH               0.325E+14  0.00   0.00E+00
HO2+H=H2+O2               1.66E+13   0.00   0.82E+03
HO2+H=OH+OH               7.08E+13   0.00   3E+02
HO2+OH=H2O+O2             2.89E+13   0.00  -5E+02
HO2+HO2=H2O2+O2           4.20E+14   0.00   1.198E+04
DUP
HO2+HO2=H2O2+O2           1.30E+11   0.00  -1.629E+03
DUP
! H2O2 REACTIONS
H2O2+O=OH+HO2             9.55E+06   2.00   3.970E+03
H2O2+H=H2O+OH             0.241E+14  0.00  0.397E+04
H2O2+H=HO2+H2             6.03E+13   0.00   7.950E+03
H2O2+OH=H2O+HO2           1.00E+12    0.00   0.00E+00
DUP
H2O2+OH=H2O+HO2           5.80E+14    0.00   9.56E+03
DUP
END
```

therm.dat:

```
THERMO ALL
200.000  1000.000  7000.000
O2                121386O   2               G  0200.00   7000.00  1000.00      1
0.03697578E+02 0.06135197E-02-0.01258842E-05 0.01775281E-09-0.01136435E-13     2
-0.01233930E+05 0.03189166E+02 0.03212936E+02 0.01127486E-01-0.05756150E-05    3
0.01313877E-07-0.08768554E-11-0.01005249E+05 0.06034738E+02                    4
O                 120186O   1               G  0200.00   7000.00  1000.00      1
0.02542060E+02-0.02755062E-03-0.03102803E-07 0.04551067E-10-0.04368052E-14     2
0.02923080E+06 0.04920308E+02 0.02946429E+02-0.01638166E-01 0.02421032E-04     3
-0.01602843E-07 0.03890696E-11 0.02914764E+06 0.02963995E+02                   4
OH                121286O   1H   1          G  0200.00   7000.00  1000.00      1
0.02882730E+02 0.01013974E-01-0.02276877E-05 0.02174684E-09-0.05126305E-14     2
```

```
0.03886888E+05 0.05595712E+02 0.03637266E+02 0.01850910E-02-0.01676165E-04     3
0.02387203E-07-0.08431442E-11 0.03606782E+05 0.01358860E+02                    4
H2O2              120186H   2O   2          G  0200.00   7000.00  1000.00      1
0.04573167E+02 0.04336136E-01-0.01474689E-04 0.02348904E-08-0.01431654E-12     2
-0.01800696E+06 0.05011370E+01 0.03388754E+02 0.06569226E-01-0.01485013E-05    3
-0.04625806E-07 0.02471515E-10-0.01766315E+06 0.06785363E+02                   4
HO2                20387H   1O   2          G  0200.00   7000.00  1000.00      1
0.04072191E+02 0.02131296E-01-0.05308145E-05 0.06112269E-09-0.02841165E-13     2
-0.01579727E+04 0.03476029E+02 0.02979963E+02 0.04996697E-01-0.03790997E-04    3
0.02354192E-07-0.08089024E-11 0.01762274E+04 0.09222724E+02                    4
H2O                20387H   2O   1          G  0200.00   7000.00  1000.00      1
0.02672146E+02 0.03056293E-01-0.08730260E-05 0.01200996E-08-0.06391618E-13     2
-0.02989921E+06 0.06862817E+02 0.03386842E+02 0.03474982E-01-0.06354696E-04    3
0.06968581E-07-0.02506588E-10-0.03020811E+06 0.02590233E+02                    4
H2                121286H   2               G  0200.00   7000.00  1000.00      1
0.02991423E+02 0.07000644E-02-0.05633829E-06-0.09231578E-10 0.01582752E-13     2
-0.08350340E+04-0.01355110E+02 0.03298124E+02 0.08249442E-02-0.08143015E-05    3
-0.09475434E-09 0.04134872E-11-0.01012521E+05-0.03294094E+02                   4
N2                121286N   2               G  0200.00   7000.00  1000.00      1
0.02926640E+02 0.01487977E-01-0.05684761E-05 0.01009704E-08-0.06753351E-13     2
-0.09227977E+04 0.05980528E+02 0.03298677E+02 0.01408240E-01-0.03963222E-04    3
0.05641515E-07-0.02444855E-10-0.01020900E+05 0.03950372E+02                    4
H                 120186H   1               G  0200.00   7000.00  1000.00      1
0.02500000E+02 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00     2
0.02547163E+06-0.04601176E+01 0.02500000E+02 0.00000000E+00 0.00000000E+00     3
0.00000000E+00 0.00000000E+00 0.02547163E+06-0.04601176E+01                    4
END
```

trans.dat:

