H2calculated_296K_CutOff_1E-34.txt

Supplementary Material attached to the paper: The vibrational absorption spectrum of H2:
CRDS measurements of the (2-0) band, review of the literature data and accurate ab initio line list up to 35000 cm-1

by

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Calculated list of the H2 transitions between 0 and 35000 cm-1 at T=296K.
The intensity cut off was fixed to 1E-34 cm/molecule.

(1) Rovibrational assignment
(2) Line position (cm-1). The number in parenthesis is the unceratinty in the unit of the last quoted digit.
(3) Transition moment (in atomic unit)
(4) Einstein coefficient (in Hz)
(5) Rotational branch
(6) Lower state energy level (cm-1)
(7) Boltzmann factor
(8) Line stength at 296 K in cm/molecule for pure H2 (100% isotopic abundance)

| (1) | (2) | (3) | (4) | (5) | (6) | (7) | (8) |
|---|---|---|---|---|---|---|---|
| (v",J") <- (v',J') | Pos (cm-1) | <v'J'\|M(R)\|v"J"> | A(Hz) | Branch | E(J') | PJ(T) | Intensity |
| ( 0,2) <- ( 0,0) | 354.37313 ( 3) | 4.8471E-1 | 2.940976E-11 | S | 0.0000 | 0.130361 | 2.026E-28 |
| ( 0,3) <- ( 0,1) | 587.03202 ( 4) | 4.8683E-1 | 4.758133E-10 | S | 118.4869 | 0.659573 | 2.820E-27 |
| ( 0,4) <- ( 0,2) | 814.42430 ( 6) | 4.9000E-1 | 2.752855E-09 | S | 354.3732 | 0.116421 | 1.154E-27 |
| ( 0,5) <- ( 0,3) | 1034.67068 ( 8) | 4.9422E-1 | 9.829497E-09 | S | 705.5189 | 0.088718 | 1.699E-27 |
| ( 0,6) <- ( 0,4) | 1246.09954 ( 9) | 4.9945E-1 | 2.641379E-08 | S | 1168.7975 | 0.004000 | 1.304E-28 |
| ( 0,7) <- ( 0,5) | 1447.28093 (11) | 5.0570E-1 | 5.875555E-08 | S | 1740.1896 | 0.000912 | 4.631E-29 |
| ( 0,8) <- ( 0,6) | 1637.04600 (13) | 5.1292E-1 | 1.141155E-07 | S | 2414.8970 | 0.000014 | 9.999E-31 |
| ( 0,9) <- ( 0,7) | 1814.49237 (14) | 5.2111E-1 | 2.000078E-07 | S | 3187.4705 | 0.000001 | 1.119E-31 |
| ( 0,0) <- ( 0,8) | 1978.97726 (15) | 5.3022E-1 | 3.233529E-07 | S | 4051.9430 | 0.000000 | 8.385E-34 |
| ( 1,5) <- ( 0,7) | 2626.4512 ( 8) | 1.3113E-1 | 1.060395E-07 | O | 3187.4705 | 0.000001 | 1.639E-32 |
| ( 1,4) <- ( 0,6) | 2856.4824 ( 8) | 1.2432E-1 | 1.496366E-07 | O | 2414.8970 | 0.000014 | 2.280E-31 |
| ( 1,3) <- ( 0,5) | 3091.2019 ( 8) | 1.1756E-1 | 2.080232E-07 | O | 1740.1896 | 0.000912 | 1.677E-29 |
| ( 1,2) <- ( 0,4) | 3329.0410 ( 9) | 1.1084E-1 | 2.893241E-07 | O | 1168.7975 | 0.004000 | 7.700E-29 |
| ( 1,1) <- ( 0,3) | 3568.2217 ( 9) | 1.0418E-1 | 4.218437E-07 | O | 705.5189 | 0.088718 | 1.672E-27 |
| ( 1,0) <- ( 0,2) | 3806.7930 ( 9) | 9.7578E-2 | 8.525013E-07 | O | 354.3732 | 0.116421 | 1.818E-27 |
| ( 1,8) <- ( 0,8) | 3955.6392 ( 9) | 9.0146E-2 | 2.226696E-07 | Q | 4051.9430 | 0.000000 | 1.170E-34 |
