A preliminary line list for methane up to 1500K

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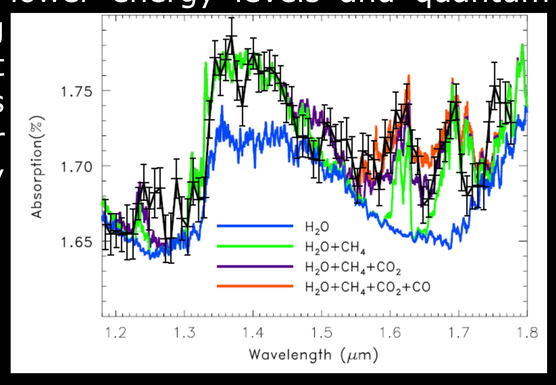
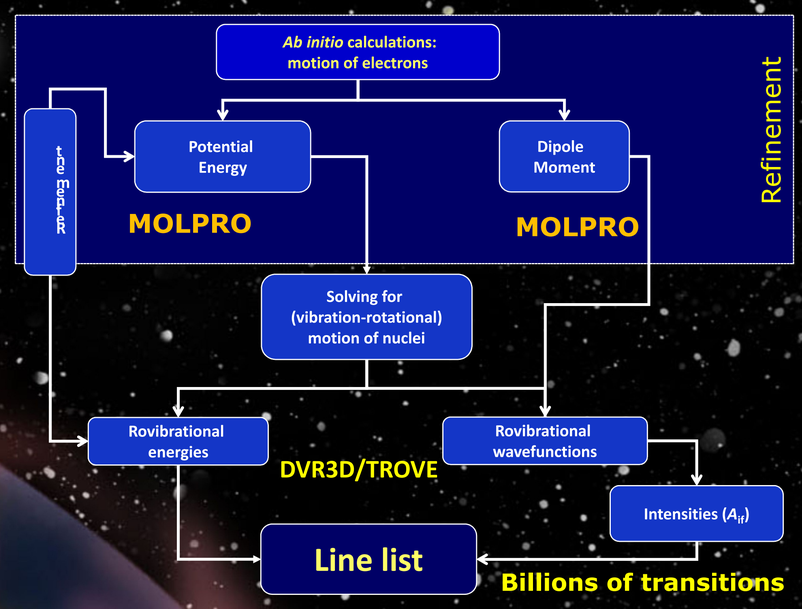
Methane plays an important role in atmospheric and astrophysical chemistry. Its rotation–vibration spectrum is of key importance for models of the atmospheres of bodies ranging from Titan to brown dwarfs. However the lack of precise data on methane spectra, particularly at higher temperatures, has severely limited models for atmospheres as diverse as Jupiter, exoplanets and brown dwarfs and made it diffifult to determine its actual quantity. Consequently we have embarked on a major project ExoMol [1] to fill this gap. Here we present a prelimenary line list for methane containing almost ten billion transition that should be sufficiently complete and accurate to replicate observed spectra at temperatures up to 1500 K. This computationally-derived line list details transition frequencies and associated Einstein coefficients, lower energy levels and quantum numbers. Hot temperature spectra of methane simulated using this line list will be presented and compared to different experimental spectra of methane available in the literature as well as generated using other line lists. Our '10to10' line list for CH4 will be suitable for use in modelling the spectra of planetary and stellar objects.

[1] J. Tennyson and S. N. Yurchenko, *Mon. Not. R. Astron. Soc.* **2012**, *425*, 21.



Primary transit spectrum of XO-1b Tinetti, ApJ 2010

Line list from first principles

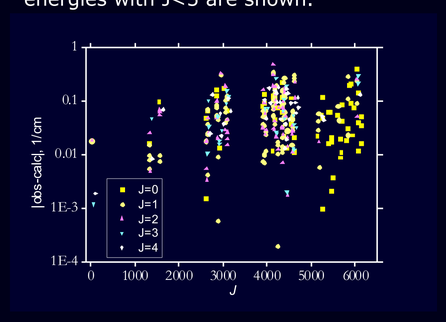


Variational calculations

The variational TROVE program was used to calculate the energy values and wavefunctions with an ab initio dipole moment surface [Yurchenko, JMS 2013] and empirically refined potential energy surface.

