HOKKAIDO UNIVERSITY

北海道大学低温科学研究所
Institute of Low Temperature Science Hokkaido University

TNU/SAGI INTERNATIONAL SUMMER SCHOOL OF RESEARCH AND EXPLORATION IN ASTRONOMY 2024

INTRODUCTION TO ASTROCHEMISTRY

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Introduction to Astrochemistry

- Astrophysics
  - The formation of the stars
  - The formation of galaxies
  - The formation of stars and planets in galaxies

- Exploring the chemical evolution of matter in the Universe is also a fundamental goal of astromony: Astrochemistrry

- Questions:
  - How are various molecules formed in the interstellar medium ?
  - How large can molecules grow in the clouds?
  - How are molecules incorporated into stars and planets?

The formation and life cycle of stars

This image shows blue stars in the constellation of Sagittarius.
Image credit: NASA / ESA / Hubble

- Stars are gaseous objects bound together by gravitational self-attraction.

What are the components of a star?

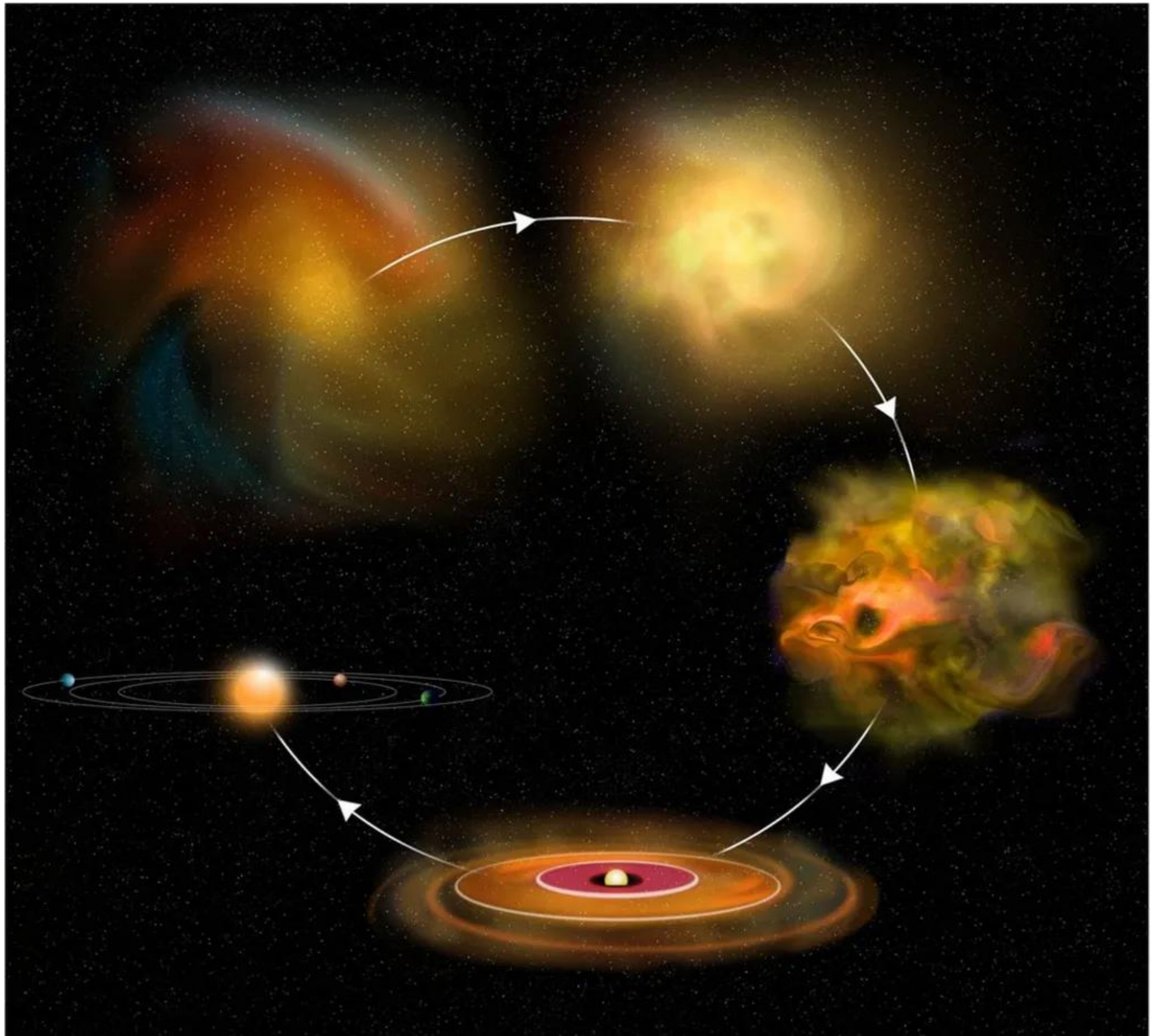
The formation and life cycle of stars

This image shows blue stars in the constellation of Sagittarius.
Image credit: NASA / ESA / Hubble