| ( 1,7) <- ( 0,7) | 4000.0551 ( 9) | 8.9670E-2 | 2.336759E-07 | Q | 3187.4705 | 0.000001 | 2.124E-32 |
| ( 1,6) <- ( 0,6) | 4039.4917 ( 9) | 8.9230E-2 | 2.441314E-07 | Q | 2414.8970 | 0.000014 | 2.686E-31 |
| ( 1,5) <- ( 0,5) | 4073.7322 ( 9) | 8.8837E-2 | 2.542654E-07 | Q | 1740.1896 | 0.000912 | 1.855E-29 |
| ( 1,4) <- ( 0,4) | 4102.5820 ( 9) | 8.8498E-2 | 2.647822E-07 | Q | | | |

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1168.7975      0.004000     8.352E-29
  ( 1,3) <- ( 0,3)  4125.8726  ( 9)   8.8218E-2     2.778835E-07     Q
705.5189       0.088718     1.922E-27
  ( 1,2) <- ( 0,2)  4143.4653  ( 9)   8.8004E-2     3.026584E-07     Q
354.3732       0.116421     2.724E-27
  ( 1,1) <- ( 0,1)  4155.2538  ( 9)   8.7859E-2     4.283675E-07     Q
118.4869       0.659573     2.172E-26
  ( 1,2) <- ( 0,0)  4497.8384  ( 9)   7.8230E-2     2.523430E-07     S
0.0000       0.130361     1.079E-26
  ( 1,3) <- ( 0,1)  4712.9046  ( 9)   7.1950E-2     3.466363E-07     S
118.4869       0.659573     3.188E-26
  ( 1,4) <- ( 0,2)  4917.0063  (10)   6.5759E-2     3.976952E-07     S
354.3732       0.116421     4.575E-27
  ( 1,5) <- ( 0,3)  5108.4029  (10)   5.9658E-2     4.201949E-07     S
705.5189       0.088718     2.979E-27
  ( 1,6) <- ( 0,4)  5285.5912  (10)   5.3642E-2     4.183665E-07     S
1168.7975      0.004000     1.148E-28
  ( 1,7) <- ( 0,5)  5447.3360  (10)   4.7705E-2     3.949522E-07     S
1740.1896      0.000912     2.198E-29
  ( 1,8) <- ( 0,6)  5592.6852  (10)   4.1835E-2     3.532757E-07     S
2414.8970      0.000014     2.652E-31
  ( 1,9) <- ( 0,7)  5720.9703  (10)   3.6019E-2     2.977432E-07     S
3187.4705      0.000001     1.676E-32
  ( 2,5) <- ( 0,7)  6466.7267  (16)   7.4880E-3     3.128659E-08     O
3187.4705      0.000001     7.978E-34
  ( 2,4) <- ( 0,6)  6725.0006  (16)   8.1916E-3     4.698724E-08     O
2414.8970      0.000014     1.292E-32
  ( 2,3) <- ( 0,5)  6982.5124  (17)   8.8635E-3     6.954163E-08     O
1740.1896      0.000912     1.099E-30
  ( 2,2) <- ( 0,4)  7237.5634  (17)   9.4917E-3     1.030523E-07     O
1168.7975      0.004000     5.802E-30
  ( 2,1) <- ( 0,3)  7488.2754  (17)   1.0065E-2     1.602968E-07     O
705.5189       0.088718     1.443E-28
  ( 2,0) <- ( 0,2)  7732.6295  (17)   1.0575E-2     3.462234E-07     O
354.3732       0.116421     1.789E-28
  ( 2,7) <- ( 0,7)  7768.1472  (17)   1.2181E-2     1.191109E-07     Q
3187.4705      0.000001     2.870E-33
  ( 2,6) <- ( 0,6)  7846.2315  (17)   1.1932E-2     1.206981E-07     Q
2414.8970      0.000014     3.520E-32
  ( 2,5) <- ( 0,5)  7914.0076  (17)   1.1719E-2     1.224280E-07     Q
1740.1896      0.000912     2.367E-30
