# Interstellar Dust : Solid $H_2$ ?

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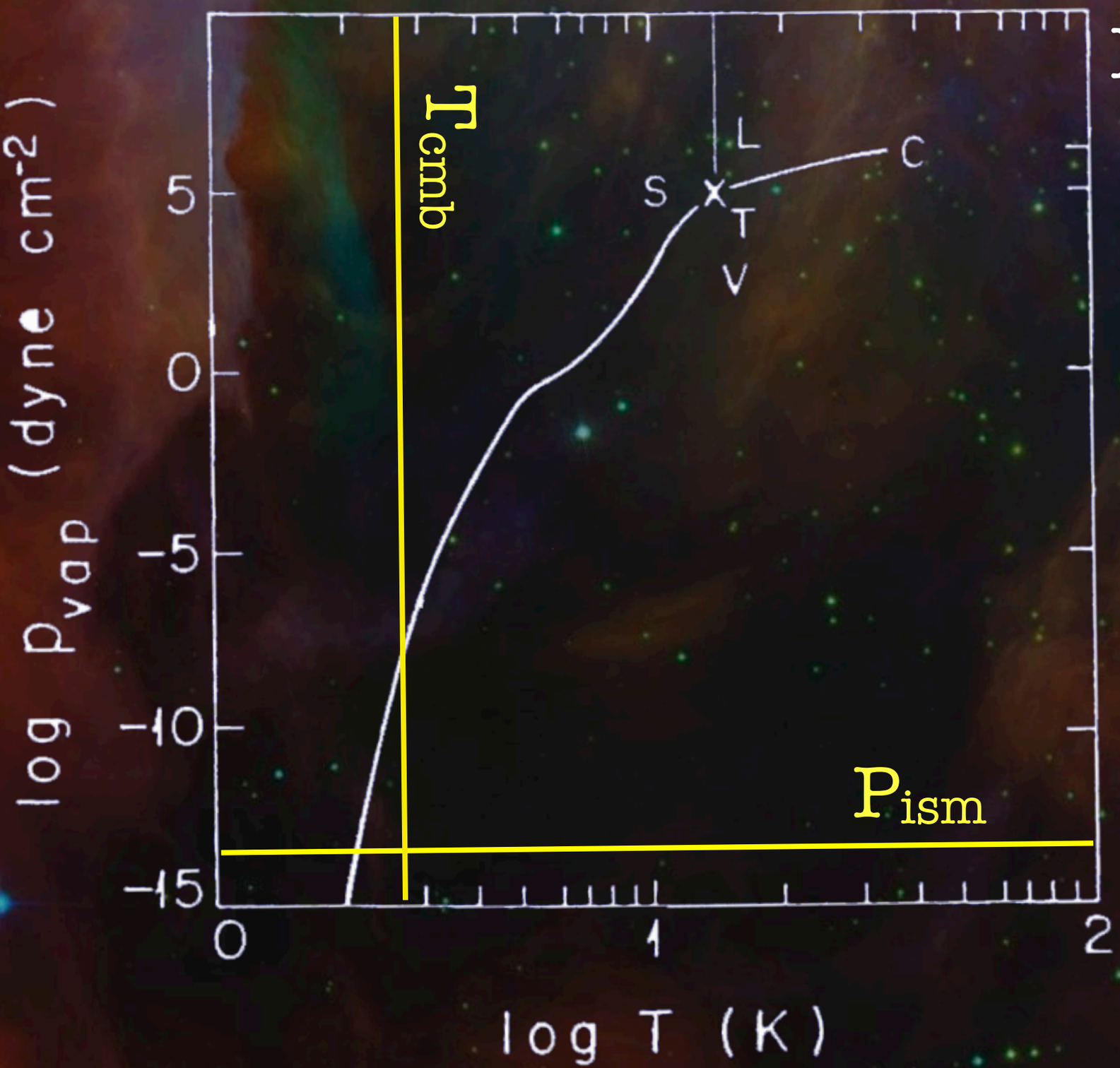
# Overview

- Motivation
- Properties of solid $H_2$
- Astrochemistry : $H_6^+$
- Q-Chem modelling of $H_6^+$ vibrations
- $H_6^+$ emission vs. astronomical data

# $H_2$ phase equilibrium

ESP 1985

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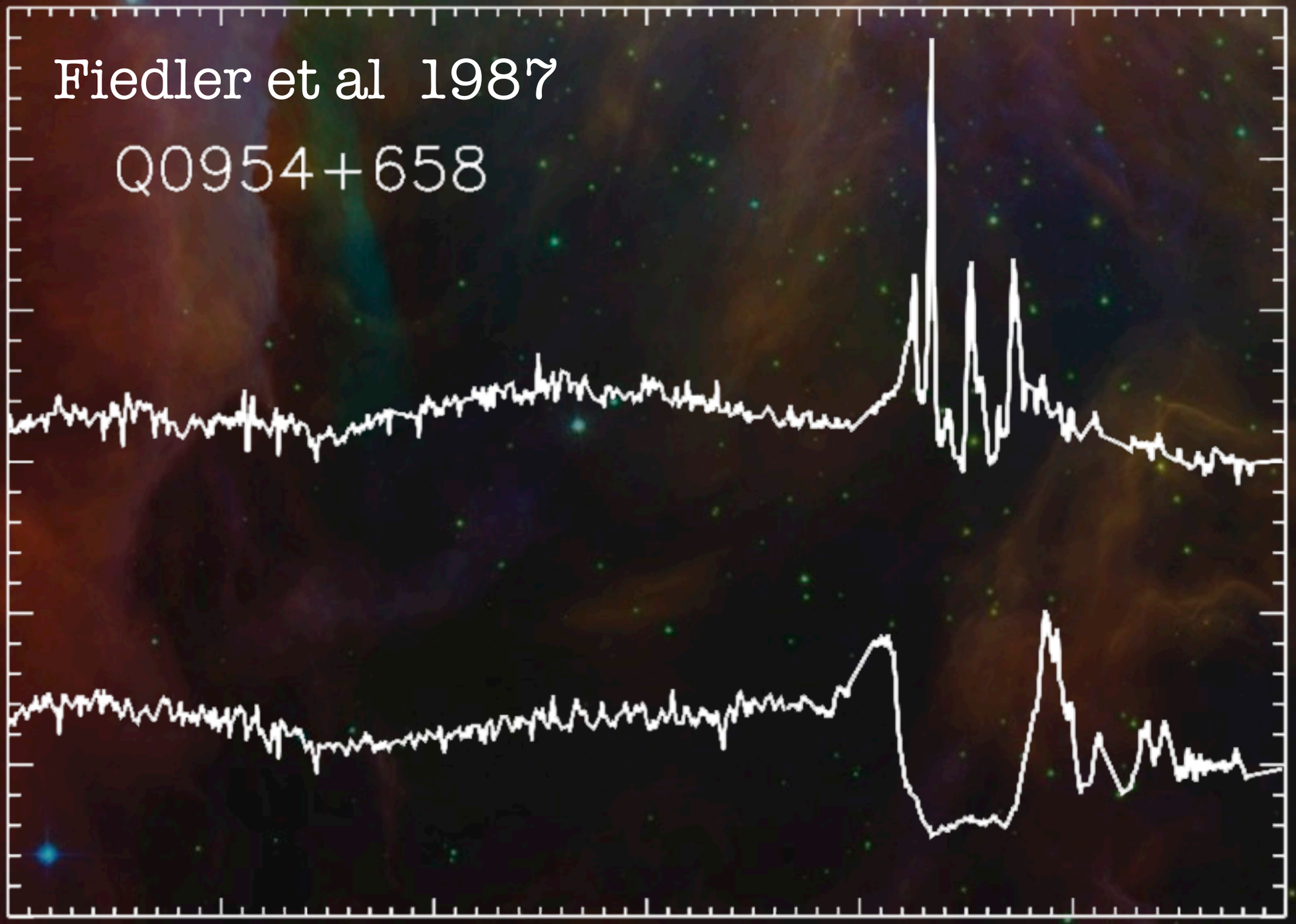
# Extreme Scattering Events