- Stars are gaseous objects bound together by gravitational self-attraction.

- Chemical components of stars is fairly constant: 73% hydrogen, 25% helium, and 2% other elements.

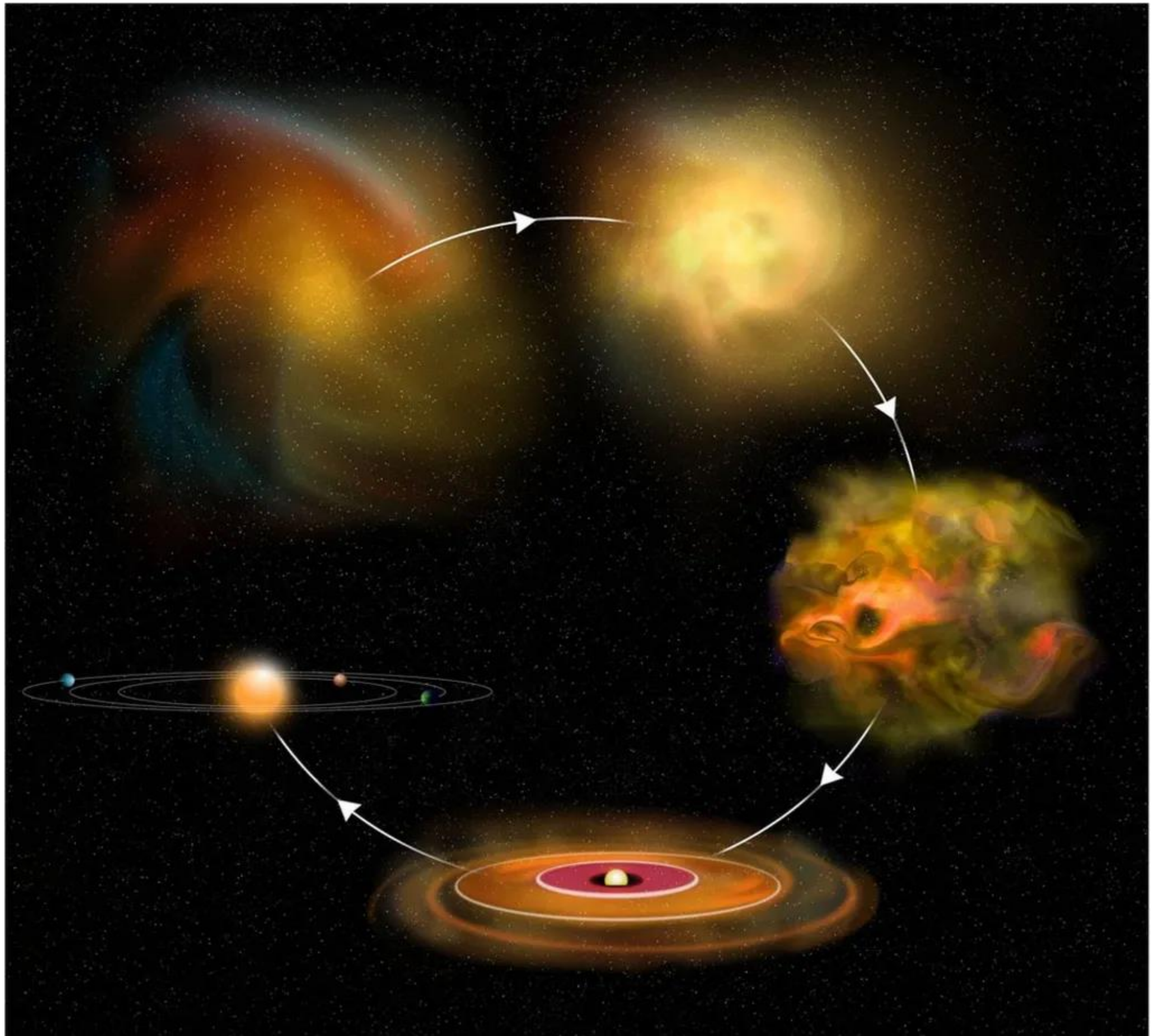
The formation and life cycle of stars



Credits: Bill Saxton, NRAO/AUI/NSF

- Stars form from the gravitational collapse of dense clouds in the interstellar medium (ISM).
- The remaining matter around the protostar forms a spinning disk → protoplanetary disk → planet orbits around a star.
- Our solar system consists a star (Sun) and 8 planets. The solar system is the result of the gravitational collapse of small part of giant molecular clouds.

The formation and life cycle of stars



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Interstellar Medium: Overview and background

