Spectrum and Opacity of CO_2. Comparison of Available Databases.

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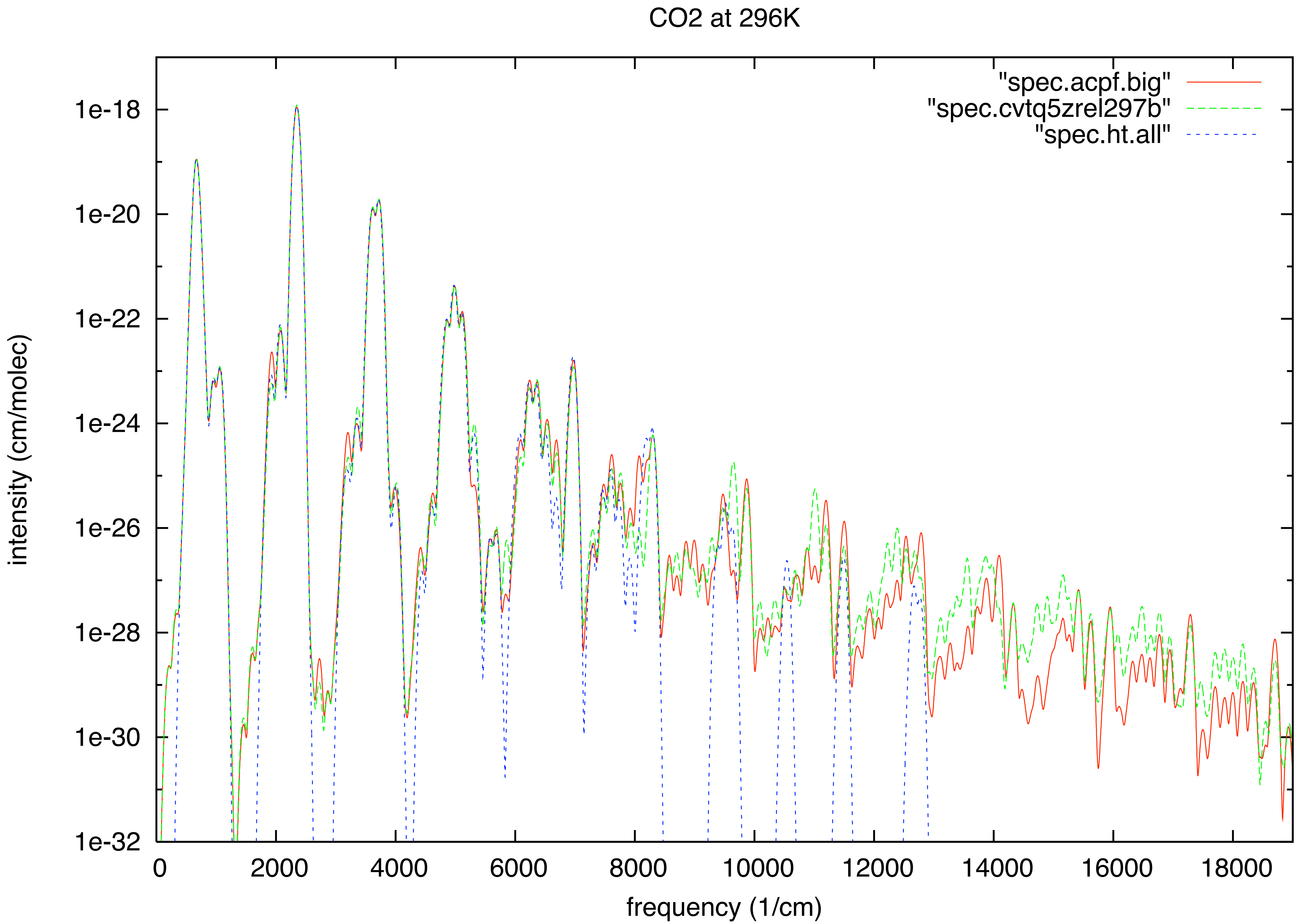
- CO2 is possibly of interest for irradiated, hot Jupiters and for extrasolar terrestrial planets
- Currently there are only a few databases available for high temperature CO_2
- New calculations are under way by David Schwenke to produce an improved and expanded version of the CO_2 linelist



A comparison of 3 different dipole moment functions for CO_2

- Hitran intensities are reproduced using the current Hitran database

- Two different dipole moment functions (DMF) are shown for CO_2 based on calculations by David Schwenke

- Note that the DMF from Schwenke extends to much higher wavenumbers than the current databases. This reflects the limits of the earlier potential energy surfaces

