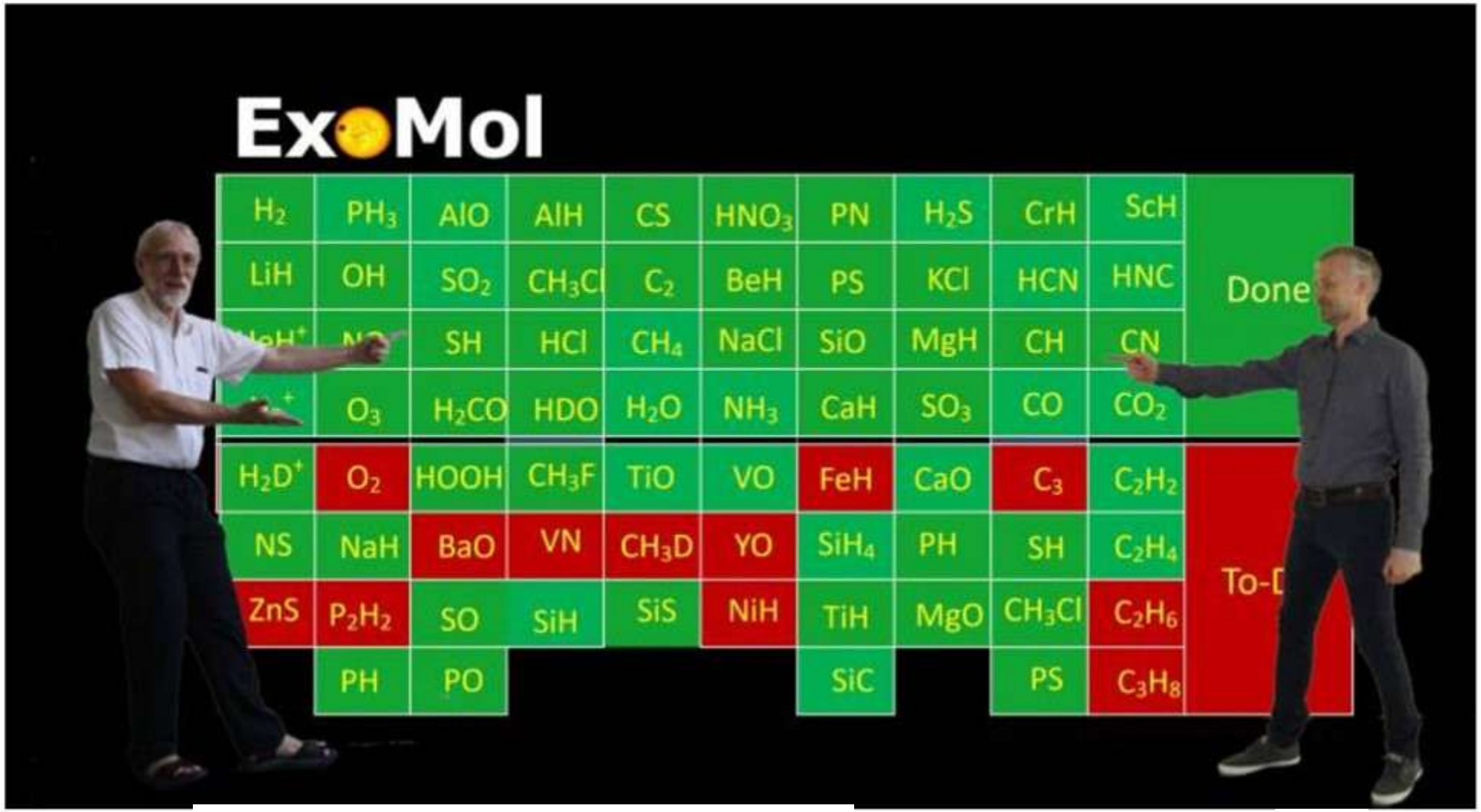
Databases : ExoMol

Tennyson et al, JQSRT 2020

Mixture of ab initio calculations and laboratory data