The

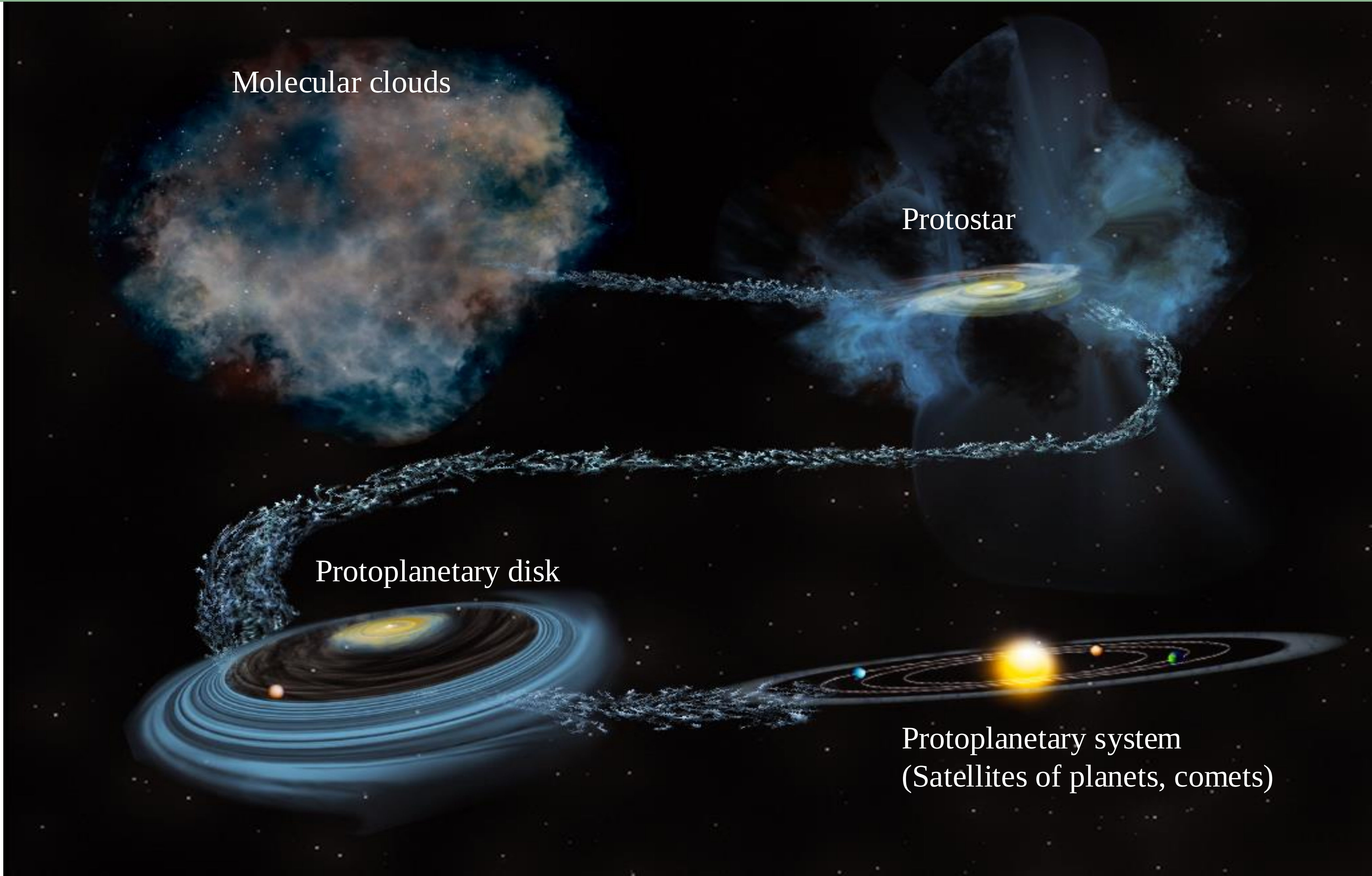
Interstellar

Medium

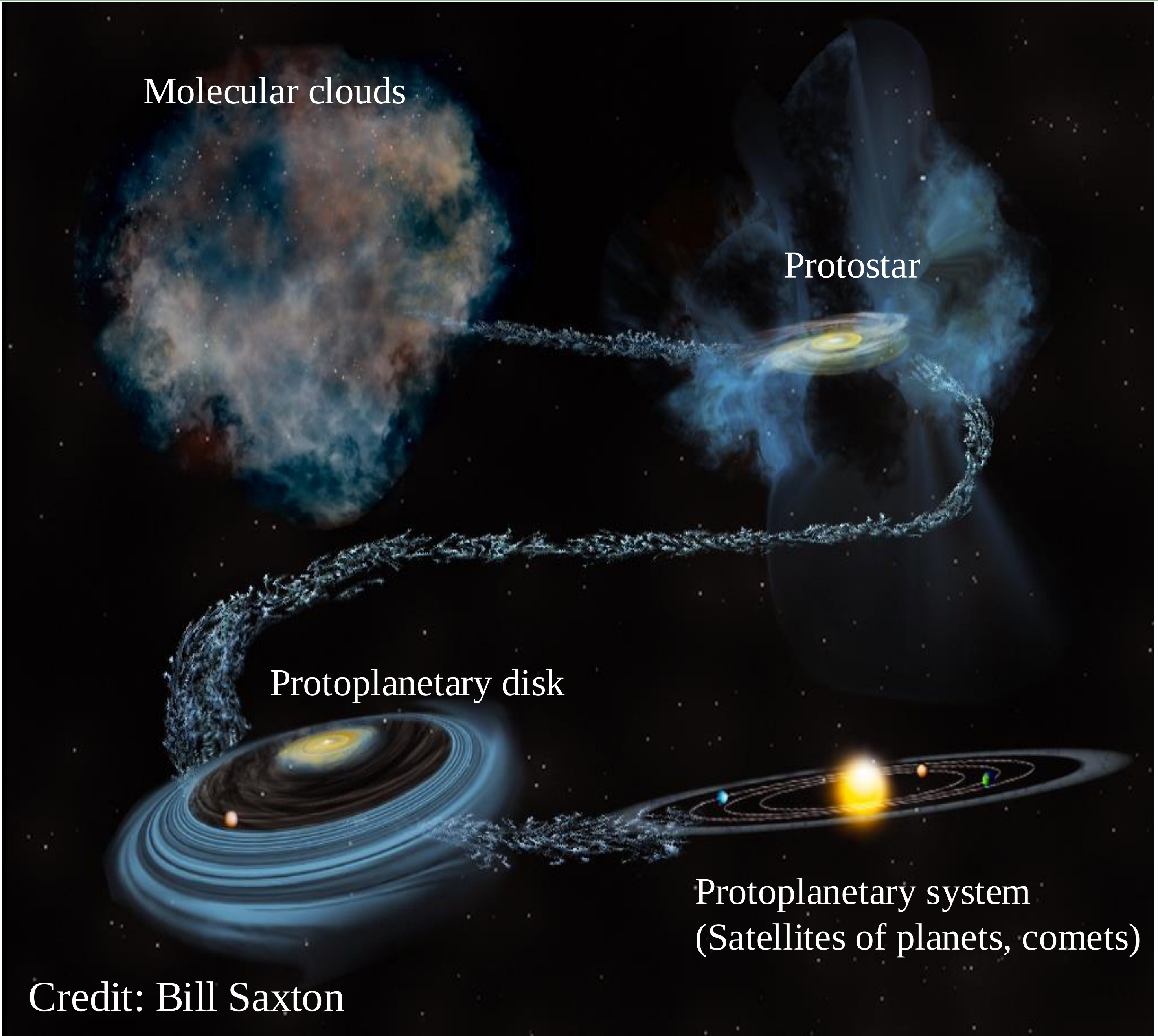
Lifecycle

Gas (300 molecules) and dust grains

Credit: Bill Saxton



Interstellar medium: overview and background



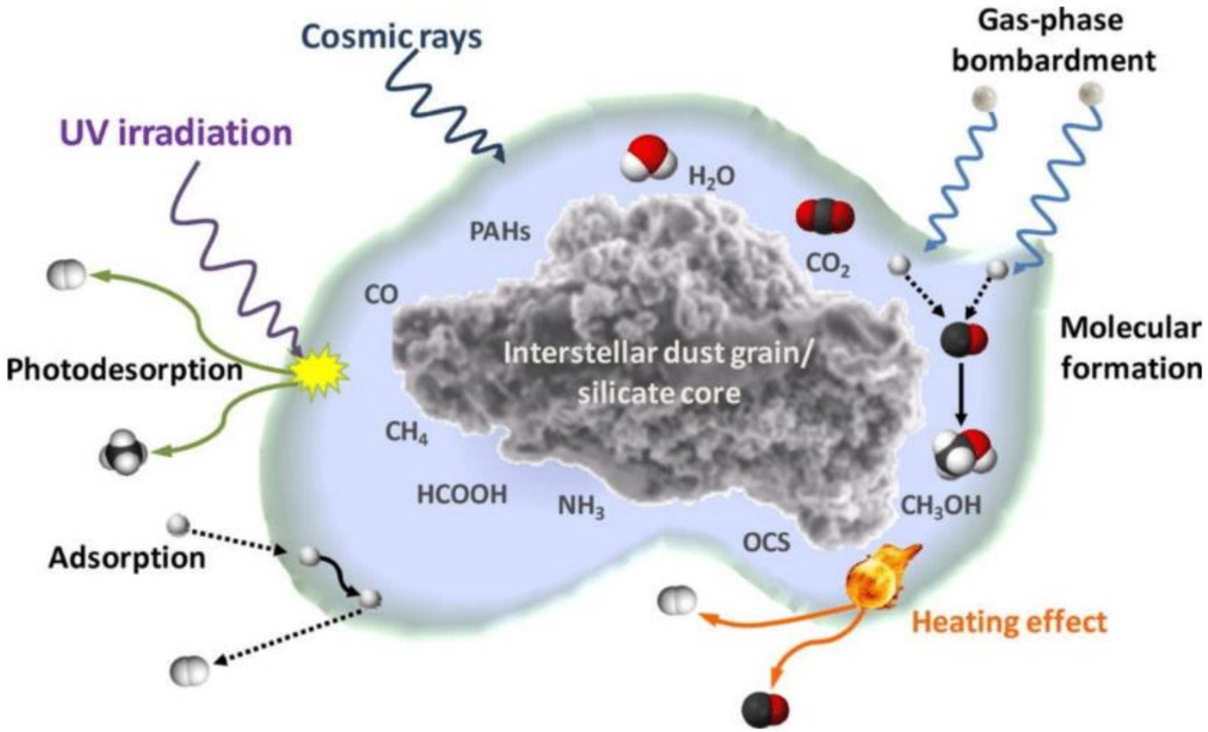
- ❑ Interstellar medium (ISM) is interstellar space where the material fills the space between stars.
- ➢ Its place is the coupling where stars are dead, and stars are born.
- ❑ The ISM components:
  - ▪ Molecular clouds (90% hydrogen, 9% helium, and 1% other heavy elements)
  - ▪ Dust
  - ▪ Photons: diverse components and roles: cosmic microwave background (CMB) (mm), starlight (eV), X-rays (keV)
  - ▪ Cosmic rays
  - ▪ Magnetic fields
- ✓ Physical processes in ISM are complicated, they can happen to phenomenon such as absorption, emission, scattering or reflection in space .

Interstellar Medium: Overview and background

- ❑ Why do we study the ISM?
  - Gas is where it all started back then at "Recombination". Part of the effort to understand the evolution of baryonic matter through time → Studying the physical processes involving gas in the ISM places a crucial role in astrophysics.
- ❑ Why is the ISM important ?
  - Stars form from the ISM, and then activate it dynamically and chemically. Gas is the active chemical ingredient of galaxies.
- ❑ Can we see the ISM the way we see the Sun and Stars shine?
  - In principle, yes, but it's hard because gas at temperatures of the surface of stars cools rapidly unless heated, e.g., by being close to a star. This kind of gas is called nebular and has characteristic emission lines.