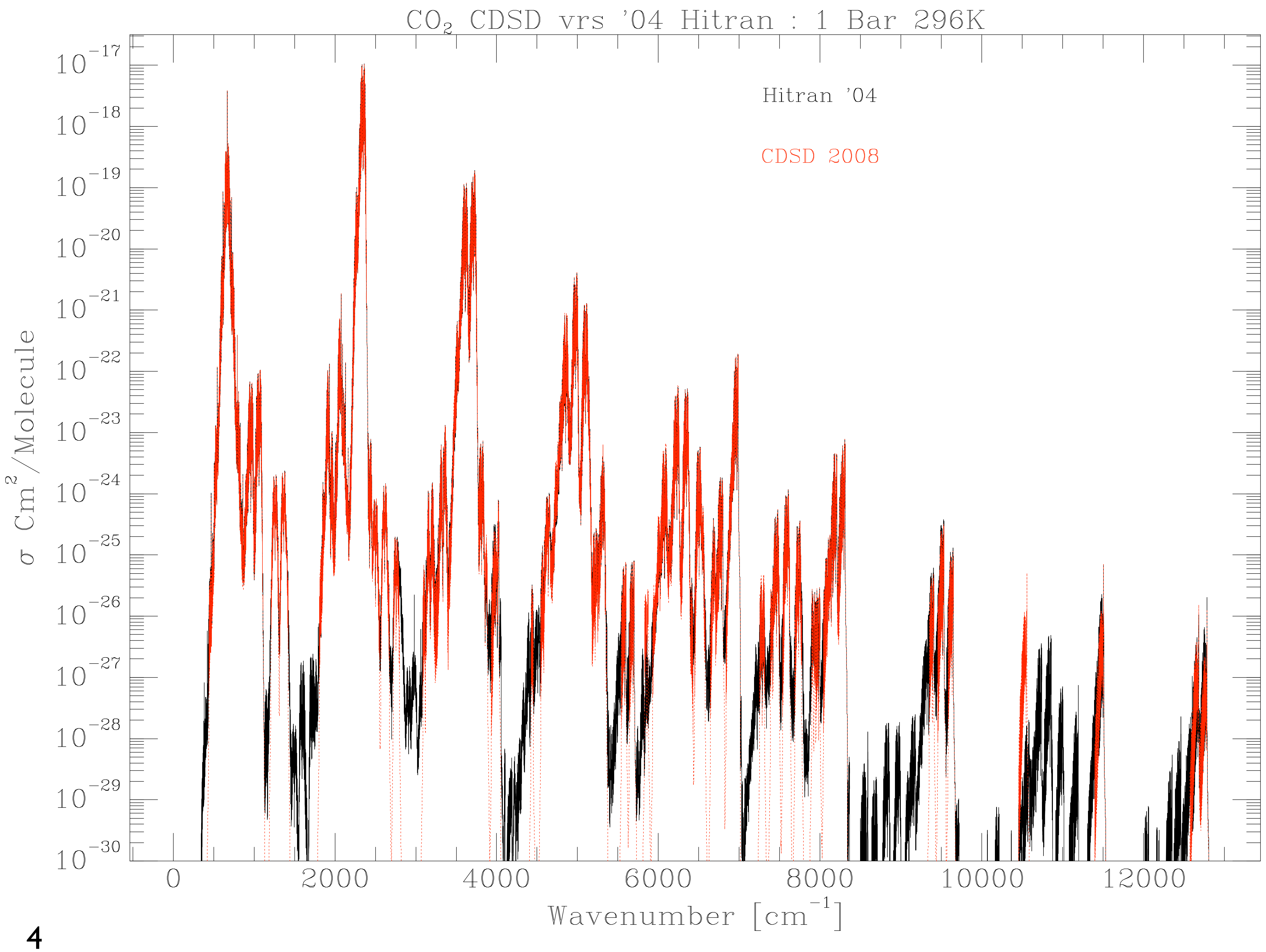
- A line list is expected by the end of 2008

Comparison of two CO_2 Spectra: Hitran 2004 vrs CDSD 2008

- Calculations are done using a Voigt profile with no adjustments (χ factor) to the far line wings

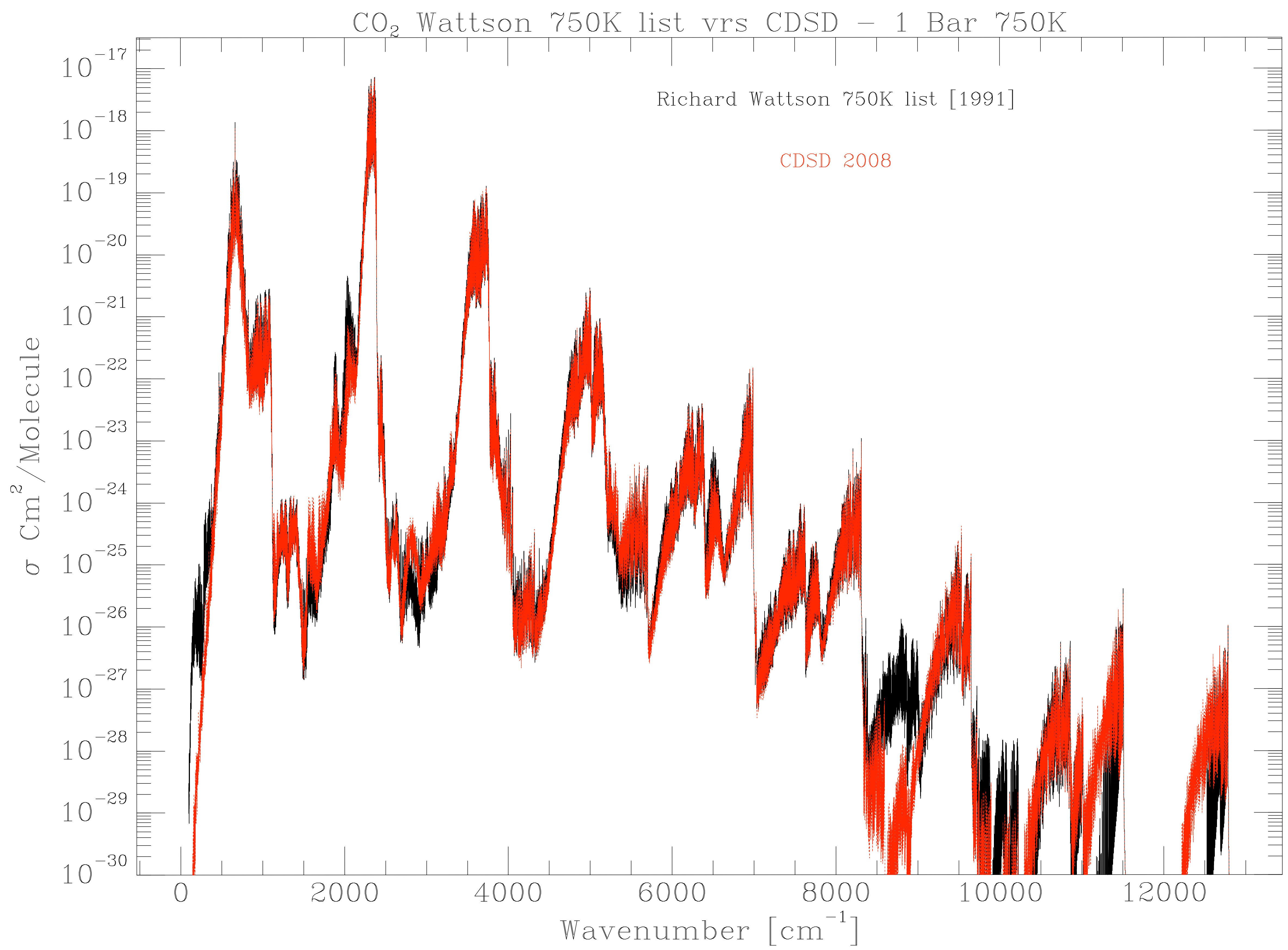
- The line widths are appropriate for "foreign" ($O_2 + N_2$) broadening