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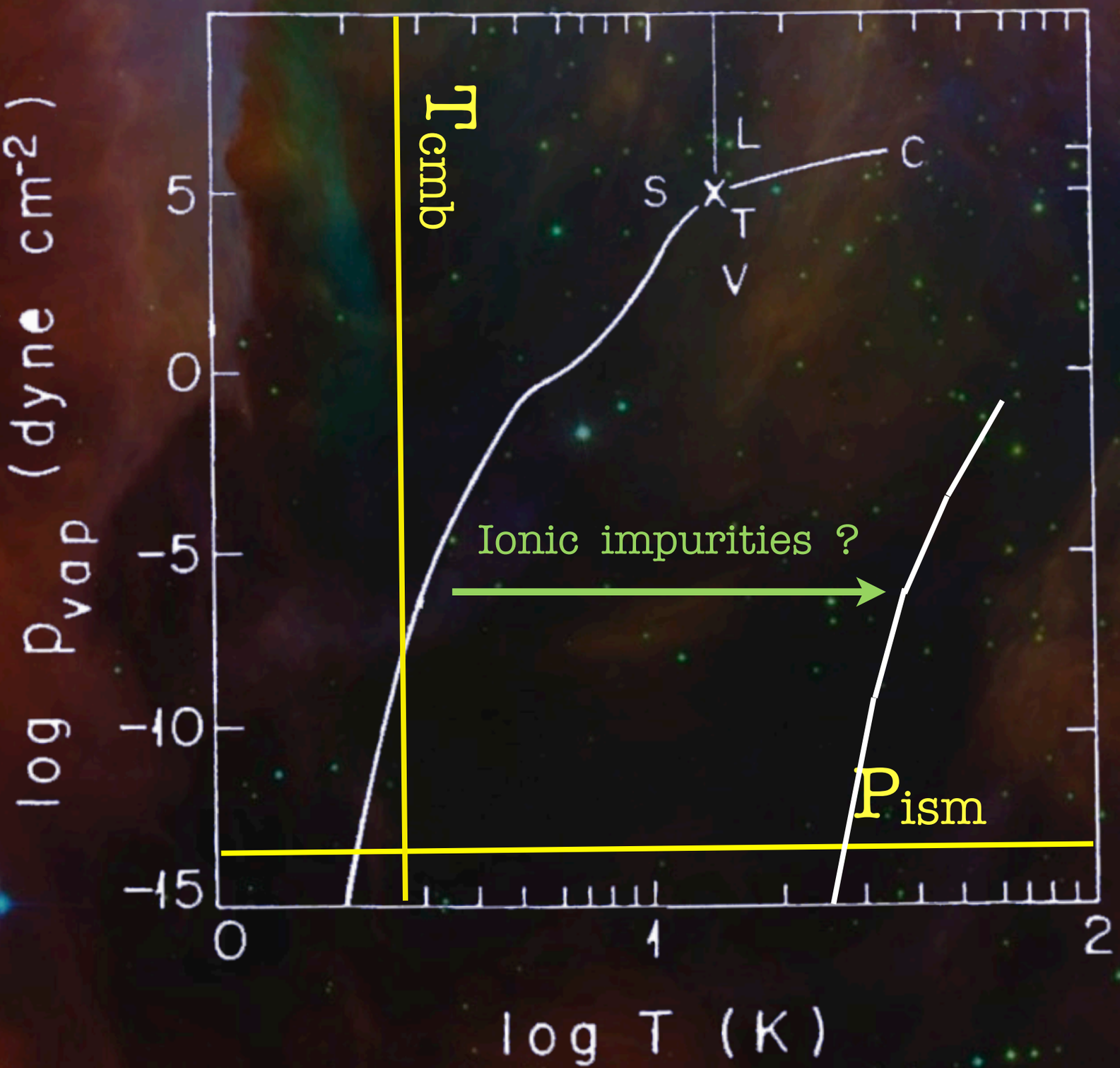
# $H_2$ with impurities

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# Properties of solid $H_2$

- Transparent in optical & IR
  - Refractive index = 1.13
  - Lyman & Werner bands in FUV
- Weak intermolecular forces
  - Used for matrix isolation spectroscopy

# Ionisation of solid $H_2$

Gas phase: $H_2^+ + H_2 \rightarrow H_3^+ + H$

Solid phase: $H_2^+ + 2\,H_2 \rightarrow H_6^+$

ESR : Miyazaki, Kumada, Kumagai, Shimizu ...
Theory : Symons, Woolley, Kurosaki, Takayanagi ...