Interstellar Medium: Physical processes

❑ Molecular clouds (MCs)



Schematic illustration of a molecular cloud in the ISM

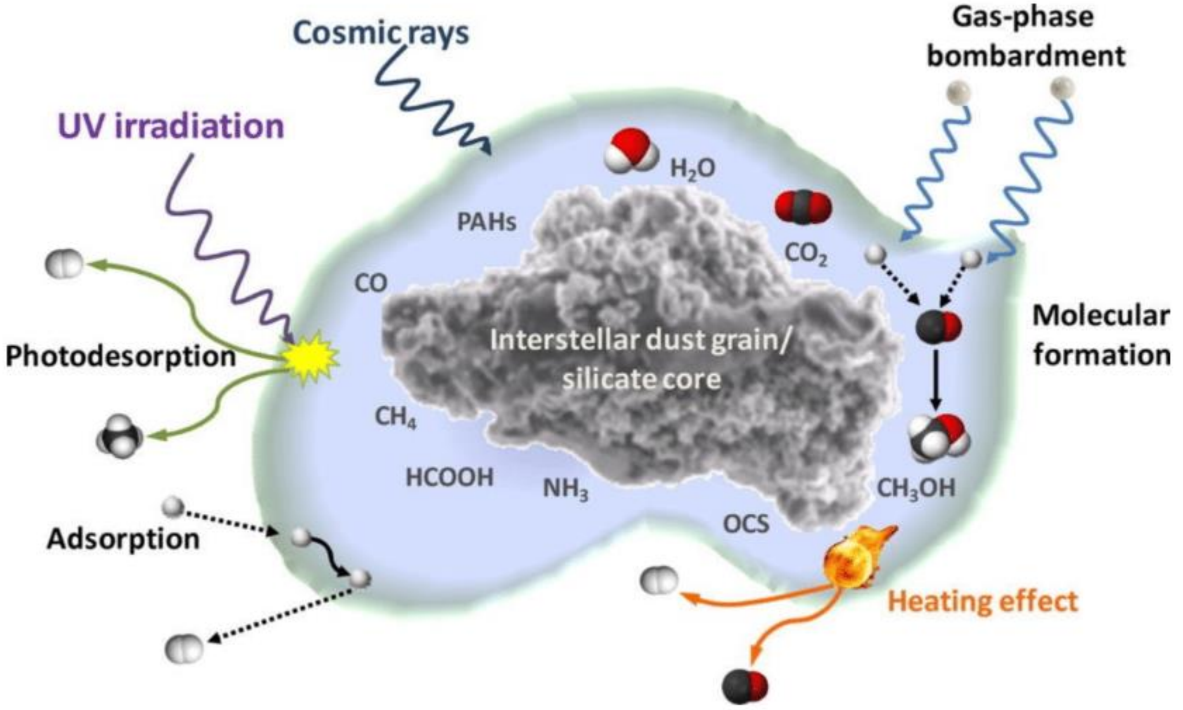
- They are the densest interstellar clouds
- Temperature: 10 – 50 K
- Number density: > 10^6 cm^{-3}
- Chemical components are H_2, CO, CO_2, and complex organic molecules.
- There are many physico-chemical processes occurring in MCs such as irradiation, photodesorption, bombardment, etc.