```
H                  0   145.000     2.050     0.000     0.000     0.000
H2                 1    38.000     2.920     0.000     0.790   280.000
H2O                2   572.400     2.605     1.844     0.000     4.000
H2O2               2   107.400     3.458     0.000     0.000     3.800
HO2                2   107.400     3.458     0.000     0.000     1.000
N                  0    71.400     3.298     0.000     0.000     0.000
N2                 1    97.530     3.621     0.000     1.760     4.
O                  0    80.000     2.750     0.000     0.000     0.000
O2                 1   107.400     3.458     0.000     1.600     3.800
OH                 1    80.000     2.750     0.000     0.000     0.000
```

3.2 Konnov

chemKonnov:

```
ELEMENTS
O  H  N
END
SPECIES
H2 O2 O H2O H OH HO2 H2O2 N2
END
!REACTIONS         BASE M=N2
REACTIONS
```

```
H+H+M=H2+M                        7.000E+17     -1.0         0.0
H2/0.0/ N2/0.0/ H/0.0/ H2O/14.3/
H+H+H2=H2+H2                      1.000E+17     -0.6         0.0
H+H+N2=H2+N2                      5.400E+18     -1.3         0.0
H+H+H=H2+H                        3.200E+15      0.0         0.0
O+O+M=O2+M                        1.000E+17     -1.0         0.0
O/71.0/ O2/20.0/ N2/5.0/
O+H+M=OH+M                        6.200E+16     -0.6         0.0
H2O/5.0/
H2+O2=OH+OH                       2.500E+12      0.0     39000.0
O+H2=OH+H                         5.060E+04      2.67     6290.0
H+O2=OH+O                         9.750E+13      0.0     14850.0
H+O2(+M)=HO2(+M)                  1.480E+12      0.6         0.0
LOW /3.50E+16 -0.41 -1116.0/
TROE /0.5 100000 10/
H2O/10.6/ H2/1.5/
H+OH+M=H2O+M                      2.200E+22     -2.0         0.0
H2O/6.4/
H2+OH=H2O+H                       1.000E+08      1.6      3300.0
OH+OH=H2O+O                       1.500E+09      1.14      100.0
HO2+OH=H2O+O2                     2.890E+13      0.0      -500.0
HO2+O=OH+O2                       1.630E+13      0.0      -445.0
H+HO2=H2+O2                       4.280E+13      0.0      1411.0
H+HO2=OH+OH                       1.700E+14      0.0       875.0
H+HO2=H2O+O                       3.000E+13      0.0      1720.0
HO2+HO2=H2O2+O2                   4.200E+14      0.0     12000.0
DUPLICATE
HO2+HO2=H2O2+O2                   1.300E+11      0.0     -1640.0
DUPLICATE
OH+OH(+M)=H2O2(+M)                7.200E+13     -0.37        0.0
LOW /2.2E+19 -0.76 0.0/
TROE /0.5 100000 10/
H2O/0.0/
OH+OH(+H2O)=H2O2(+H2O)            7.200E+13     -0.37        0.0
LOW /1.45E+18 0.0 0.0/
H2O2+OH=HO2+H2O                   1.000E+12      0.0         0.0
DUPLICATE
H2O2+OH=HO2+H2O                   5.800E+14      0.0      9560.0
DUPLICATE
H2O2+H=HO2+H2                     1.700E+12      0.0      3755.0
H2O2+H=H2O+OH                     1.000E+13      0.0      3575.0
H2O2+O=HO2+OH                     2.800E+13      0.0      6400.0

END
```

therm.dat:

```
THERMO ALL
200.000  1000.000  7000.000
O2                121386O   2               G  0200.00   7000.00  1000.00      1
0.03697578E+02 0.06135197E-02-0.01258842E-05 0.01775281E-09-0.01136435E-13     2
-0.01233930E+05 0.03189166E+02 0.03212936E+02 0.01127486E-01-0.05756150E-05    3
0.01313877E-07-0.08768554E-11-0.01005249E+05 0.06034738E+02                    4
O                 120186O   1               G  0200.00   7000.00  1000.00      1
0.02542060E+02-0.02755062E-03-0.03102803E-07 0.04551067E-10-0.04368052E-14     2
```

```
0.02923080E+06 0.04920308E+02 0.02946429E+02-0.01638166E-01 0.02421032E-04     3
-0.01602843E-07 0.03890696E-11 0.02914764E+06 0.02963995E+02                    4
OH                120286O   1H   1          G  0200.00   7000.00  1000.00      1
0.02882730E+02 0.01013974E-01-0.02276877E-05 0.02174684E-09-0.05126305E-14     2
0.03886888E+05 0.05595712E+02 0.03637266E+02 0.01850910E-02-0.01676165E-04     3
0.02387203E-07-0.08431442E-11 0.03606782E+05 0.01358860E+02                    4
H2O2              120186H   2O   2          G  0200.00   7000.00  1000.00      1
0.04573167E+02 0.04336136E-01-0.01474689E-04 0.02348904E-08-0.01431654E-12     2
-0.01800696E+06 0.05011370E+01 0.03388754E+02 0.06569226E-01-0.01485013E-05    3
-0.04625806E-07 0.02471515E-10-0.01766315E+06 0.06785363E+02                    4
HO2                20387H   1O   2          G  0200.00   7000.00  1000.00      1
0.04072191E+02 0.02131296E-01-0.05308145E-05 0.06112269E-09-0.02841165E-13     2
-0.01579727E+04 0.03476029E+02 0.02979963E+02 0.04996697E-01-0.03790997E-04    3
0.02354192E-07-0.08089024E-11 0.01762274E+04 0.09222724E+02                    4
H2O                20387H   2O   1          G  0200.00   7000.00  1000.00      1
0.02672146E+02 0.03056293E-01-0.08730260E-05 0.01200996E-08-0.06391618E-13     2
-0.02989921E+06 0.06862817E+02 0.03386842E+02 0.03474982E-01-0.06354696E-04    3
0.06968581E-07-0.02506588E-10-0.03020811E+06 0.02590233E+02                    4
H2                121286H   2               G  0200.00   7000.00  1000.00      1
0.02991423E+02 0.07000644E-02-0.05633829E-06-0.09231578E-10 0.01582752E-13     2
-0.08350340E+04-0.01355110E+02 0.03298124E+02 0.08249442E-02-0.08143015E-05    3
-0.09475434E-09 0.04134872E-11-0.01012521E+05-0.03294094E+02                    4
N2                121286N   2               G  0200.00   7000.00  1000.00      1
0.02926640E+02 0.01487977E-01-0.05684761E-05 0.01009704E-08-0.06753351E-13     2
-0.09227977E+04 0.05980528E+02 0.03298677E+02 0.01408240E-01-0.03963222E-04    3
0.05641515E-07-0.02444855E-10-0.01020900E+05 0.03950372E+02                    4
H                 120186H   1               G  0200.00   7000.00  1000.00      1
0.02500000E+02 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00     2
0.02547163E+06-0.04601176E+01 0.02500000E+02 0.00000000E+00 0.00000000E+00     3
0.00000000E+00 0.00000000E+00 0.02547163E+06-0.04601176E+01                    4
END
```

trans.dat:

```
H                    0   145.000     2.050     0.000     0.000     0.000
H2                   1    38.000     2.920     0.000     0.790   280.000
H2O                  2   572.400     2.605     1.844     0.000     4.000
H2O2                 2   107.400     3.458     0.000     0.000     3.800
HO2                  2   107.400     3.458     0.000     0.000     1.000
N2                   1    97.530     3.621     0.000     1.760     4.000
O                    0    80.000     2.750     0.000     0.000     0.000
O2                   1   107.400     3.458     0.000     1.600     3.800
OH                   1    80.000     2.750     0.000     0.000     0.000
```