```
# The list of spectral lines. HITRAN-2004 format
# HITRAN. Molecule CH4. Isotopologue(s): 211.
# Wavenumber range: 2000.000000-4000.000000 cm-1, T: 296 K, P: 1 atm, Scut: 1e-20 cm/molecule
#MI WN,cm-1     S,cm/mol  A,s-1    Lenv Lself El,cm-1  Nt  Pshift  GQNup          GQNlow         LQNup          LQNlow         Ierr  Iref          * SWup   SWlow

 61 2894.996098 1.109e-20 1.913e+01.04700.067  815.14360.65-.002000    0 0 1 0 1F2    0 0 0 0 1A1   11A2 15        12A1  2     765343463631 3 2 2   115.0  125.0
 61 2895.233319 1.102e-20 1.901e+01.04950.067  815.08900.65-.012300    0 0 1 0 1F2    0 0 0 0 1A1   11A1 14        12A2  1     765343463631 3 2 2   115.0  125.0
 61 2896.990180 1.116e-20 1.923e+01.04760.067  814.64600.65-.009250    0 0 1 0 1F2    0 0 0 0 1A1   11A2 16        12A1  1     765343463633 3 4 4   115.0  125.0
 61 2905.633661 1.132e-20 1.955e+01.05000.068  690.04920.65-.001200    0 0 1 0 1F2    0 0 0 0 1A1   10F2 41        11F1  3     765343463631 3 2 2    63.0   69.0
 61 2905.813742 1.140e-20 1.969e+01.05000.068  690.01740.65-.006000    0 0 1 0 1F2    0 0 0 0 1A1   10F1 39        11F2  3     765343464731 3 2 2    63.0   69.0
 61 2906.282471 1.106e-20 1.910e+01.05410.068  689.95670.65-.007700    0 0 1 0 1F2    0 0 0 0 1A1   10F2 42        11F1  2     765343463631 3 2 2    63.0   69.0
 61 2906.647628 1.110e-20 1.916e+01.05360.068  689.87670.65-.005000    0 0 1 0 1F2    0 0 0 0 1A1   10F1 40        11F2  2     765343463631 3 2 2    63.0   69.0