- The Russian (CDSD) data is missing some minor isotopes present in Hitran



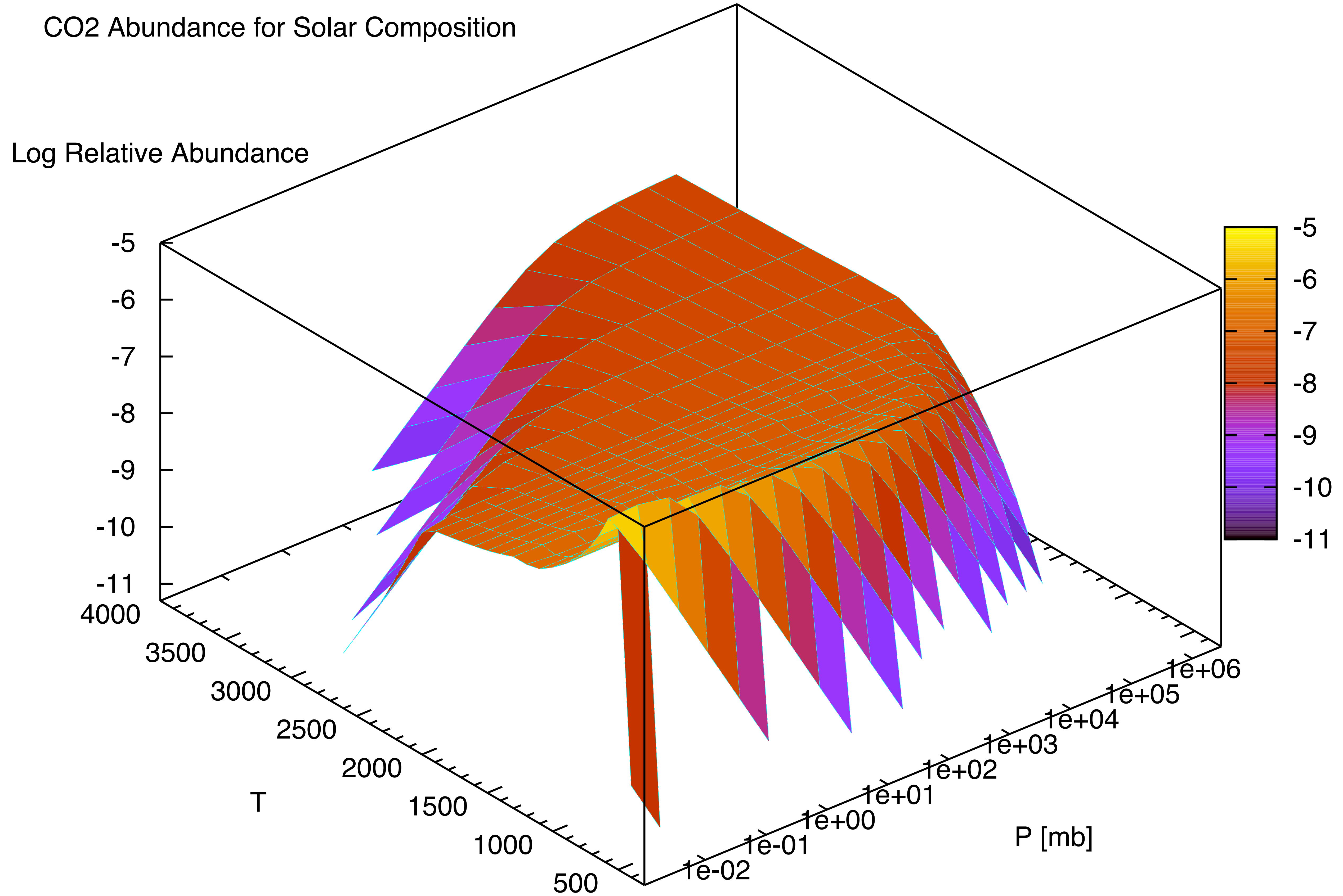
CO_2 absorption at 750K & 1 Bar: Comparison of a 1991 calculation of Wattson and 2008 CDSD data

- Both calculations use a pure Voigt profile
- Assumes foreign broadening
- The Wattson data includes some bands added by Freedman at high wavenumbers
- The Hitran and Wattson data show better agreement as they share some common computational history (based on DND calculations and similar dipole moments)