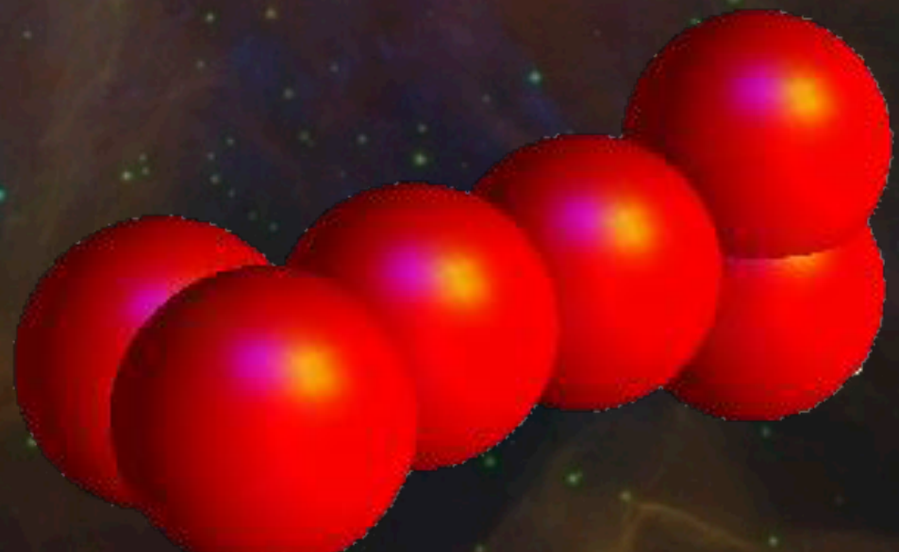
Isotopic condensation: $H_6^+ + 3\,HD \rightarrow (HD)_3^+ + 3\,H_2$

NO LAB SPECTROSCOPY !

# Ab Initio modelling of $H_6^+$

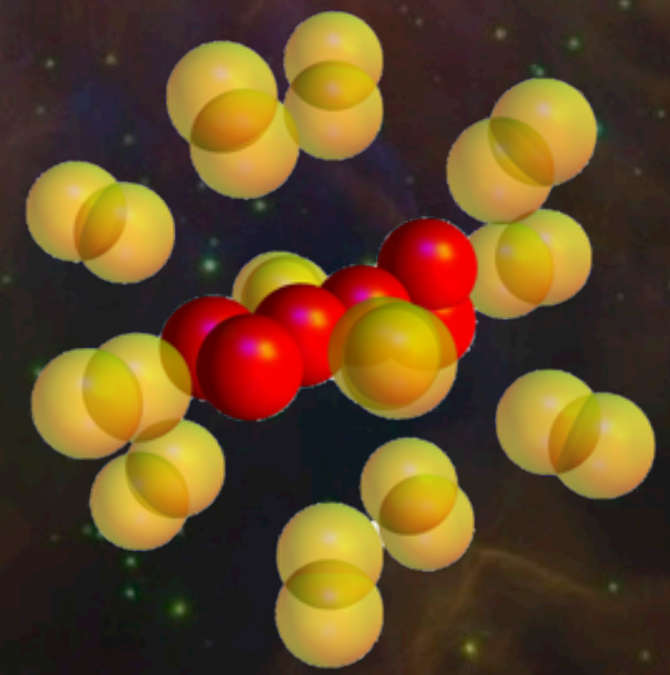
(Kurosaki & Takayanagi 1998)

Minimum energy configuration: $D_{2d}$



# Ab Initio modelling of $H_6^+$

(Kurosaki & Takayanagi 1998)



Minimum energy configuration: $D_{2d}$

On solvation :

Drastic change in rotational states

Drastic change in electronic states

Little change in vibrational states

# Ab Initio modelling of $H_6^+$

12 vibration modes

Can only model 5

CCSD + cc-pVTZ

Highly anharmonic :