 61 2906.734957 1.859e-20 1.926e+01.05380.068  689.86210.65-.008520    0 0 1 0 1F2    0 0 0 0 1A1   10A1 15        11A2  1     765343463633 3 4 4   105.0  115.0
 61 2907.321273 1.141e-20 1.969e+01.05020.068  689.70750.65-.008960    0 0 1 0 1F2    0 0 0 0 1A1   10F1 41        11F2  1     765343463633 3 4 4    63.0   69.0
 61 2907.336088 1.141e-20 1.969e+01.04980.068  689.70520.65-.009000    0 0 1 0 1F2    0 0 0 0 1A1   10F2 43        11F1  1     765343463633 3 4 4    63.0   69.0
 61 2916.201625 1.836e-20 2.021e+01.05910.070  575.28520.670.000300    0 0 1 0 1F2    0 0 0 0 1A1    9F1 37        10F2  3     765343464731 3 2 2    57.0   63.0
 61 2916.301842 1.207e-20 1.992e+01.04270.070  575.27170.64-.005500    0 0 1 0 1F2    0 0 0 0 1A1    9E  24        10E   2     765343463631 3 2 2    38.0   42.0
 61 2916.396322 1.787e-20 1.967e+01.05690.070  575.25960.67-.011200    0 0 1 0 1F2    0 0 0 0 1A1    9F2 36        10F1  2     765343463631 3 2 2    57.0   63.0
 61 2916.753786 2.962e-20 1.956e+01.05650.070  575.22270.67-.008280    0 0 1 0 1F2    0 0 0 0 1A1    9A2 14        10A1  1     765343463633 3 4 4    95.0  105.0
 61 2916.966220 1.770e-20 1.948e+01.05910.070  575.18410.67-.004300    0 0 1 0 1F2    0 0 0 0 1A1    9F2 37        10F1  1     765343463631 3 2 2    57.0   63.0
 61 2917.066127 1.788e-20 1.968e+01.05550.070  575.16990.67-.008400    0 0 1 0 1F2    0 0 0 0 1A1    9F1 38        10F2  2     765343463631 3 2 2    57.0   63.0
 61 2917.629074 3.055e-20 2.017e+01.05440.070  575.05550.67-.008680    0 0 1 0 1F2    0 0 0 0 1A1    9A1 12        10A2  1     765343463631 3 2 2    95.0  105.0
