# Adapting ExoMol line lists for high-resolution studies: Methane as an example

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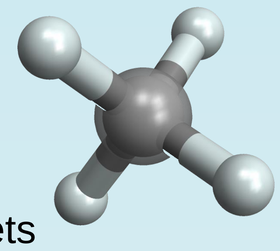
The **ExoMolHD** (ExoMol in High Definition) project delivers accurate molecular line lists tailored for the studies of exoplanetary atmospheres in the current era of high-resolution (R=100000) observations.

## Methane in Astrochemistry



- ✓ Brown dwarfs
- ✓ Hot atmospheres of exoplanets
- ✓ Biosignature on terrestrial planets

## **MARVELous Methane** line list

82000 experimental transitions from 100 sources [2]

Over 50 billion transitions were calculated with the variational program **TROVE** [3]

23000 Empirical energy levels computed with the **MARVEL**

Over 1 million line positions with experimental accuracy

## The **MARVEL** procedure

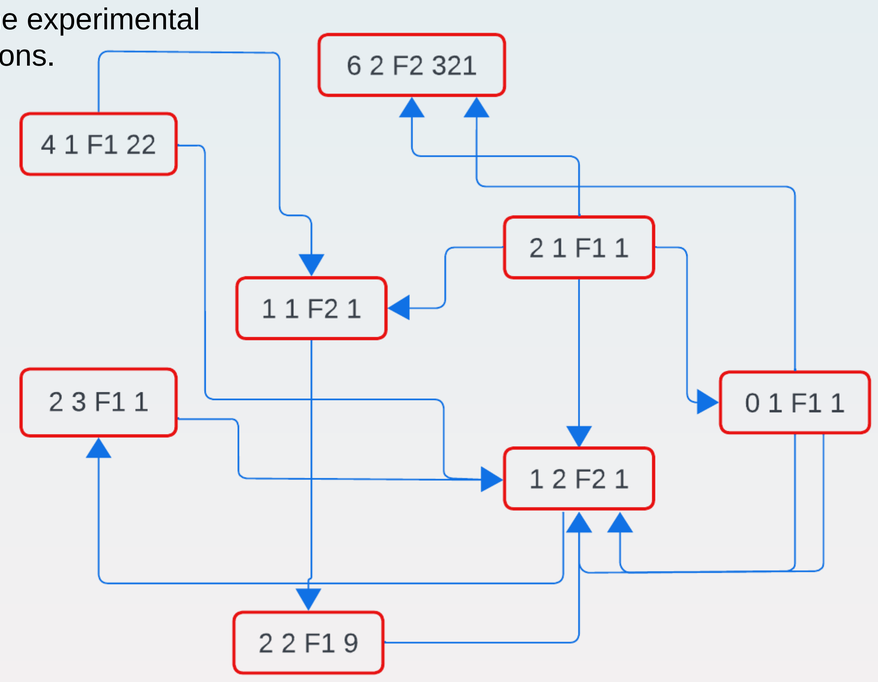
We are using **M**easured **A**ctive **V**ibration **E**nergy **L**evel algorithm [1] to determine accurate empirical energy levels for methane. The algorithm evaluates the self-consistency of our database and adjusts the uncertainties accordingly until a non-conflicting **spectroscopic network** of energy levels is achieved. MARVEL performs the inversion of the input transitions to compute the energy levels with their respective uncertainties.

## Quantum Numbers

The quantum numbers we are using here for methane are: p, J, C, n

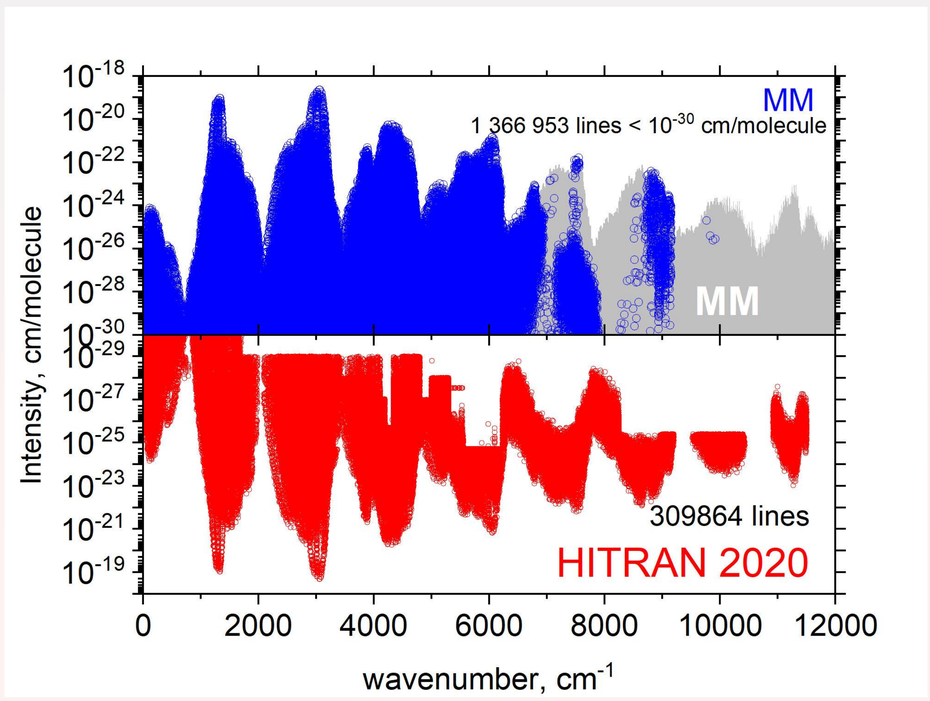
- p: Determining the vibrational level.
- J: The rotational quantum number
- C: The total symmetry: $A_1$, $A_2$, E, $F_1$, $F_2$
- n: A number that counts the levels with the same (C, J) within a polyad from lower to higher energy