  ( 2,4) <- ( 0,4)  7971.1001  (17)   1.1541E-2     1.246865E-07     Q
1168.7975      0.004000     1.042E-29
  ( 2,3) <- ( 0,3)  8017.1831  (17)   1.1399E-2     1.285272E-07     Q
705.5189       0.088718     2.355E-28
  ( 2,2) <- ( 0,2)  8051.9877  (17)   1.1292E-2     1.380999E-07     Q
354.3732       0.116421     3.291E-28
  ( 2,1) <- ( 0,1)  8075.3074  (17)   1.1221E-2     1.936902E-07     Q
118.4869       0.659573     2.600E-27
  ( 2,2) <- ( 0,0)  8406.3608  (18)   1.1637E-2     1.273300E-07     S
0.0000       0.130361     1.559E-27
  ( 2,3) <- ( 0,1)  8604.2152  (18)   1.1819E-2     1.897171E-07     S
118.4869       0.659573     5.234E-27
  ( 2,4) <- ( 0,2)  8785.5244  (18)   1.1912E-2     2.376675E-07     S
354.3732       0.116421     8.564E-28
  ( 2,5) <- ( 0,3)  8948.6783  (18)   1.1917E-2     2.765727E-07     S
705.5189       0.088718     6.391E-28
  ( 2,6) <- ( 0,4)  9092.3310  (18)   1.1835E-2     3.067375E-07     S
1168.7975      0.004000     2.845E-29
  ( 2,7) <- ( 0,5)  9215.4281  (18)   1.1669E-2     3.274350E-07     S
1740.1896      0.000912     6.366E-30
  ( 2,8) <- ( 0,6)  9317.2177  (18)   1.1422E-2     3.379724E-07     S
2414.8970      0.000014     9.142E-32
  ( 2,9) <- ( 0,7)  9397.2457  (18)   1.1100E-2     3.380900E-07     S
3187.4705      0.000001     7.051E-33
  ( 3,3) <- ( 0,5) 10643.8922  (24)   4.7818E-4     1.665982E-09     O
1740.1896      0.000912     1.133E-32
  ( 3,2) <- ( 0,4) 10915.8996  (24)   7.3464E-4     4.817869E-09     O
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1168.7975      0.004000     1.193E-31
  ( 3,1) <- ( 0,3) 11177.9689  (24)   9.8951E-4     1.148170E-08     O
705.5189       0.088718     4.637E-30
  ( 3,7) <- ( 0,7) 11307.9726  (24)   1.8142E-3     1.726957E-08     Q
3187.4705      0.000001     1.964E-34
  ( 3,6) <- ( 0,6) 11424.2163  (24)   1.7595E-3     1.717436E-08     Q
2414.8970      0.000014     2.363E-33
  ( 3,0) <- ( 0,2) 11428.0177  (25)   1.2399E-3     3.355810E-08     O
354.3732       0.116421     7.941E-30
  ( 3,5) <- ( 0,5) 11525.0786  (24)   1.7129E-3     1.713274E-08     Q
1740.1896      0.000912     1.562E-31
  ( 3,4) <- ( 0,4) 11610.0178  (25)   1.6742E-3     1.720029E-08     Q
1168.7975      0.004000     6.774E-31
  ( 3,3) <- ( 0,3) 11678.5629  (25)   1.6434E-3     1.752186E-08     Q
705.5189       0.088718     1.513E-29
  ( 3,2) <- ( 0,2) 11730.3239  (25)   1.6202E-3     1.865673E-08     Q
354.3732       0.116421     2.095E-29
  ( 3,1) <- ( 0,1) 11765.0009  (25)   1.6048E-3     2.600597E-08     Q
118.4869       0.659573     1.645E-28
  ( 3,2) <- ( 0,0) 12084.6970  (25)   1.9322E-3     2.155403E-08     S
0.0000       0.130361     1.277E-28