 61 2917.652561 1.831e-20 2.015e+01.04830.070  575.05250.67-.002700    0 0 1 0 1F2    0 0 0 0 1A1    9F1 39        10F2  1     765343463631 3 2 2    57.0   63.0
 61 2917.662838 1.222e-20 2.017e+01.04830.070  575.05110.64-.005835    0 0 1 0 1F2    0 0 0 0 1A1    9E  25        10E   1     765343463631 3 2 2    38.0   42.0
 61 2926.700231 4.583e-20 2.051e+01.06110.073  470.87270.67-.000200    0 0 1 0 1F2    0 0 0 0 1A1    8A1 12         9A2  1     765343463631 3 2 2    85.0   95.0
 61 2926.782987 2.736e-20 2.040e+01.05820.073  470.86490.67-.007690    0 0 1 0 1F2    0 0 0 0 1A1    8F1 32         9F2  2     765343463633 3 4 4    51.0   57.0
 61 2926.885111 2.709e-20 2.020e+01.05830.073  470.85480.67-.007740    0 0 1 0 1F2    0 0 0 0 1A1    8F2 33         9F1  3     765343463633 3 4 4    51.0   57.0
 61 2927.076189 4.546e-20 2.034e+01.05850.073  470.83080.67-.007600    0 0 1 0 1F2    0 0 0 0 1A1    8A2 10         9A1  1     765343463633 3 4 4    85.0   95.0
 61 2927.372646 2.682e-20 2.000e+01.05750.073  470.80510.67-.008040    0 0 1 0 1F2    0 0 0 0 1A1    8F2 34         9F1  2     765343463633 3 4 4    51.0   57.0
 61 2927.429168 1.800e-20 2.014e+01.05000.073  470.79880.65-.005800    0 0 1 0 1F2    0 0 0 0 1A1    8E  23         9E   1     764332 53638 7 1 7    34.0   38.0
 61 2927.932131 2.765e-20 2.062e+01.06330.073  470.72020.67-.008390    0 0 1 0 1F2    0 0 0 0 1A1    8F1 33         9F2  1     765343463631 3 2 2    51.0   57.0
 61 2927.963557 2.765e-20 2.062e+01.05370.073  470.71680.67-.008480    0 0 1 0 1F2    0 0 0 0 1A1    8F2 35         9F1  1     765343463633 3 4 4    51.0   57.0