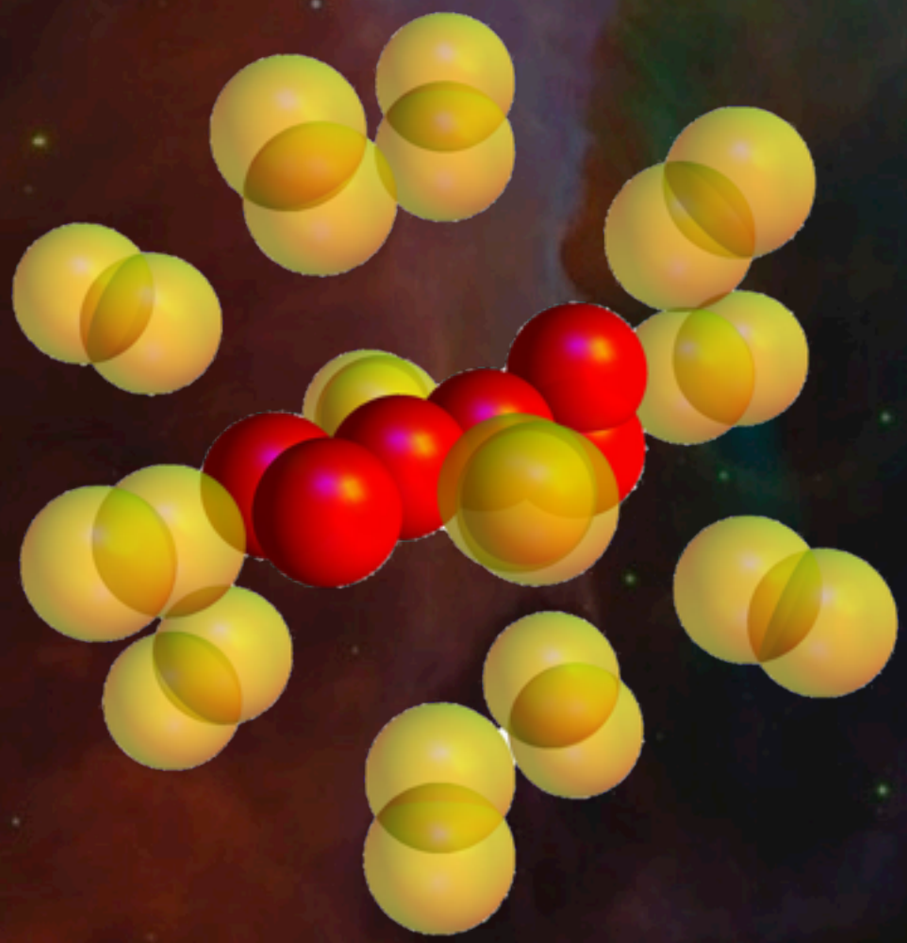
Include cubic & quartic

Use VCI method

Large isotopic shifts

Solvation shifts by reference to $H_6^+(H_2)_4$

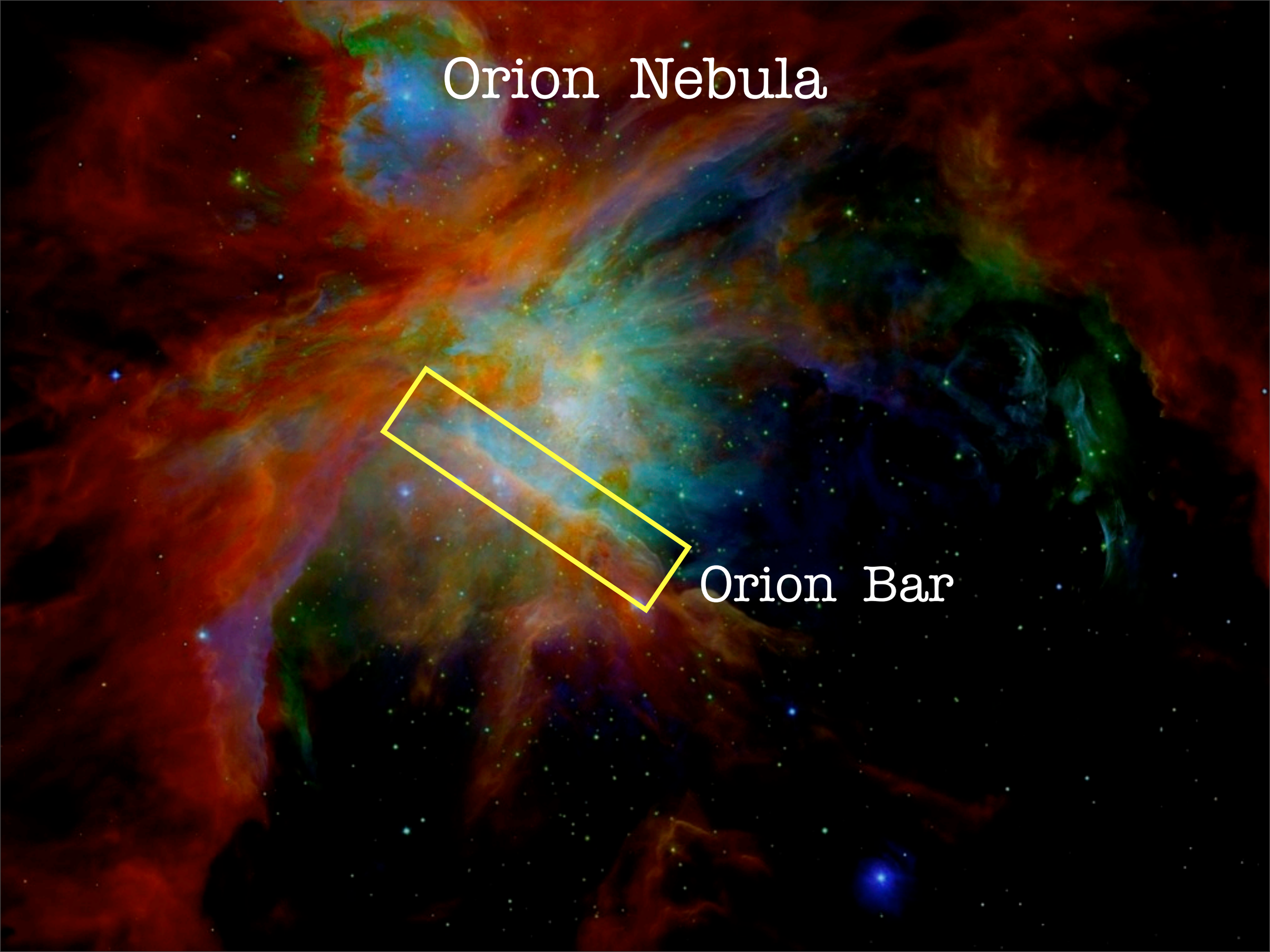
# Exciting mid-IR emission



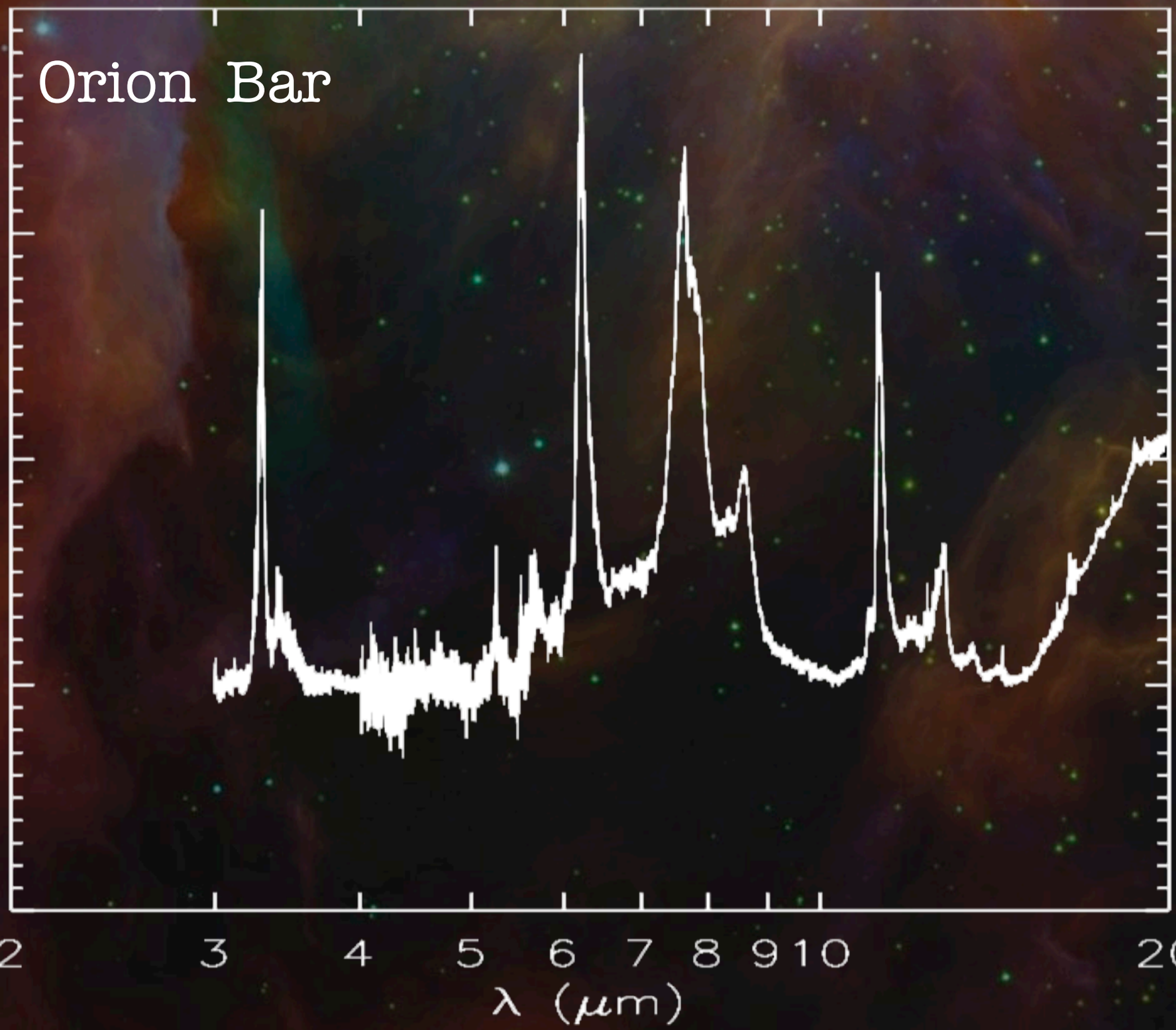
Photon energies >> kT
Non-thermal excitation