  ( 3,3) <- ( 0,1) 12265.5949  (25)   2.1333E-3     3.638613E-08     S
118.4869       0.659573     4.940E-28
  ( 3,4) <- ( 0,2) 12424.4421  (25)   2.3152E-3     5.078207E-08     S
354.3732       0.116421     9.150E-29
  ( 3,5) <- ( 0,3) 12559.7492  (25)   2.4760E-3     6.502856E-08     S
705.5189       0.088718     7.628E-29
  ( 3,6) <- ( 0,4) 12670.3158  (25)   2.6143E-3     7.865514E-08     S
1168.7975      0.004000     3.757E-30
  ( 3,7) <- ( 0,5) 12755.2535  (25)   2.7292E-3     9.099591E-08     S
1740.1896      0.000912     9.235E-31
  ( 3,8) <- ( 0,6) 12813.9923  (25)   2.8203E-3     1.013814E-07     S
2414.8970      0.000014     1.450E-32
  ( 3,9) <- ( 0,7) 12846.2712  (25)   2.8877E-3     1.092460E-07     S
3187.4705      0.000001     1.219E-33
  ( 4,3) <- ( 0,5) 14078.0983  (31)   5.2561E-5     8.147604E-11     O
1740.1896      0.000912     3.168E-34
  ( 4,2) <- ( 0,4) 14366.9458  (31)   2.2902E-5     1.849187E-11     O
1168.7975      0.004000     2.642E-34
  ( 4,1) <- ( 0,3) 14640.2910  (31)   1.0153E-4     4.658524E-10     O
705.5189       0.088718     1.097E-31
  ( 4,6) <- ( 0,6) 14775.4941  (31)   3.4904E-4     2.445790E-09     Q
2414.8970      0.000014     2.012E-34
  ( 4,0) <- ( 0,2) 14895.9925  (31)   1.8261E-4     2.739046E-09     O
354.3732       0.116421     3.815E-31
  ( 4,5) <- ( 0,5) 14909.2792  (31)   3.3676E-4     2.399154E-09     Q
1740.1896      0.000912     1.307E-32
  ( 4,4) <- ( 0,4) 15021.9052  (31)   3.2654E-4     2.372688E-09     Q
1168.7975      0.004000     5.582E-32
  ( 4,3) <- ( 0,3) 15112.7690  (31)   3.1837E-4     2.386405E-09     Q
705.5189       0.088718     1.230E-30
  ( 4,2) <- ( 0,2) 15181.3701  (31)   3.1223E-4     2.515584E-09     Q
354.3732       0.116421     1.687E-30
  ( 4,1) <- ( 0,1) 15227.3230  (32)   3.0814E-4     3.482288E-09     Q
118.4869       0.659573     1.315E-29
  ( 4,2) <- ( 0,0) 15535.7432  (32)   4.3098E-4     3.765329E-09     S
0.0000       0.130361     1.350E-29
  ( 4,3) <- ( 0,1) 15699.8010  (32)   5.1170E-4     7.192533E-09     S
118.4869       0.659573     5.960E-29
  ( 4,4) <- ( 0,2) 15836.3295  (32)   5.8946E-4     1.107402E-08     S
354.3732       0.116421     1.228E-29
  ( 4,5) <- ( 0,3) 15943.9499  (32)   6.6317E-4     1.537852E-08     S
705.5189       0.088718     1.119E-29
  ( 4,6) <- ( 0,4) 16021.5936  (32)   7.3193E-4     1.993137E-08     S
1168.7975      0.004000     5.954E-31
  ( 4,7) <- ( 0,5) 16068.5214  (32)   7.9497E-4     2.449544E-08     S
1740.1896      0.000912     1.566E-31
  ( 4,9) <- ( 0,7) 16068.9109  (31)   9.0185E-4     3.263016E-08     S
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3187.4705 0.000001 2.328E-34
