Input file for the TRAPRB code [Jarmain&McCallum1970]

Variable descriptions found in program “FCF486.FOR” (sent by Prof. Amaury)

```
C...  NI = 0 ALLOWS DENSITY GRAPHS TO BE PRODUCED.OTHER VALUES DO NO
C...  NS  GIVES ORTHOGONALITY TEST IF = 1
C...  IGRAPH
C...  IENERG
C...  ISTATE = 2 FOR A TRANSITION = 1 FOR A SINGLE STATE
C...  RMIN   MINIMUM RADIUS FOR CALCULATION OF WAVEFUNCTIONS
C...  RMAX   MAXIMUM RADIUS FOR CALCULATION OF WAVEFUNCTIONS
C...  DELR   RADIAL INTERVAL FOR CALCULATION OF WAVEFUNCTIONS
C...  MAXV   MAXIMUM QUANTUM NUMBER FOR CALCULATION OF RESULTS
C...  BE     EQUILBRIUM ROTATIONAL CONSTANT
C...  DE     DISSOCIATION ENERGY OR ESTIMATE THEREOF
C...  KDMAXV MAXIMUM QUANTUM NUMBER FOR CALCULATION OF KLEIN DUNHAM
C...         POTENTIAL.MUST BE AT LEAST 2 AND NOT MORE THAN 30
C...  NEIG   USED FOR WORK IN THE CONTINUUM, NUMBER OF ENERGY LEVELS
C...         TO CALCULATE CONTINUUM WAVEFUNCTIONS AT


C...  READ IN EXPERIMENTAL EIGENVALUES AND ROTATIONAL CONSTANTS

(JT) EV: experimental eigenvalues (dimension 32 in program, but only 14 values present in file)
(JT) BV: rotational constants (dimension 32 in program, but only 14 values present in file)
```

Annotated input file (“oh.dat”)

Green – found in NIST Chemistry Web Book

```
                                                      ISTATE
                                                  IENERG  |
                                              IGRAPH  |   |
                                           NI NS  |   |   |
TITLE--------------------------------------  |  |  |   |   |
1  OH A DOUBLET SIGMA UPPER STATE             0  1  0   0   2

ZMU-------RMIN------RMAX------DELR------
0.9480871     0.750     3.500     0.005


MAXV
---       BE        DE                                    KDMAXV NEIG
  |       ----------==========                                ===---
 12           17.358  35000.00                                   12

EV(32)
     00.00   1565.99   4554.82   7351.07   9959.53  12392.75  14671.06  16822.54
  18883.03  20896.17  22913.33  24993.67  27204.10  29619.32

BV(32)
   17.3580   16.9606   16.1418   15.2910   14.4082   13.4934   12.5466   11.5678
   10.5570    9.5142    8.4394    7.3326    6.1938    5.0230

FINAL STATE: SAME STRUCTURE AS BEFORE
1  OH X DOUBLET PI  GROUND STATE                   0  1  0  0  2
0.9480871      0.650   3.500     0.005
 12          18.9108  39162.18                                  12
      0.00   1847.73   5417.37   8821.40  12061.76  15139.53  18054.80  20806.55
  23392.49  25808.94  28050.69  30110.87  31980.82  33649.91


   18.9108   18.5504   17.8387   17.1366   16.4411   15.7493   15.0581   14.3645
   13.6655   12.9581   12.2394   11.5063   10.7557    9.9849
```