Electronic absorption
of optical photons .
Solvation is critical

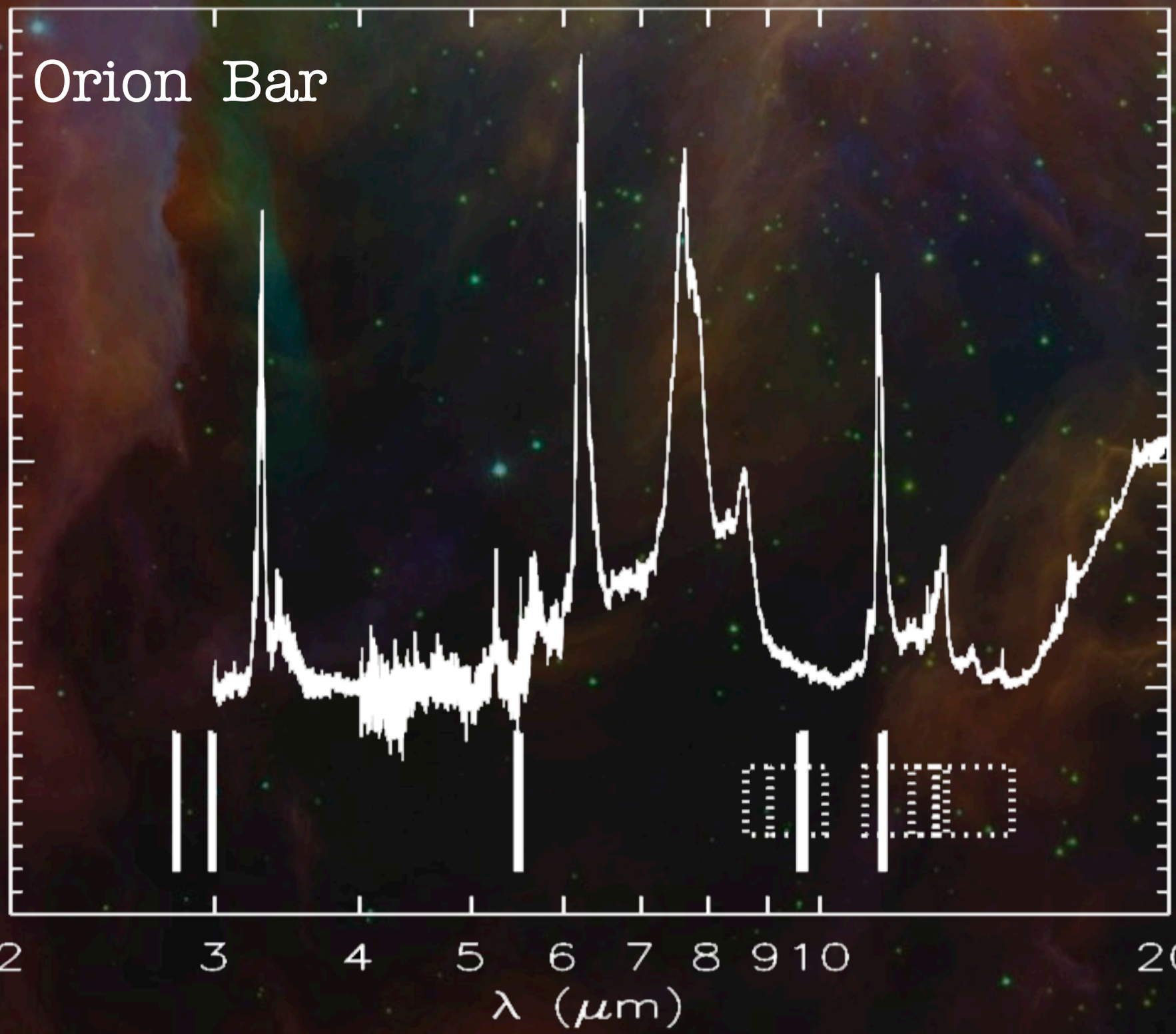
Line strengths fixed by Franck-Condon


Orion Nebula
Orion Bar

Peeters et al 2004



Peeters et al 2004 : $H_6^+$