( 4,8) <- ( 0,6) 16084.3247 (31) 8.5174E-4 2.881139E-08 S
2414.8970 0.000014 2.615E-33
( 5,3) <- ( 0,5) 17285.8147 (37) 5.2629E-5 2.279726E-10 O
1740.1896 0.000912 5.879E-34
( 5,2) <- ( 0,4) 17591.5461 (37) 2.7877E-5 7.540858E-11 O
1168.7975 0.004000 7.187E-34
( 5,5) <- ( 0,5) 18066.8060 (37) 8.3701E-5 3.872579E-10 Q
1740.1896 0.000912 1.437E-33
( 5,0) <- ( 0,2) 18137.5564 (37) 2.7544E-5 1.667845E-10 O
354.3732 0.116421 1.567E-32
( 5,4) <- ( 0,4) 18207.2310 (37) 8.0215E-5 3.745179E-10 Q
1168.7975 0.004000 5.998E-33
( 5,3) <- ( 0,3) 18320.4854 (37) 7.7422E-5 3.694737E-10 Q
705.5189 0.088718 1.296E-31
( 5,2) <- ( 0,2) 18405.9704 (37) 7.5323E-5 3.835099E-10 Q
354.3732 0.116421 1.749E-31
( 5,1) <- ( 0,1) 18463.2234 (37) 7.3920E-5 5.251980E-10 Q
118.4869 0.659573 1.349E-30
( 5,2) <- ( 0,0) 18760.3435 (38) 1.2190E-4 7.734007E-10 S
0.0000 0.130361 1.901E-30
( 5,3) <- ( 0,1) 18907.5174 (38) 1.5481E-4 1.667898E-09 S
118.4869 0.659573 9.530E-30
( 5,4) <- ( 0,2) 19021.6553 (38) 1.8769E-4 2.807054E-09 S
354.3732 0.116421 2.158E-30
( 5,5) <- ( 0,3) 19101.4767 (37) 2.2004E-4 4.178545E-09 S
705.5189 0.088718 2.119E-30
( 5,8) <- ( 0,6) 19127.2227 (37) 3.0977E-4 9.062850E-09 S
2414.8970 0.000014 5.817E-34
( 5,6) <- ( 0,4) 19146.0288 (37) 2.5142E-4 5.731584E-09 S
1168.7975 0.004000 1.199E-31
( 5,7) <- ( 0,5) 19154.7014 (37) 2.8144E-4 7.390092E-09 S
1740.1896 0.000912 3.326E-32
( 6,3) <- ( 0,5) 20265.3607 (42) 3.0434E-5 1.688324E-10 O
1740.1896 0.000912 3.168E-34
( 6,2) <- ( 0,4) 20588.2094 (42) 2.1079E-5 9.467054E-11 O
1168.7975 0.004000 6.587E-34
( 6,1) <- ( 0,3) 20884.3046 (42) 1.0655E-5 3.030803E-11 O
705.5189 0.088718 3.507E-33
( 6,5) <- ( 0,5) 20995.3964 (42) 2.4067E-5 6.785544E-11 Q
1740.1896 0.000912 1.864E-34
( 6,4) <- ( 0,4) 21164.0583 (42) 2.2645E-5 6.334199E-11 Q
1168.7975 0.004000 7.508E-34
( 6,3) <- ( 0,3) 21300.0314 (42) 2.1506E-5 6.056053E-11 Q
705.5189 0.088718 1.572E-32
( 6,2) <- ( 0,2) 21402.6337 (42) 2.0649E-5 6.127446E-11 Q
354.3732 0.116421 2.067E-32
( 6,1) <- ( 0,1) 21471.3366 (43) 2.0077E-5 8.240355E-11 Q
118.4869 0.659573 1.565E-31
( 6,2) <- ( 0,0) 21757.0068 (43) 4.0822E-5 1.819732E-10 S
0.0000 0.130361 3.326E-31
( 6,3) <- ( 0,1) 21887.0634 (43) 5.5521E-5 4.458820E-10 S
118.4869 0.659573 1.901E-30
( 6,8) <- ( 0,6) 21938.9866 (42) 1.3033E-4 3.184773E-09 S
2414.8970 0.000014 1.554E-34
( 6,4) <- ( 0,2) 21978.4826 (43) 7.0584E-5 8.175825E-10 S
354.3732 0.116421 4.707E-31
( 6,7) <- ( 0,5) 22010.6553 (42) 1.1585E-4 2.508741E-09 S
1740.1896 0.000912 8.550E-33
( 6,5) <- ( 0,3) 22030.0671 (42) 8.5797E-5 1.296321E-09 S
705.5189 0.088718 4.942E-31
( 6,6) <- ( 0,4) 22040.9602 (42) 1.0095E-4 1.868295E-09 S
1168.7975 0.004000 2.949E-32