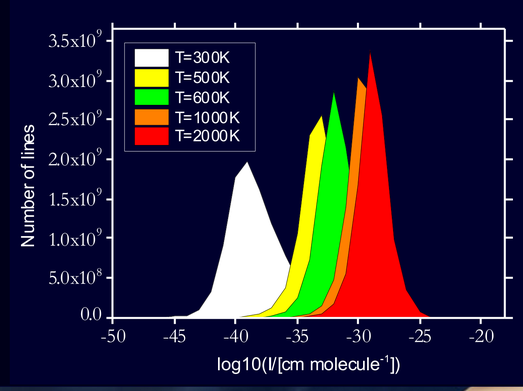
The accuracy of the 'spectroscopic' PES:

The obs-calc. residuals for all experimental energies with J<5 are shown.

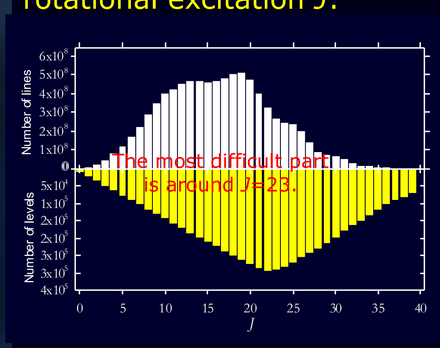


Weak transitions become strong at high *T*:

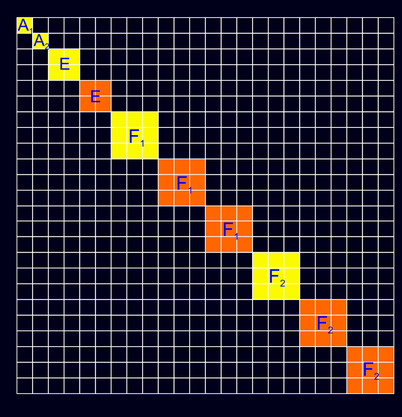
The number of strong lines grows significantly at high temperatures. For example, at *T*=2000K the maximal number of transitions have intensities of 10^{-28} cm/molecule.



The number of lines and energies against the rotational excitation *J*:

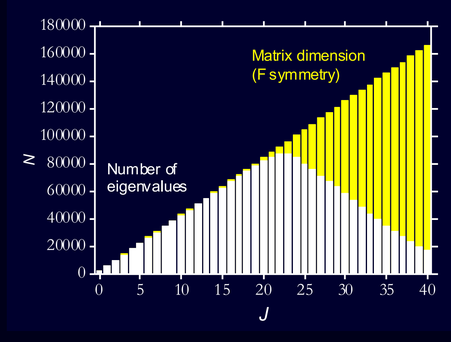


A general structure of the Hamiltonian matrix



The size of the F_2 matrix to be diagonalized and the number of eigenstates energies against *J*:

The number of states is controlled by the energy threshold, *E*=18000 cm^{-1}. The maximal *J*=39 value is defined by the lower state energy threshold, E=8000 cm^{-1}. At J>30 all energies are higher than 8000 cm^{-1}.