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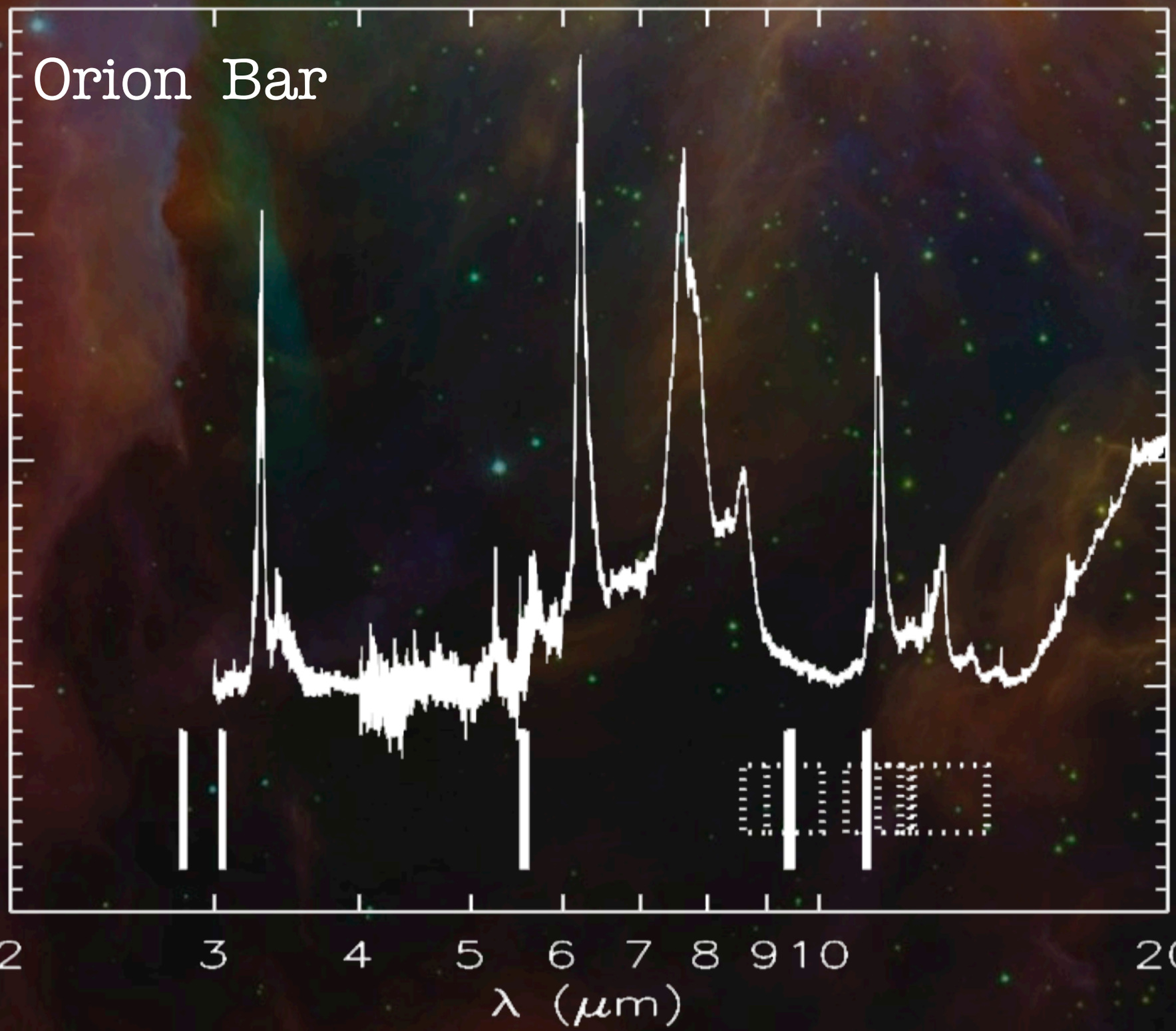
Peeters et al 2004 : $H_6^+ (H_2)_4$

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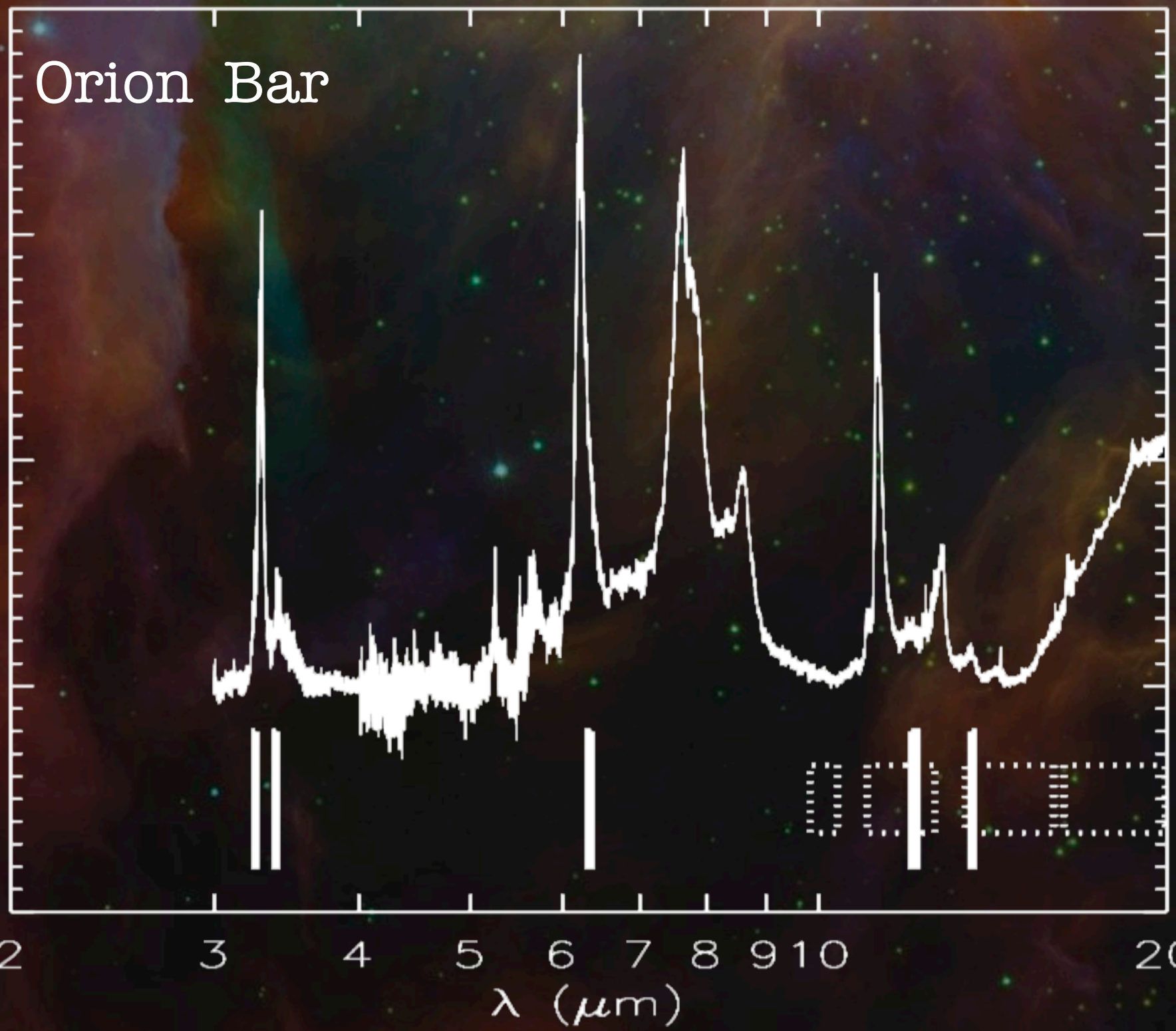
Peeters et al 2004 : $(HD)_3^+$