Equilibrium abundances of CO_2 for an assumed solar composition

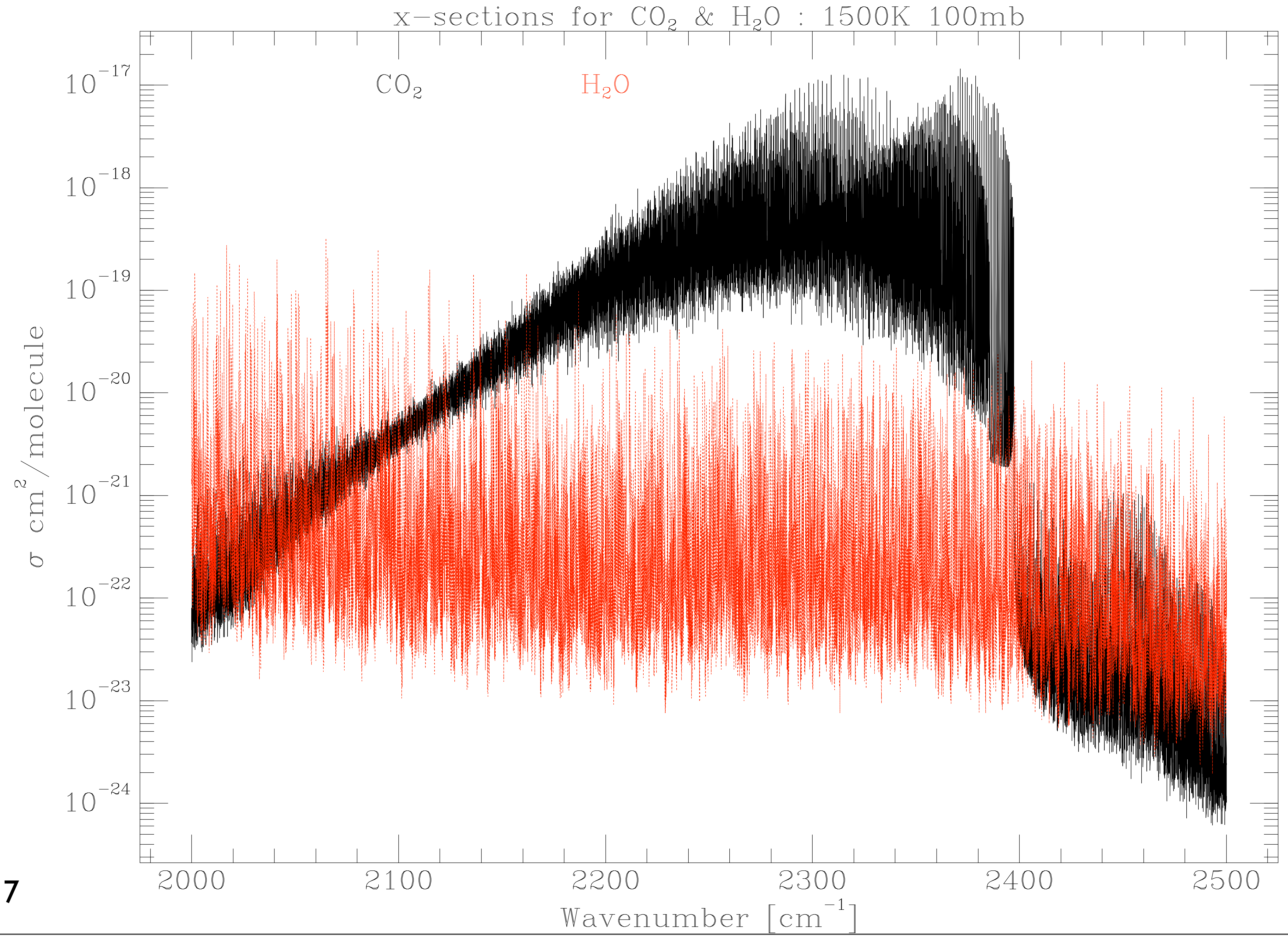
- In chemical equilibrium the most significant abundances are at moderate temperatures and low pressures
- For temperatures > ~ 1200K the largest abundances are at the higher pressures
- At high temperatures the abundance is greatest at high pressures
- Non-equilibrium abundances may be quite different in certain P:T regimes



Comparison of absorption cross sections for CO_2 & H_2O

- Cross-sections are shown per molecule without any adjustment for the relative abundance