 61 2937.234649 3.880e-20 2.091e+01.05500.074  376.82610.72-.006700    0 0 1 0 1F2    0 0 0 0 1A1    7F1 30         8F2  2     765343463631 3 2 2    45.0   51.0
 61 2937.308180 2.571e-20 2.079e+01.04770.074  376.82110.69-.005200    0 0 1 0 1F2    0 0 0 0 1A1    7E  19         8E   2     765343463631 3 2 2    30.0   34.0
 61 2937.495038 3.853e-20 2.077e+01.05680.074  376.80460.72-.002000    0 0 1 0 1F2    0 0 0 0 1A1    7F2 28         8F1  2     765343463631 3 2 2    45.0   51.0
 61 2937.767224 3.817e-20 2.058e+01.05890.074  376.78570.72-.006700    0 0 1 0 1F2    0 0 0 0 1A1    7F1 31         8F2  1     765343463631 3 2 2    45.0   51.0
 61 2938.192639 2.606e-20 2.107e+01.05890.074  376.73550.69-.001000    0 0 1 0 1F2    0 0 0 0 1A1    7E  20         8E   1     765343463631 3 2 2    30.0   34.0
 61 2938.215410 3.910e-20 2.108e+01.05610.074  376.73360.72-.008360    0 0 1 0 1F2    0 0 0 0 1A1    7F2 29         8F1  1     765343463633 3 4 4    45.0   51.0
 61 2938.251832 6.530e-20 2.112e+01.05250.074  376.73030.72-.008000    0 0 1 0 1F2    0 0 0 0 1A1    7A2 11         8A1  1     765343463631 3 2 2    75.0   85.0
 61 2947.667995 5.128e-20 2.139e+01.05710.075  293.17850.73-.005100    0 0 1 0 1F2    0 0 0 0 1A1    6F2 26         7F1  2     765343463631 3 2 2    39.0   45.0
 61 2947.810950 3.406e-20 2.131e+01.04850.075  293.17000.70-.005100    0 0 1 0 1F2    0 0 0 0 1A1    6E  17         7E   1     765343463631 3 2 2    26.0   30.0