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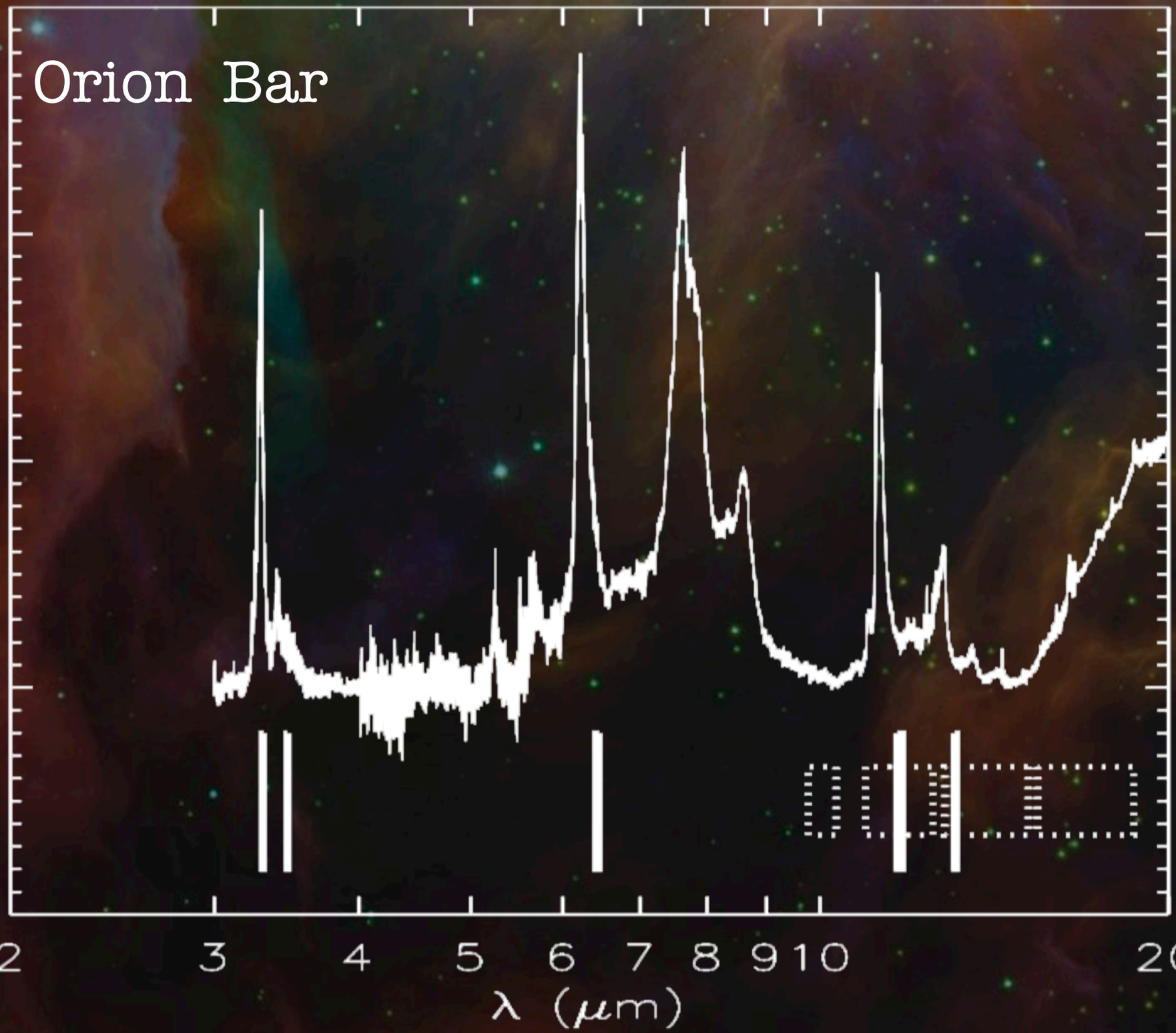