- The region shown is in the CO_2 4.3 µm band

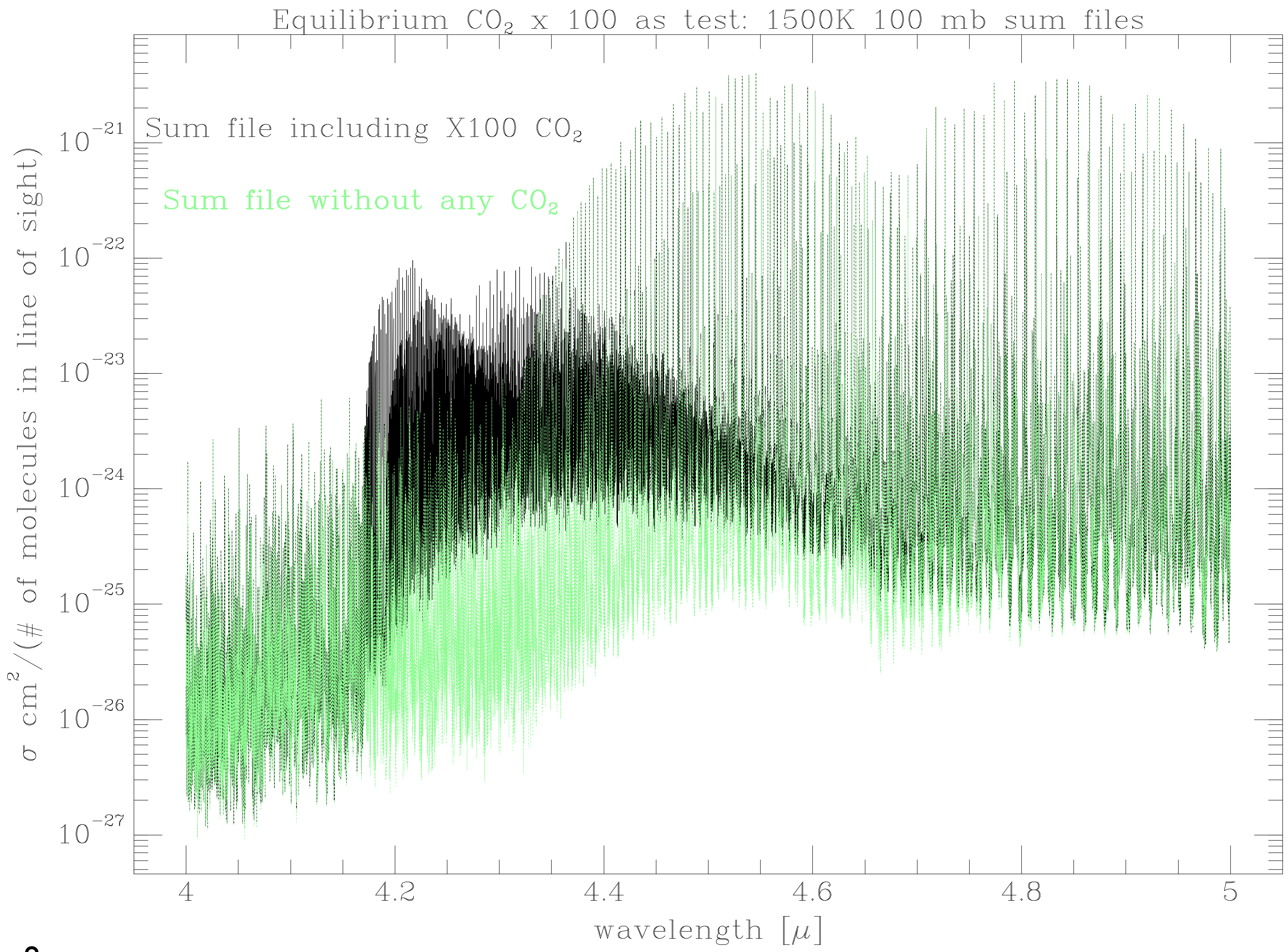


Sum of opacities of 10 molecules and alkali atoms + CO_2 x 100

- For this test the relative abundance of CO_2 has been increased by a factor of 100 from the chemical equilibrium abundance

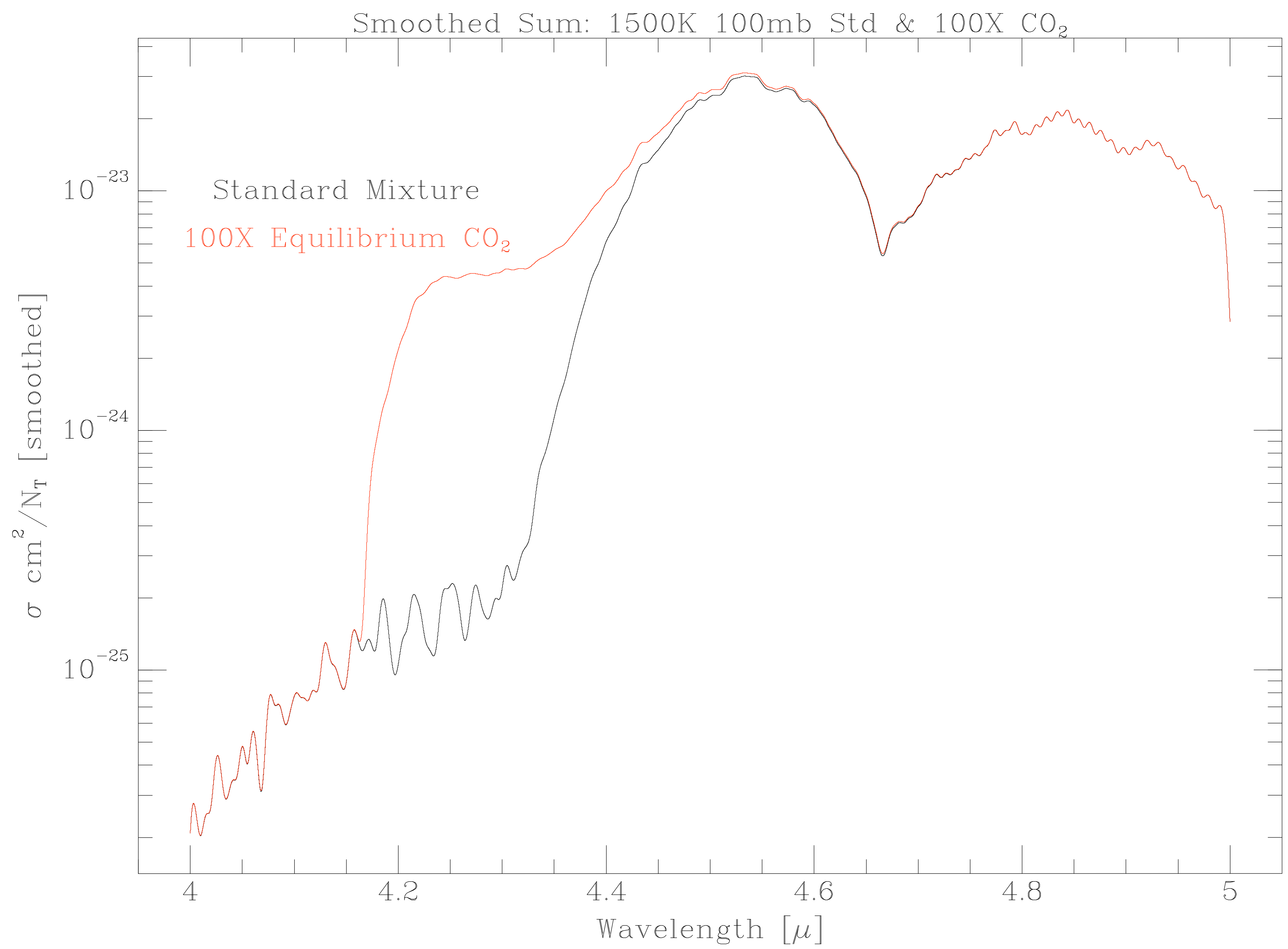
- This may be appropriate for upper regions of an exoplanet atmosphere affected by UV radiation from the central star