 61 2947.912105 5.069e-20 2.114e+01.06340.075  293.16440.73-.003800    0 0 1 0 1F2    0 0 0 0 1A1    6F1 24         7F2  2     765343463631 3 2 2    39.0   45.0
 61 2948.107945 8.412e-20 2.105e+01.05990.075  293.15410.73-.007090    0 0 1 0 1F2    0 0 0 0 1A1    6A1 10         7A2  1     765343463631 3 2 2    65.0   75.0
 61 2948.421423 5.149e-20 2.148e+01.06340.075  293.12640.73-.003800    0 0 1 0 1F2    0 0 0 0 1A1    6F1 25         7F2  1     765343463631 3 2 2    39.0   45.0
 61 2948.474107 5.171e-20 2.157e+01.05780.075  293.12290.73-.006880    0 0 1 0 1F2    0 0 0 0 1A1    6F2 27         7F1  1     765343463631 3 2 2    39.0   45.0
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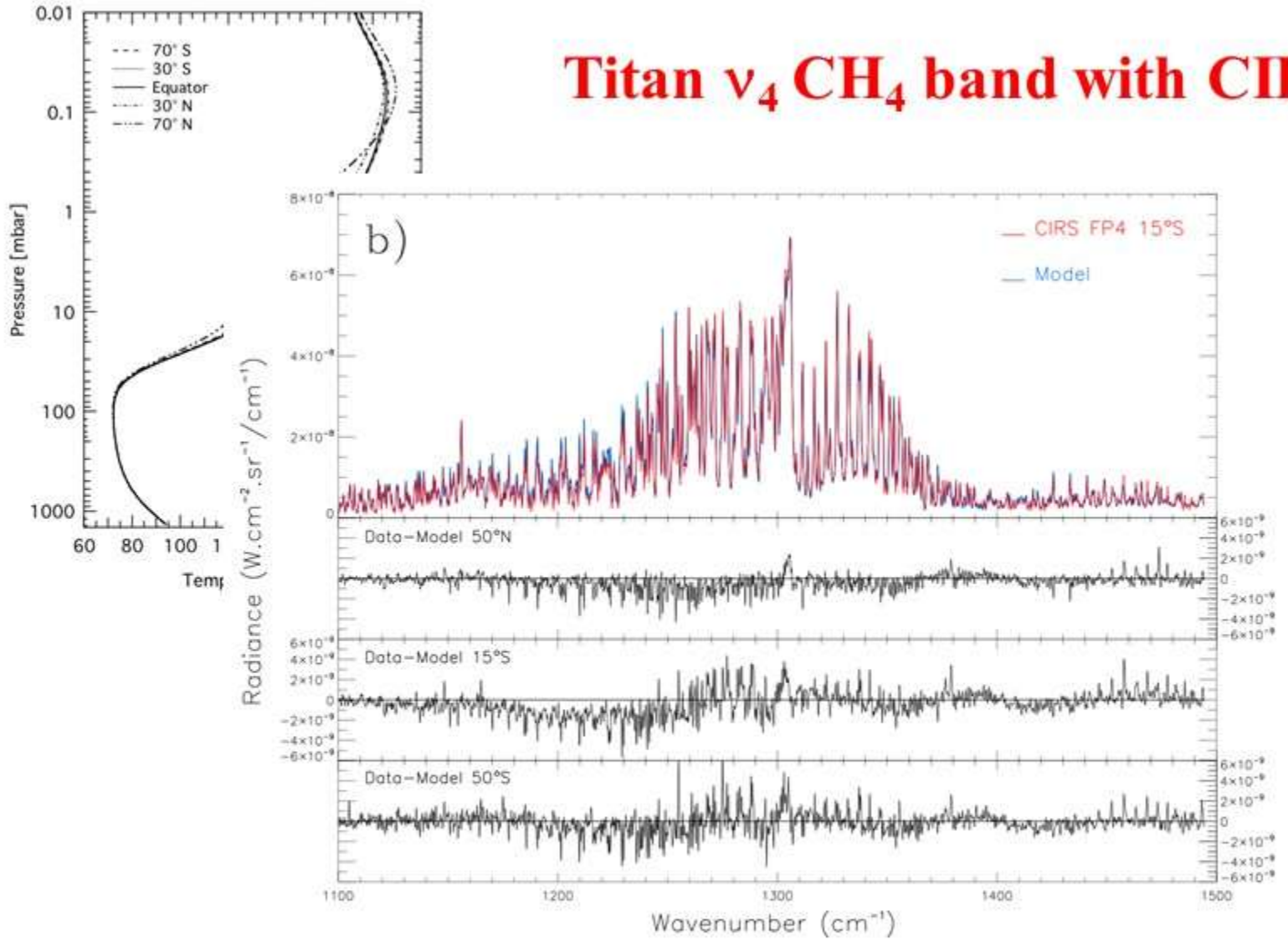
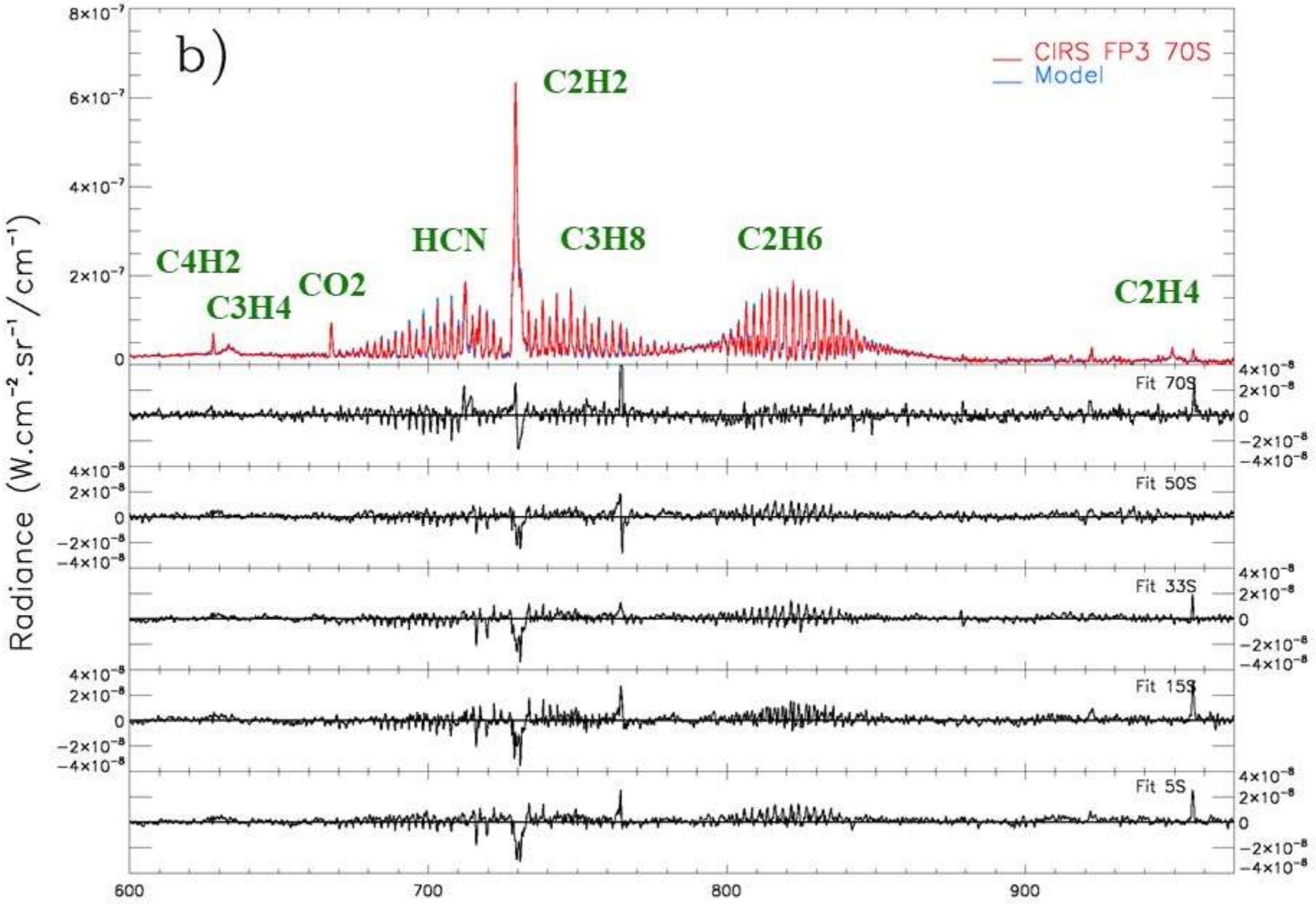
Application to planetary spectroscopy

Infrared spectra are the main domain for identifying molecular composition of planets from their rotation-vibration transitions

Titan ν_4 CH_4 band with CIRS



Coustenis et al., 2007



Coustenis et al., 2009

Application to exoplanets

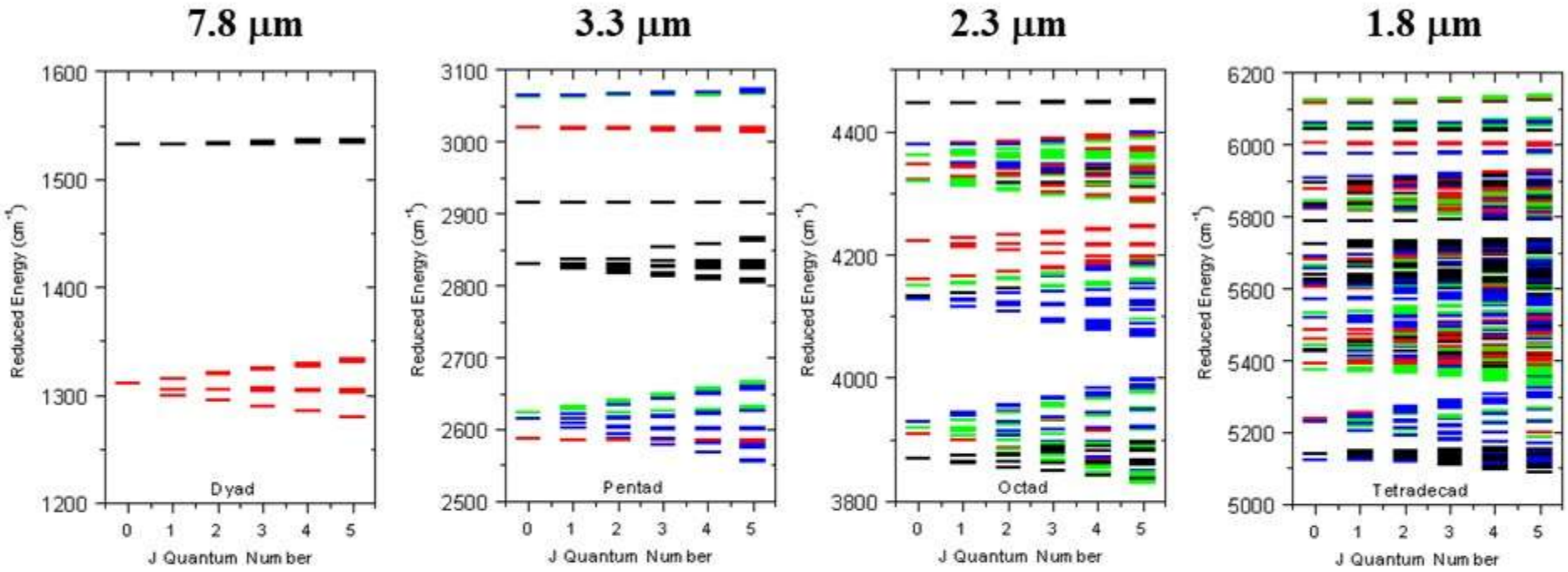
The spectroscopy of exoplanets collect the most challenging parts for spectroscopy : high temperatures (=> high J, hot vibrational bands), large number of molecules and complex atmospheric structures

Difficulties for high temperature spectra

- Large number of overtones
- Accuracy of the database (missing bands, accuracy of coefficients at high temperatures)

The need for continued research in cooperation with spectroscopic group is mandatory to adapt the needs of exoplanets community with spectroscopic research !