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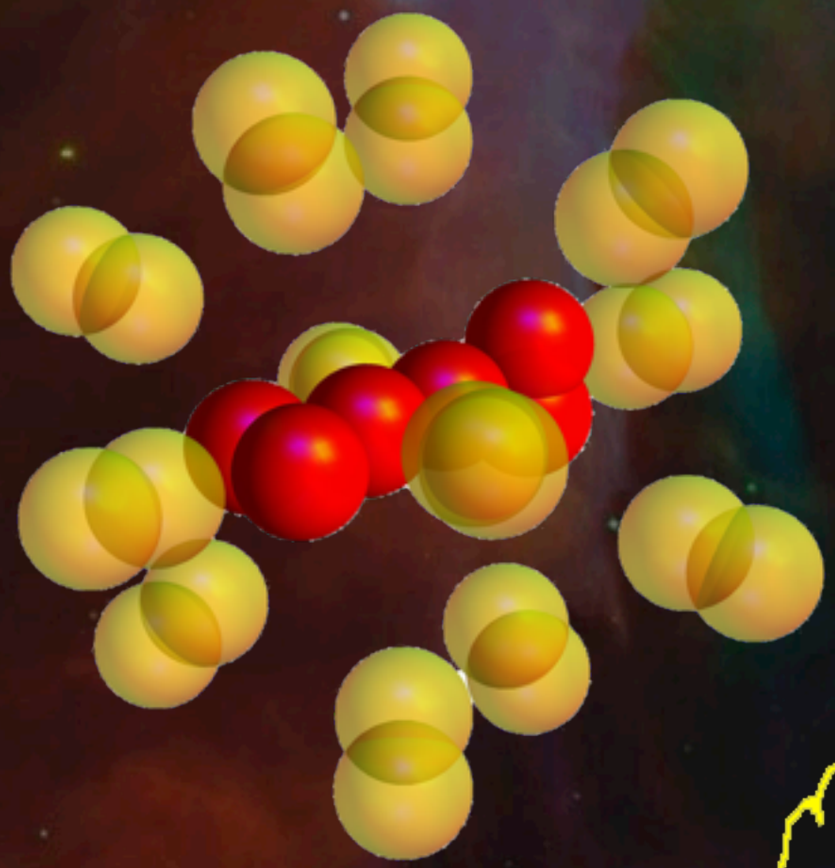
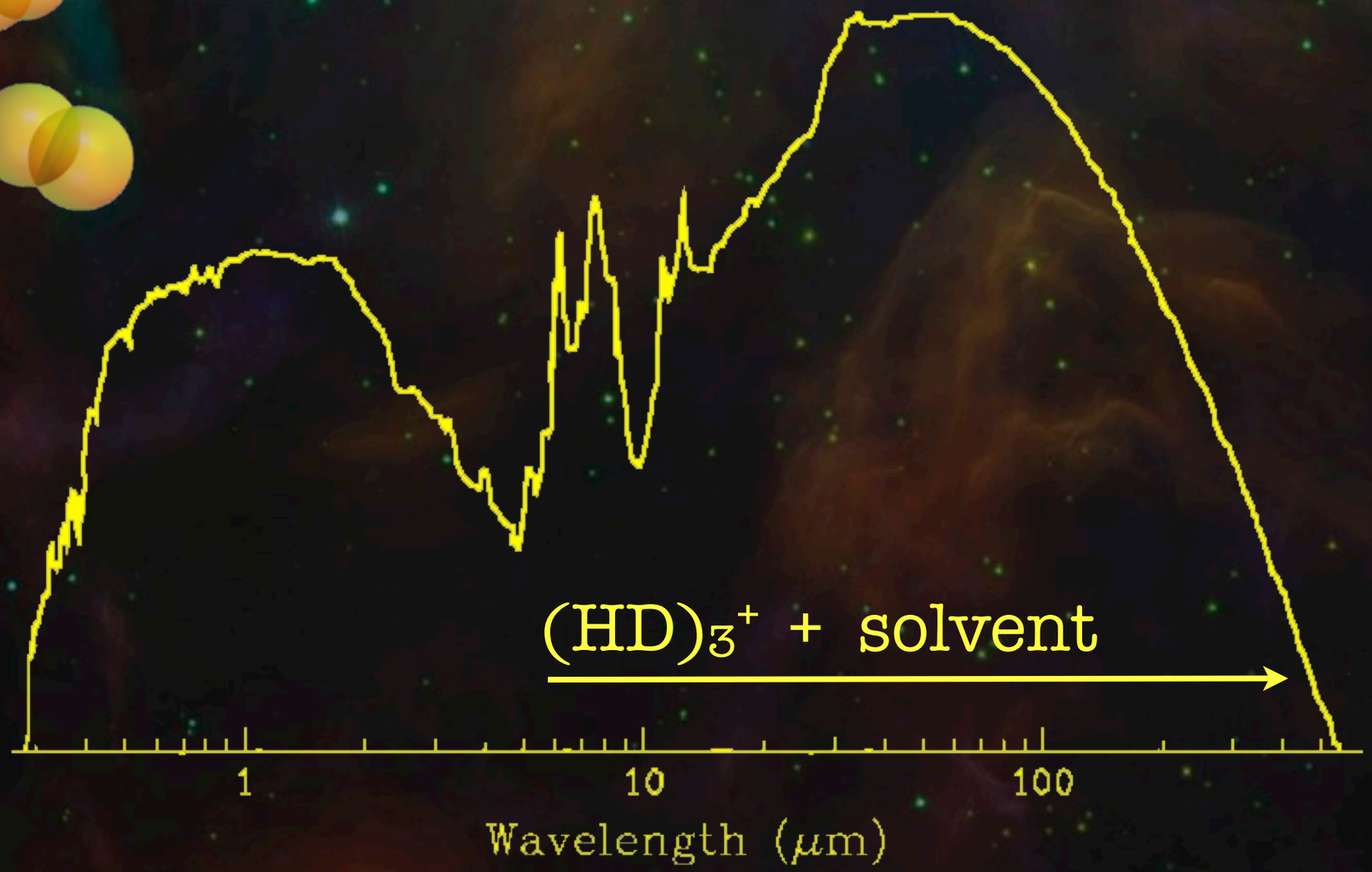
# Far-IR emission

FIR from cluster modes.
Many modes :
quasi - continuum FIR.



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# Summary

- ESEs demand population of spherical clouds
  - Solid $H_2$ confers thermal stability
- Solid $H_2$ + cr → $H_6^+$ → $(HD)_3^+$ → $(HD)_3^+ (H_2)_{54}$
  - $H_6^+$ etc unique to condensed phase
- Ab initio models: 5 predictable vibration lines
- $(HD)_3^+(H_2)_4$ : 3.3, 3.5, 6.4, 11.7, 13.1 μm
  - All close to UIR bands
- FIR emission from cluster modes
- Encourages a dust model based on solid $H_2$