Description of the SCAN-H_2O line list.

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The computation of the SCAN-H_2O line list has been described in detail in our papers ”H_2O in stellar atmospheres”, U.G.Jørgensen, P.Jensen, G.O.Sørensen, B.Aringer, A&A, in press, 2001, and ”The Dipole Moment Surface and the Vibrational Transition Moments of H_2O”, U.G.Jørgensen & P.Jensen, J.Mol.Spectr., 161, 219−242, 1993, which you are requested to refer to if you want to use the data.

We kindly ask you not to distribute the lists, but instead refer interested friends and colleagues to the ftp site where you found the data (stella.nbi.dk, anonymous login with your userid as password, cd to pub/scan). The data are occasionally updated if errors are discovered or improved molecular constants etc have become available which can influence the line list data. New lists are added to the old ones when time permits. To optimise the completeness and to minimise the risk of circulating data with errors, please try to be a bit unfriendly in sharing our data with your friends, but be friendly in advising them the ftp address if they asks you for a copy of the data. Of course we are also curious about the possible use you have of the data, so we gladly hear about your projects and results. Some of the SCAN molecular data base have been described in general and compared to other available data, in U.G.Jørgensen, “Cool Star Models”, In: E.F.vanDishoeck (ed.), *Molecules in Astrophysics: Probes and Processes* (IAU Symp. 178), Kluwer, 1997, p.441−456.

There are 3 H_2O line list available at this anonymous ftp site:

(1) A full 100 million lines list meant for computation of stellar opacities, and other high temperature purposes. This list includes all lines in the spectral interval $400\,\mathrm{cm}^{-1}$−$15000\,\mathrm{cm}^{-1}$ ($\approx 6700\,\text{Å}$−25μm) which have an intensity larger than 10^{-9} km/mol at 3500 K. It contains basically the complete total absorption coefficient at temperatures up to at least 4000 K, in the definition of completeness described in Jørgensen et al. 2001 cited above. Test computations of up to 3 billion lines (i.e., all lines stronger than 10^{-20}km/mol) gave the same effect on stellar atmospheric structures and synthetic spectra, as did the available 100 million lines list. The three columns in the file, lists (a) the line center wavenumber ν_0 in cm^{-1}, (b) the temperature independent line strength s_0 in km/mol, (c) the excitation energy E_{low} in cm^{-1}.

(2) A 1.2 million lines list with spectroscopic information. This list is computed in the same way as list (1), but only the lines with intensity larger than 10^{-5} km/mol at 3500 K are listed. The first three columns in this file is organised in the same way as list (1), but for each transition the first three columns are then followed first by 6 columns describing the upper eigenstate of the transition, and then 6 columns describing the lower state. The 6 columns list first the 3 v-quantum numbers, then the J quantum

number, and finally K_a and K_c.

(3) A 1.1 million lines list aimed at planetary and other relatively low temperature research. It is computed for the same spectral interval as the above lists, but all lines with intensity larger than 10^{-18} km/mol at 300 K are included. This list has strong similarity to the HITEMP line list, but it is purely *ab initio.* The line frequencies will be more accurate in HITEMP than in the present list, but the line intensities will some times be more accurate in HITEMP and some times be more accurate in the present list. The organisation of the columns is identical to list (2) above.

The temperature dependent line intensity $s(T)$ is calculated from the 3 listed quantities ν_0, s_0, E_{low}, as:

$$s(T) = s_0 * exp(-E_{low} * hc/kT) * (1 - exp(-\nu_0 * hc/kT))/Q_{vib}(T)Q_{rot}(T) \tag{1}$$

where h,c, and k are Planck's constant, the speed of light, and Boltzman's constant. With $\mathrm{E}_{\mathrm{low}}$ and ν_0 in units of cm^{-1}, hc/k takes the numerical value 1.43877.

Q_{vib}(T) has to be calculated consistently with the line list, and values of Q_{vib}(T) that corresponds to the present line list therefore follows here, for values of T from 200 K in steps of 200 K to 8000 K:

1.0000, 1.0032, 1.0227, 1.0633, 1.1239, 1.2036, 1.3018, 1.4186, 1.5541, 1.7085, 1.8825, 2.0767, 2.2919, 2.5289, 2.7886, 3.0721, 3.3804, 3.7144, 4.0752, 4.4637, 4.8807, 5.3272, 5.8038, 6.3112, 6.8499, 7.4203, 8.0227, 8.6572, 9.3238, 10.0225, 10.7531, 11.5153, 12.3085, 13.1325, 13.9864, 14.8698, 15.7819, 16.7218, 17.6889, 18.6821

At 300 K $\mathrm{Q}_{vib}(300) = 1.0005$.