CH_4 : vibration/rotation bands

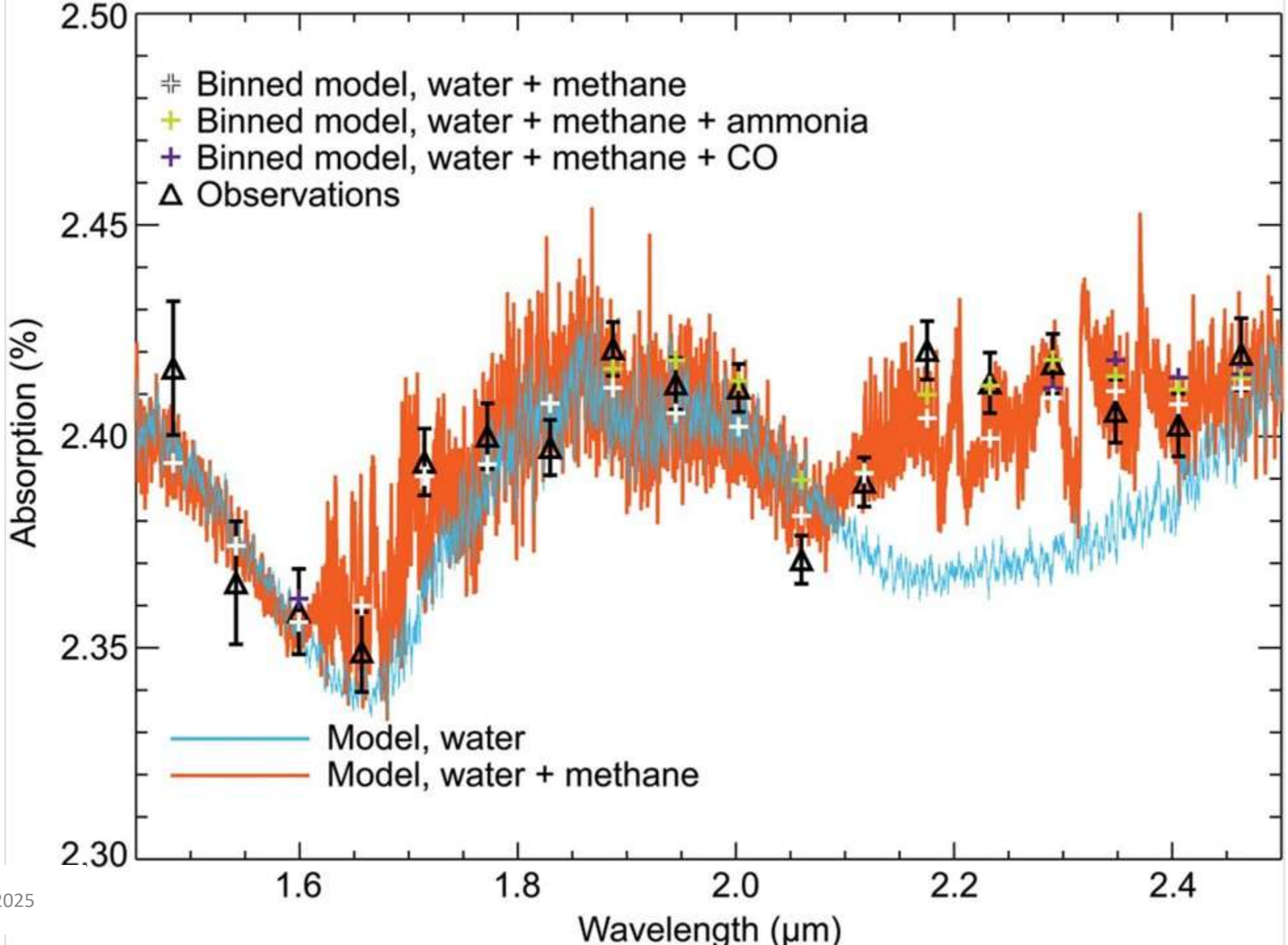


Dyad
2 vibrational states
2 sublevels

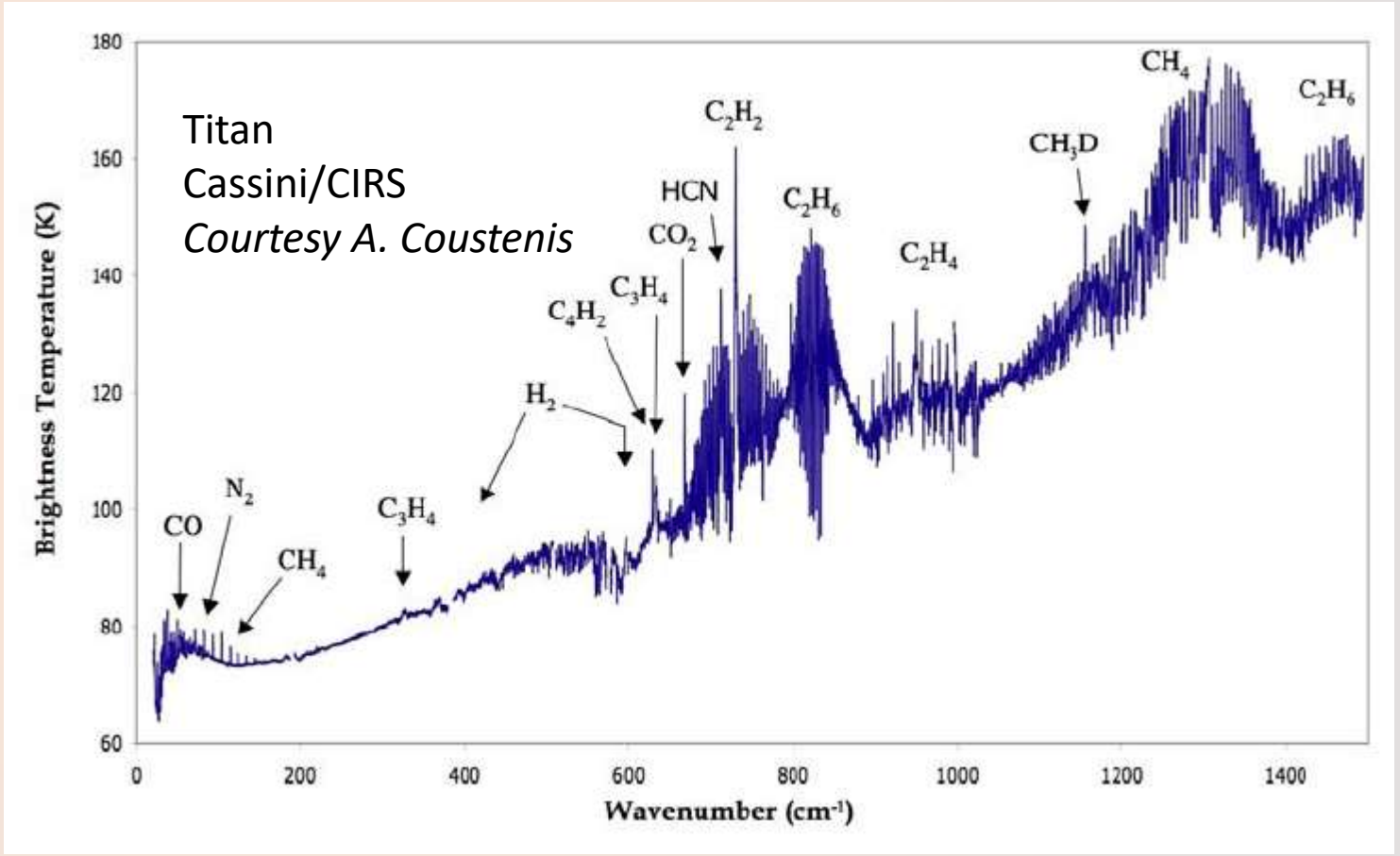
Pentad
5 vibrational states
9 sublevels

Octad
8 vibrational states
20 sublevels

Tetradecad
14 vibrational states
60 sublevels


Binned model, water + methane
Binned model, water + methane + ammonia
Binned model, water + methane + CO
Observations
Model, water
Model, water + methane
Absorption (%)
Wavelength (μm)
2.50
2.45
2.40
2.35
2.30
1.6
1.8
2.0
2.2
2.4

Are you ready to include molecular spectroscopy in your preferred radiative transfer model ?



Credits

- Isabelle Kleiner, Les Houches course (Ariel school 2022)
- Herzberg : Infrared and Raman spectra of polyatomic molecules
- Hanson, Summer School on Combustion and the Environment, June 19-24, 2022, Princeton, NJ, USA

https://cefrc.princeton.edu/sites/g/files/toruqf1071/files/documents/Lecture%20Notes%20-%20Hanson.pdf

- Exomol : Tennyson et al, JQSRT 2020 (The 2020 release of the ExoMol database: Molecular line lists for exoplanet and other hot atmospheres)
- The spectroscopic community : I. Kleiner, M. Rey, V. Boudon, J. Tennyson, V. Tyuterev,… – *(Paris, Reims, Dijon, Rennes, London, Omsk)*

- Site of the University of Geneva : https://dace.unige.ch

The end