- This shows the raw absorption coefficients unsmoothed



Sum file smoothed to simulate an observation - resolution ~ 1200

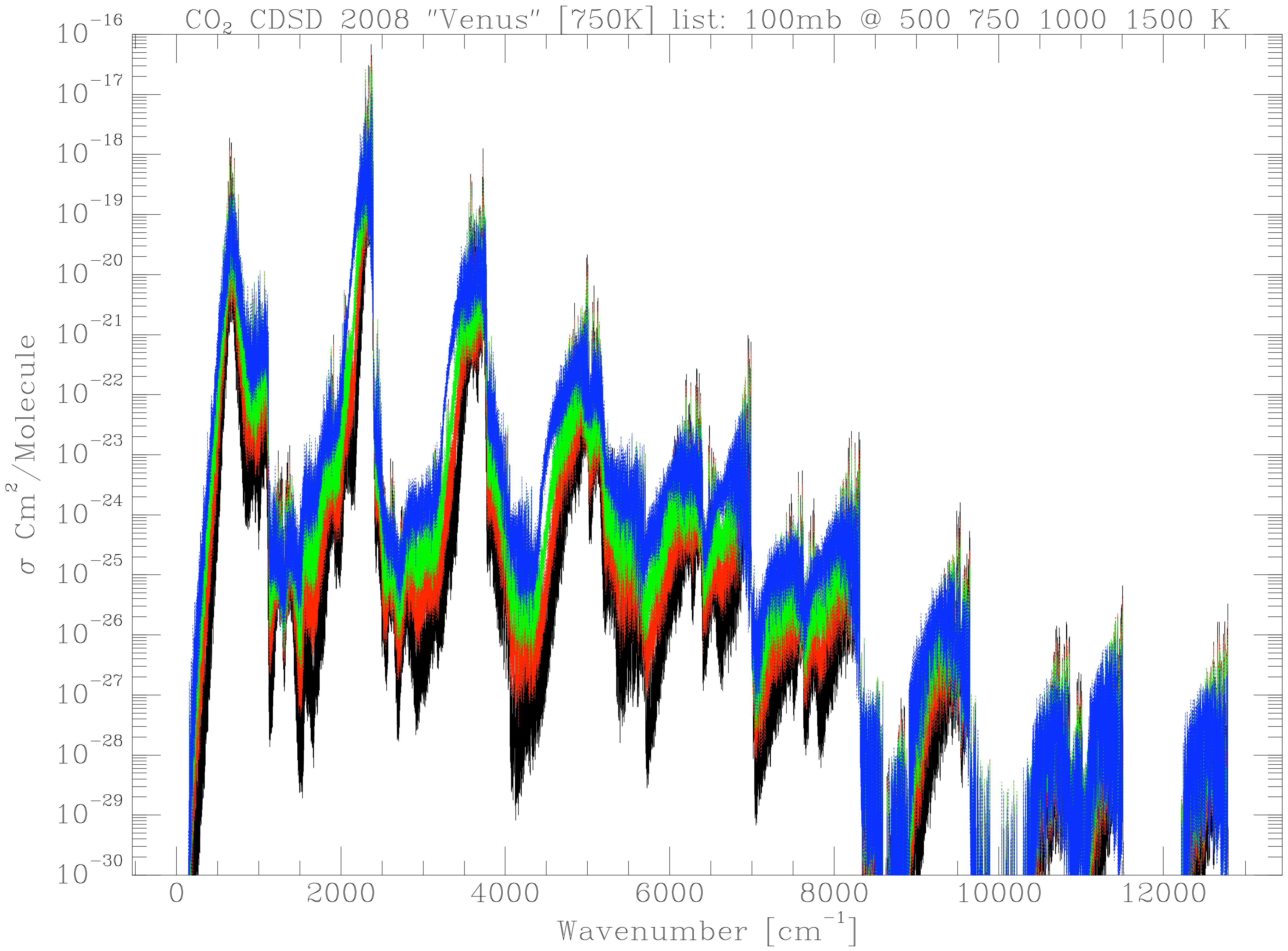
- This plot shows more clearly the affect that enhanced CO_2 abundance can have on the total opacity
- To calculate the total optical depth multiply the absorption cross-section by the total number of particles in the line of sight
- CIA has not been included [H_2-H_2 and H_2-He] as the total pressure is so low



Absorption coefficient of CO_2 for 4 different temperatures : 100 mb

- Classical Voigt profile was used with no adjustment for sub-Lorenztian wings of CO_2

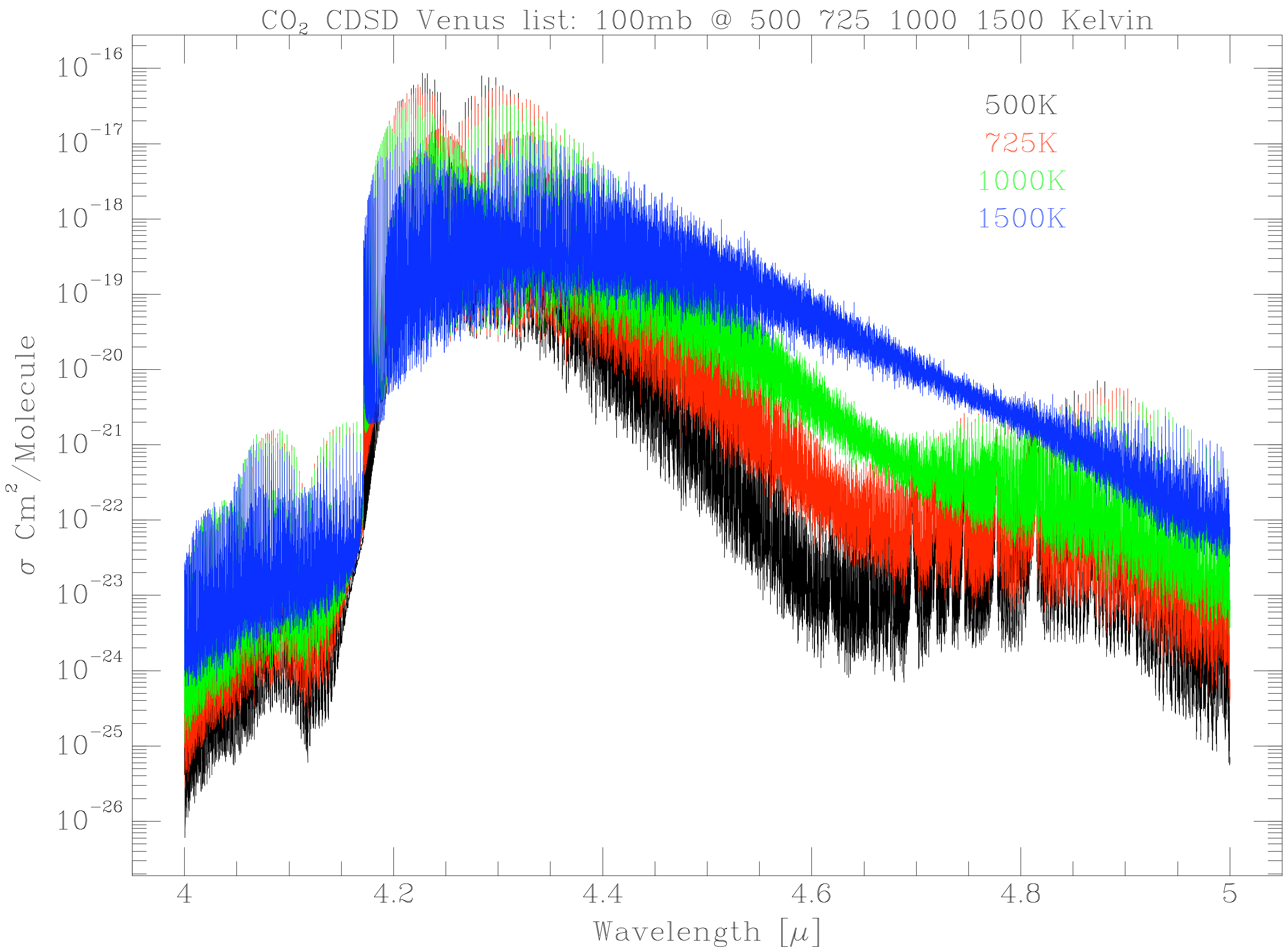
- Only the region around the 4.3 µm band is being considered as that region is also near a minimum of H_2O absorption and is therefore suitable for a search for the presence of CO_2