( 7,3) <- ( 0,5) 23012.2739 (46) 1.6969E-5 9.910340E-11 O
1740.1896 0.000912 1.442E-34
( 7,2) <- ( 0,4) 23352.7060 (46) 1.2969E-5 6.727787E-11 O
1168.7975 0.004000 3.639E-34
( 7,1) <- ( 0,3) 23660.5543 (46) 8.4003E-6 3.516089E-11 O

705.5189 0.088718 3.170E-33
( 7,0) <- ( 0,2) 23933.5421 (47) 3.2481E-6 9.278962E-12 O
354.3732 0.116421 5.006E-34
( 7,3) <- ( 0,3) 24046.9446 (46) 6.2981E-6 9.525582E-12 Q
705.5189 0.088718 1.940E-33
( 7,2) <- ( 0,2) 24167.1303 (47) 5.9020E-6 9.188596E-12 Q
354.3732 0.116421 2.431E-33
( 7,1) <- ( 0,1) 24247.5864 (47) 5.6373E-6 1.193274E-11 Q
118.4869 0.659573 1.777E-32
( 7,2) <- ( 0,0) 24521.5035 (47) 1.5529E-5 4.789186E-11 S
0.0000 0.130361 6.890E-32
( 7,7) <- ( 0,5) 24630.1107 (46) 5.3772E-5 9.482954E-10 S
1740.1896 0.000912 2.581E-33
( 7,3) <- ( 0,1) 24633.9766 (47) 2.2719E-5 1.348434E-10 S
118.4869 0.659573 4.539E-31
( 7,6) <- ( 0,4) 24700.7121 (46) 4.5864E-5 6.816533E-10 S
1168.7975 0.004000 8.567E-33
( 7,4) <- ( 0,2) 24702.0338 (47) 3.0238E-5 2.690965E-10 S
354.3732 0.116421 1.227E-31
( 7,5) <- ( 0,3) 24724.5412 (46) 3.7987E-5 4.524781E-10 S
705.5189 0.088718 1.370E-31
( 8,2) <- ( 0,4) 25877.4995 (49) 7.8560E-6 4.124901E-11 O
1168.7975 0.004000 1.817E-34
( 8,1) <- ( 0,3) 26197.5981 (49) 5.6416E-6 2.639094E-11 O
705.5189 0.088718 1.940E-33
( 8,0) <- ( 0,2) 26476.7175 (50) 3.0948E-6 1.395701E-11 O
354.3732 0.116421 6.153E-34
( 8,3) <- ( 0,3) 26553.3932 (49) 1.7392E-6 1.192538E-12 Q
705.5189 0.088718 1.992E-34
( 8,2) <- ( 0,2) 26691.9238 (50) 1.5372E-6 1.024482E-12 Q
354.3732 0.116421 2.222E-34
( 8,1) <- ( 0,1) 26784.6301 (50) 1.4024E-6 1.214556E-12 Q
118.4869 0.659573 1.482E-33
( 8,7) <- ( 0,5) 27002.9037 (48) 2.7566E-5 3.947349E-10 S
1740.1896 0.000912 8.938E-34
( 8,2) <- ( 0,0) 27046.2970 (50) 6.5450E-6 1.388643E-11 S
0.0000 0.130361 1.642E-32
( 8,6) <- ( 0,4) 27115.8975 (49) 2.3075E-5 2.750811E-10 S
1168.7975 0.004000 2.869E-33
( 8,3) <- ( 0,1) 27140.4253 (50) 1.0363E-5 4.554093E-11 S
118.4869 0.659573 1.263E-31
( 8,5) <- ( 0,3) 27176.1508 (49) 1.8677E-5 1.754814E-10 S
705.5189 0.088718 4.397E-32
( 8,4) <- ( 0,2) 27184.0758 (49) 1.4423E-5 9.880794E-11 S
354.3732 0.116421 3.719E-32
( 9,1) <- ( 0,3) 28484.0451 (51) 3.7121E-6 1.736188E-11 O
705.5189 0.088718 1.080E-33
( 9,0) <- ( 0,2) 28769.6672 (51) 2.3429E-6 1.211671E-11 O
354.3732 0.116421 4.524E-34
( 9,7) <- ( 0,5) 29113.8774 (49) 1.5372E-5 1.788315E-10 S
1740.1896 0.000912 3.484E-34
( 9,6) <- ( 0,4) 29272.4119 (50) 1.2656E-5 1.213335E-10 S
1168.7975 0.004000 1.086E-33
( 9,2) <- ( 0,0) 29319.7424 (51) 3.0072E-6 4.388857E-12 S
0.0000 0.130361 4.417E-33
( 9,5) <- ( 0,3) 29371.6485 (50) 1.0036E-5 7.472541E-11 S