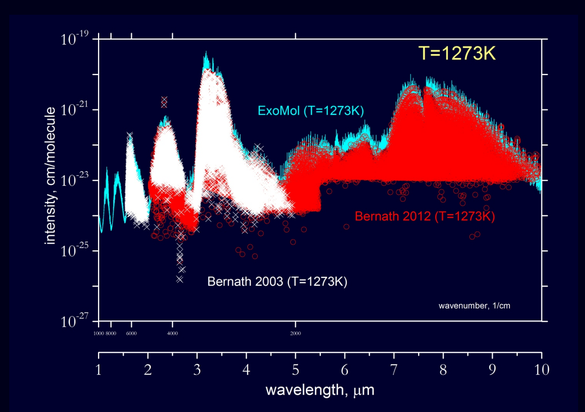


Size of the problem

Results

CH_4 hot spectrum

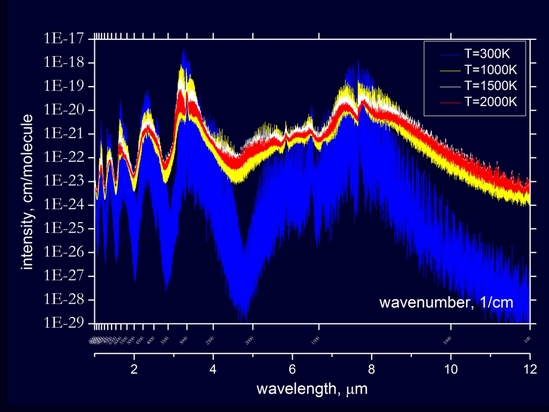
Here we compare our intensities (T=1275) with the experimental spectra of methane at T=1300K.



Nassar and Bernath, *JQSRT* **82**, 279 (2003)
Hargreaves et al, *ApJ* **757**, 46 (2003)

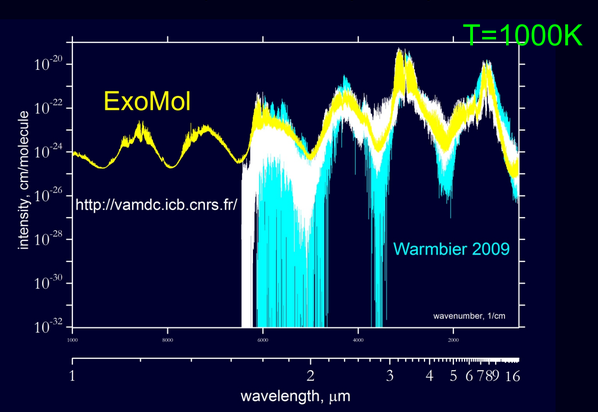
CH_4 spectra: Temperature effect

At high temperatures the band structure of the spectrum is flattened.



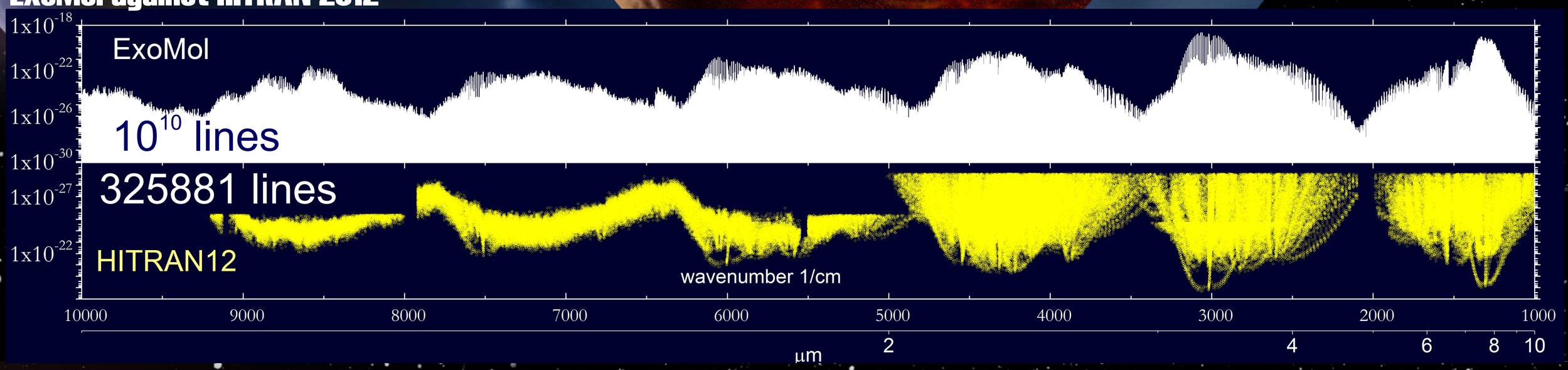
Comparison with other theoretical line lists (T=1000K):

Here we compare the ExoMol room temperature cross sections with that by Nikitin 2013 (VAMDC).



Nikitin, Boudon, Wenger, Albert, Brown, Bauerecker, Quack, *PCCP* **15**, 10071 (2013)
Warmbier, Schneider, Sharma, Braams, Bowman, P. H. Hauschildt A&A 495, 655 (2009)

ExoMol against HITRAN 2012



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