CO_2 in the 4.3 μ band at 4 temperatures

- Note that it is the weaker transitions which originate from excited energy levels that increase the most in a relative sense at high temperatures

- These calculations were applied to the file of the summed opacity of all molecules and the alkali atoms to show the effect of including CO_2 at a non-equilibrium abundance



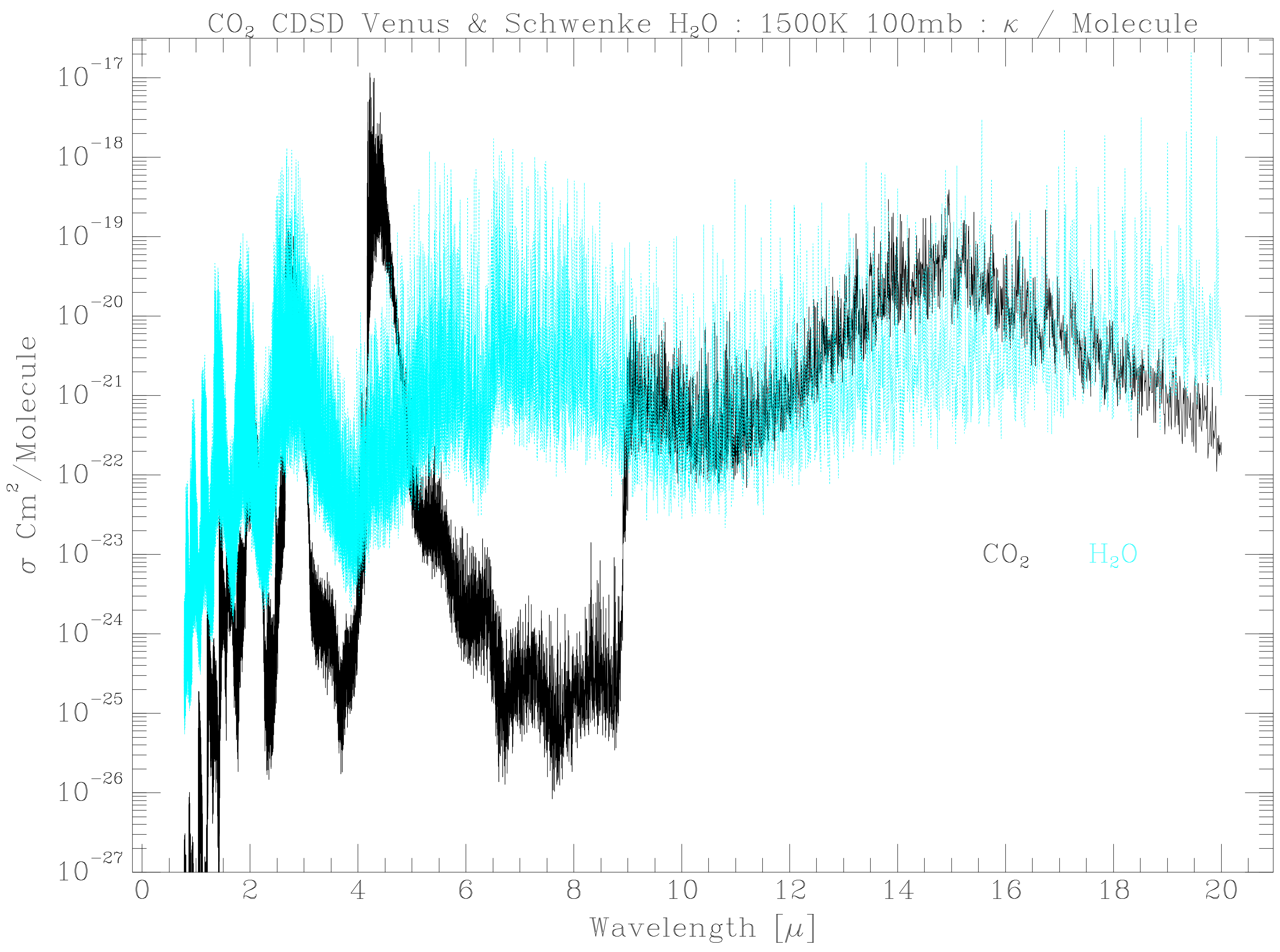
- Because the 4.3 µm band is opaque even at the operating altitude of SOFIA, observations from space will be required to observe in the 4.3µm wavelength region

- There is another region at ~ 1.05 µm which is near a minimum in the H_2O opacity that could be used to detect CO_2 if its abundance were high enough. This region is also relatively transparent in the earth's atmosphere, however the intrinsic strength of CO_2 absorption in this region is not really large enough for a detection unless the abundance greatly exceeds the equilibrium value and is much greater than the 100X case show here.