705.5189 0.088718 1.603E-32
( 9,3) <- ( 0,1) 29394.3770 (51) 5.1867E-6 1.700093E-11 S
118.4869 0.659573 4.019E-32
( 9,4) <- ( 0,2) 29412.0461 (51) 7.5376E-6 4.001537E-11 S
354.3732 0.116421 1.287E-32
(10,1) <- ( 0,3) 30503.3511 (51) 2.4793E-6 1.090806E-11 O
705.5189 0.088718 5.916E-34
(10,0) <- ( 0,2) 30796.0178 (51) 1.6872E-6 8.831125E-12 O
354.3732 0.116421 2.878E-34
(10,7) <- ( 0,5) 30941.2209 (48) 9.2043E-6 8.693029E-11 S
1740.1896 0.000912 1.499E-34
(10,6) <- ( 0,4) 31149.9497 (49) 7.4722E-6 5.771110E-11 S

H2calculated_296K_CutOff_1E-34.txt

```
1168.7975      0.004000     4.561E-34
  (10,5) <- ( 0,3) 31291.9341  (50)   5.8206E-6     3.449659E-11     S
705.5189       0.088718     6.519E-33
  (10,2) <- ( 0,0) 31324.9505  (51)   1.4911E-6     1.502014E-12     S
0.0000       0.130361     1.324E-33
  (10,4) <- ( 0,2) 31367.7960  (50)   4.2640E-6     1.766817E-11     S
354.3732       0.116421     4.994E-33
  (10,3) <- ( 0,1) 31378.4126  (51)   2.8168E-6     6.950790E-12     S
118.4869       0.659573     1.442E-32
  (11,1) <- ( 0,3) 32232.2305  (48)   1.6955E-6     6.720634E-12     O
705.5189       0.088718     3.264E-34
  (11,0) <- ( 0,2) 32532.7252  (48)   1.2078E-6     5.953271E-12     O
354.3732       0.116421     1.738E-34
  (11,6) <- ( 0,4) 32719.7041  (45)   4.6853E-6     2.901321E-11     S
1168.7975      0.004000     2.078E-34
  (11,1) <- ( 0,1) 32819.2626  (48)   3.0267E-7     1.562589E-13     Q
118.4869       0.659573     1.270E-34
  (11,5) <- ( 0,3) 32910.0105  (46)   3.5979E-6     1.695942E-11     S
705.5189       0.088718     2.897E-33
  (11,4) <- ( 0,2) 33025.7288  (47)   2.5810E-6     8.374549E-12     S
354.3732       0.116421     2.136E-33
  (11,2) <- ( 0,0) 33038.1431  (48)   7.9302E-7     5.544606E-13     S
0.0000       0.130361     4.394E-34
  (11,3) <- ( 0,1) 33067.9934  (48)   1.6437E-6     3.076394E-12     S
118.4869       0.659573     5.746E-33
  (12,1) <- ( 0,3) 33638.3294  (42)   1.1814E-6     4.039399E-12     O
705.5189       0.088718     1.801E-34
  (12,0) <- ( 0,2) 33947.8009  (42)   8.6653E-7     3.791653E-12     O
354.3732       0.116421     1.017E-34
  (12,5) <- ( 0,3) 34187.6897  (38)   2.3239E-6     8.560171E-12     S
705.5189       0.088718     1.355E-33
  (12,1) <- ( 0,1) 34225.3614  (42)   2.7509E-7     1.592010E-13     Q
118.4869       0.659573     1.190E-34
  (12,4) <- ( 0,2) 34349.9117  (40)   1.6431E-6     4.131090E-12     S
354.3732       0.116421     9.738E-34
  (12,2) <- ( 0,0) 34426.2179  (42)   4.4932E-7     2.186718E-13     S
0.0000       0.130361     1.596E-34
  (12,3) <- ( 0,1) 34428.8463  (41)   1.0161E-6     1.438267E-12     S
118.4869       0.659573     2.478E-33
```