Part of the ortho network of methane. The energy levels are labelled with the quantum numbers and the links between them represent the experimental transitions.

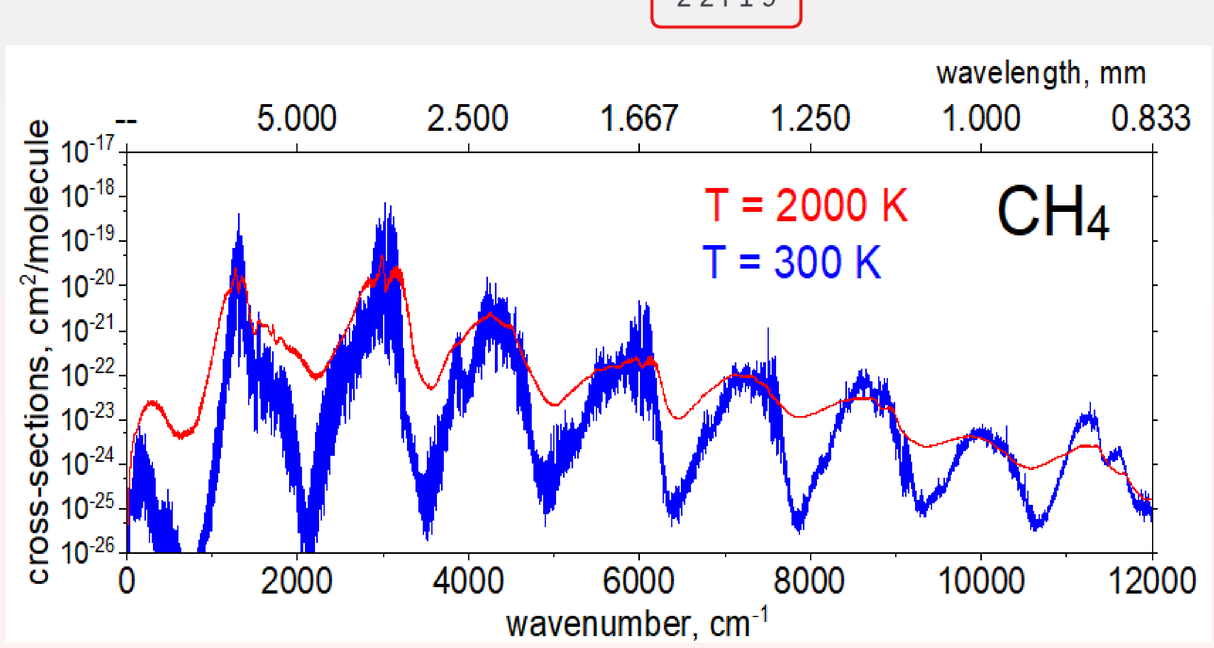



## Results

- ✓The MARVEL procedure derived over 23000 assigned energy levels with experimental accuracy for polyads 0 to 7.
- ✓The MARVELous Methane line list contains over 50 billion transitions in the range from 0 to 12000 $cm^{-1}$ with rotational excitation up to J= 60.




Comparison of the HITRAN (bottom) and MM (top) T=296 K spectra. The blue points on the top display show line intensities (cm/molecule) computed for the MARVELised states only, while the grey area indicates the full coverage in the line list. [4]




Cross sections of methane generated using the ExoMol line list 'MARVELous Methane' at T=300 K and 2000 K.

[1] Furtenbacher+ (2007 J. Molec. Spectrosc., 245, 115)
[2] Kefala+ (2024 J. Quant. Spectrosc. Radiat. Transf., 316, 108897)
[3] Yurchenko + (2007 J. Molec. Spectrosc, 245, 126)
[4] Yurchenko+ (2024 Mon. Not. Roy. Astron. Soc., 528, 3719)

**Looking for a postdoc!**

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The line list paper

The MARVEL paper