Comparison of the opacity of CO_2 and H_2O per molecule

- The 4.3μm band of CO_2 is the best placed to be detected in relation to the opacity of H_2O which is a major source of opacity

- The 4.3μm cannot be observed from the ground because the atmosphere is opaque in this band even at aircraft altitudes

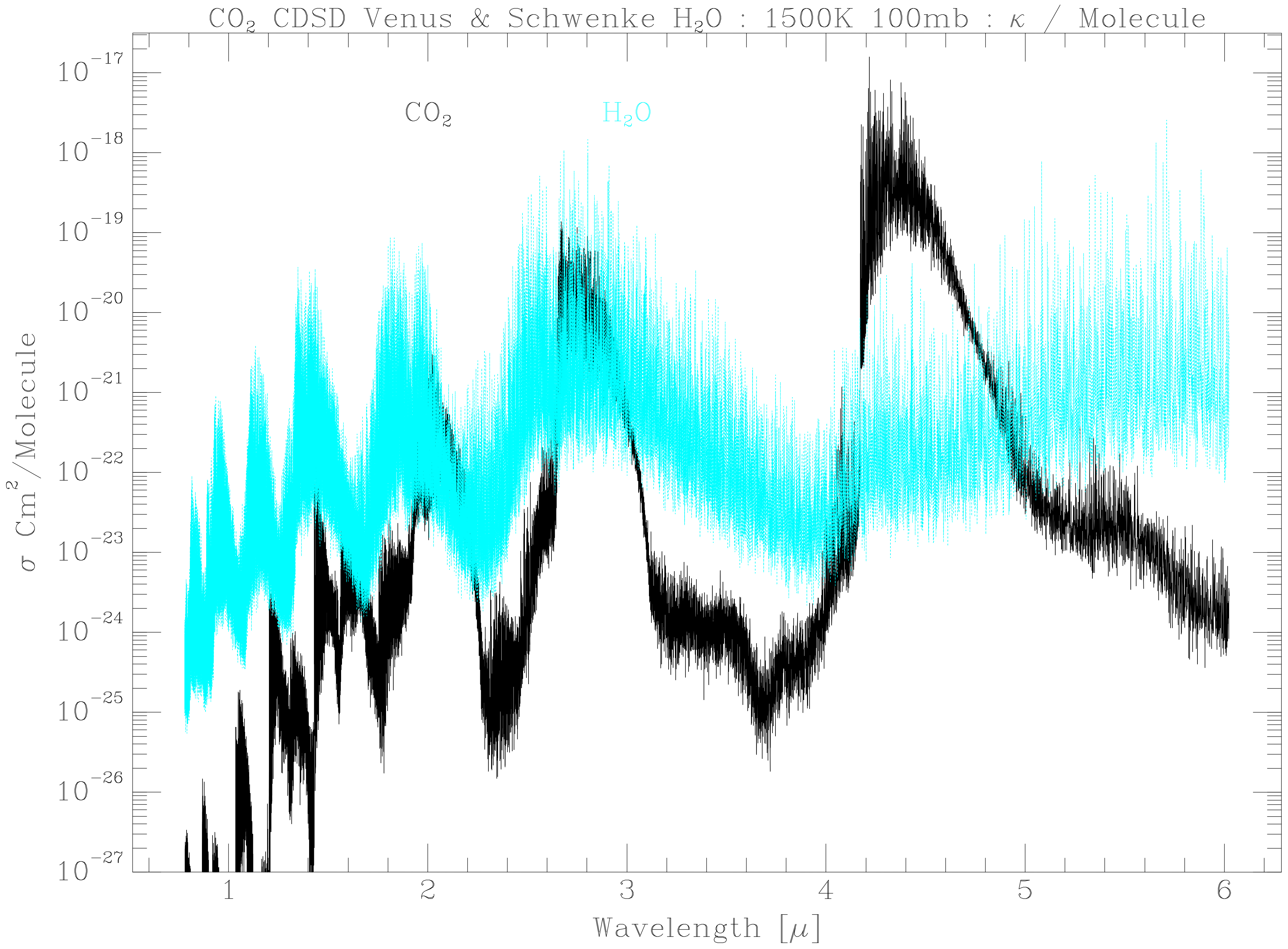


A blowup of the short wavelength region

- Assuming equilibrium chemistry and solar abundances the relative abundance of CO_2 is less than that of H_2O by at least a factor of 1000 in most of the regions where it exists in any appreciable quantity

- Non-equilibrium situations may allow detection of CO_2

- Although the atmosphere is relatively transparent at ~ 1.05µm the CO_2 opacity there is still too low relative to H_2O to be important in most cases



Notes and References

- Russian CO_2 data: JQSRT 82 (2003) 165-196, CDSD-1000, the high temperature carbon dioxide spectroscopic databank, S.A. Tashkuna, V.I. Perevalova, J-L. Tebob, A.D. Bykova, N.N. Lavrentievaa

- JQSRT 48 (1992) 537-566, Energy levels, intensities, and linewidths of atmospheric carbon dioxide bands, Rothman, L. S. and Hawkins, R.L. and Wattson, R.B. and Gamache, R.R.

- There are other articles about the techniques used by Wattson and Rothman in their calculations as applied to CO_2 & H_2O

- The technique used by Wattson and Rothman is known as the DND or direct numerical diagonalization technique

- The methods used by D. Schwenke involve techniques closer to ab-initio quantum mechanical techniques