Q_{rot}(T) can be computed as *Qrb* at the temperature T=*temp* from the following small program loop:

```
pi = 3.14159
RC01 = 27.88063
RC02 = 14.52177
RC03 = 9.27771
hck = 1.43877
hckt = hck / temp
Qra = RC01*RC02*RC03
Qra = sqrt(pi/Qra*(1.D0/hckt)**3)
A = RC01
B = sqrt(RC02*RC03)
Qrb = B*hckt
B = (1.D0-B/A)*Qrb
Qrb = Qra*exp(0.25D0*Qrb)*(1.D0+B/12.D0+B*B*7.D0/480.D0)
Qrb = Qrb + Qrb
```

For the two smaller lists, higher accuracy can be obtained by substituting the molecular B_0-values (RC01, RC02, RC03 above) with the B_v values, which can be calculated by use of Eq. 8 and Tab. 1 in Jørgensen et al. 2001. However this cannot be done based on the 100 million lines list (because the v quantum numbers are not listed), and here the B_0 values in the above program piece will do.

Remark that the temperature independent part of the partition function is included in the listed value of s_0 in the line lists. The use of partition functions from the literature together with the SCAN lists can therefore result in considerable errors in the computed opacities, and it is therefore important to adopt the above consistent definitions of the partition functions. For this reason, the user will also not have to multiply the listed line strengths with any spin-, weight-, degeneration- or other factors (like e.g. 2J+1). Also note that the degeneration of the lines in the list is treated consistently with the above definition of the partition functions. This results for example in that degenerated transitions of high J-number but different K_a, K_c values will be listed separately, even though they have identical wavenumber. Such lines should be treated as individual lines, although at identical frequency. There are also other pairs of lines that will be listed with the same frequency. Some of these just accidentally happens to have the same frequency (recall that at the 100 million lines list, there are on average 100 listed spectral lines per cm^{-1}). At high eigenenergies, there is not a unique description of the eigenstates in terms of harmonic quantum numbers, and some different high-energy states can therefore be described best by the same set of harmonic quantum numbers. You can therefore find lines belonging to such states, which have the same transition frequency, the same quantum numbers (in list 2 and 3), but different excitation energies. These lines and all other "multiple" lines should be treated as they are listed, although some of them at first glance could look erroneously. Remark also that intensity borrowing is not included, so some of such line pairs can appear with the two lines having quite different line strengths.

The conversion from s_0 in the line lists to the often used gf value, is given by $gf = s_0$*1.87572 10^{-7}.

The figures below illustrate the correspondance between the 3 available lists. At room temperature the absorption coefficient from the planetary list is basically identical to the full 100 million lines list (although based on only 1% the number of lines), while at high temperature the spectroscopic list equals the 100 million lines list in the infrared, and the planetary list deviate much more from the 100 million lines list than at room temperature. While at this resolution it is indicated that the planetary list is sufficient at low temperatures, it is also clear that at high temperatures only the full 100 million lines list is sufficient for opacity as well as for low resolution spectroscopic purposes. The plots are in colours, so they are easiest inspected in a colour print, but you can also easily view them in black and white.

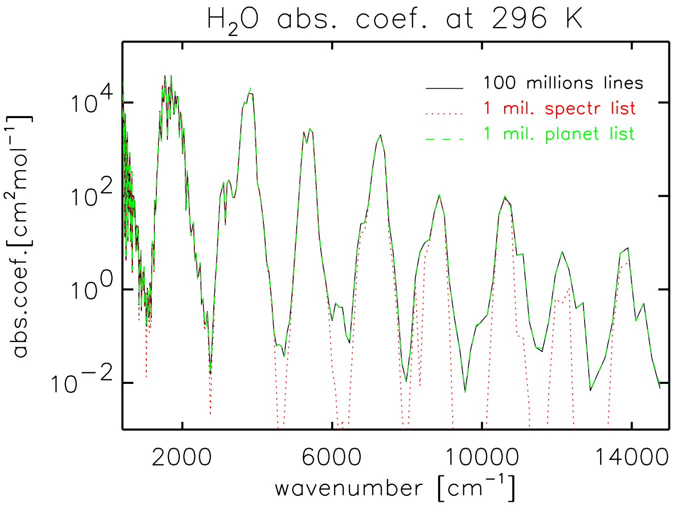

Figure 1: The absorption coefficient for H_2O at T=296 K.

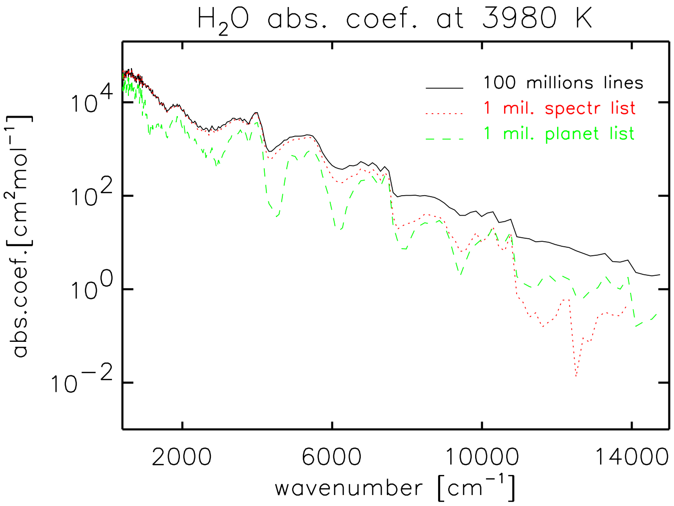

Figure 2: The absorption coefficient for H_2O at T=3980 K.