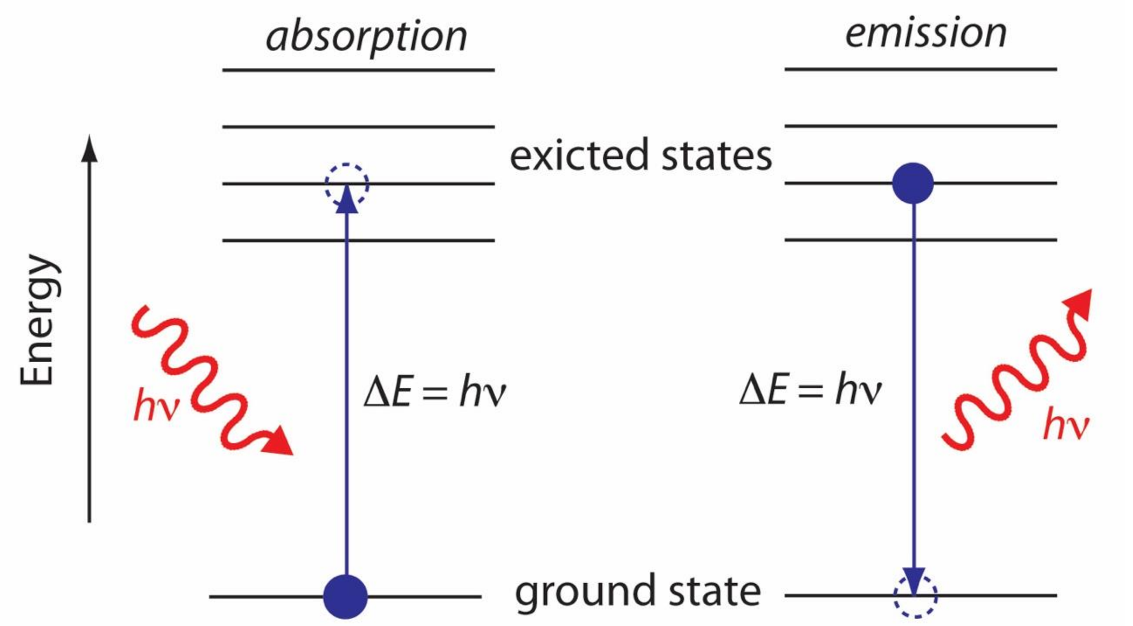
➢ MCs plays an important role for the formation of stars.

➢ Studying physico-chemical behavior of MCs contributes understanding the evolution of the Universe.

Interstellar Medium: Physical processes

❑ Molecular clouds: Absorption and emission

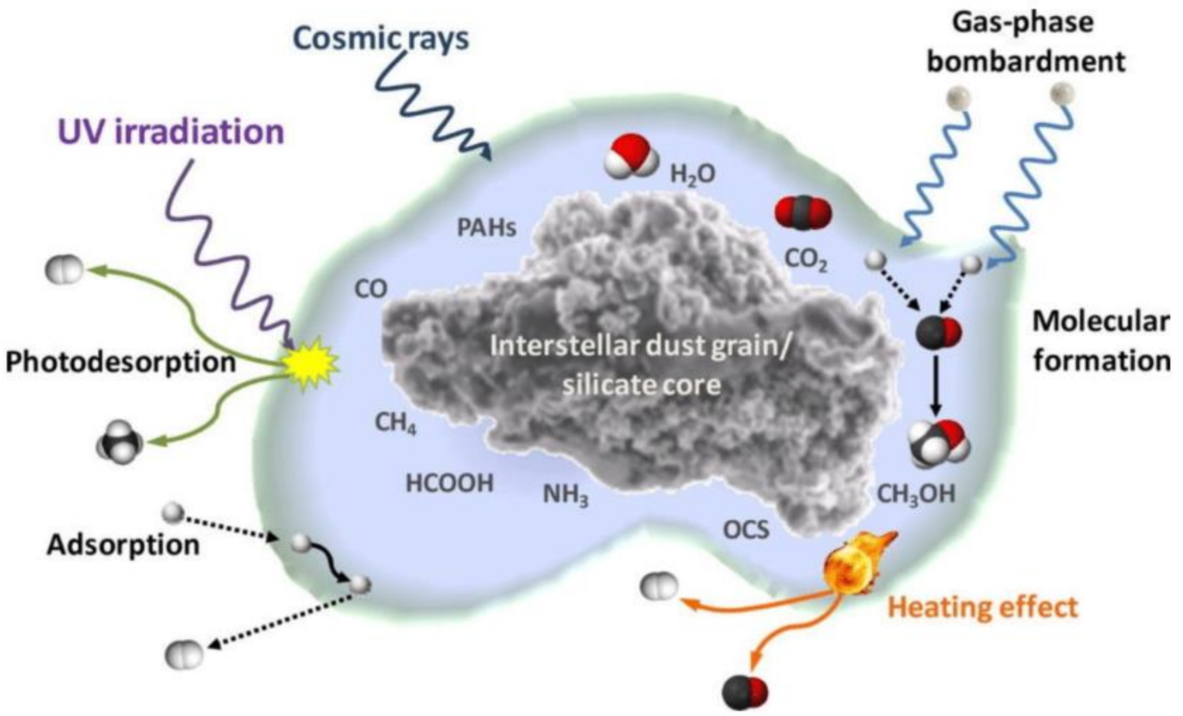


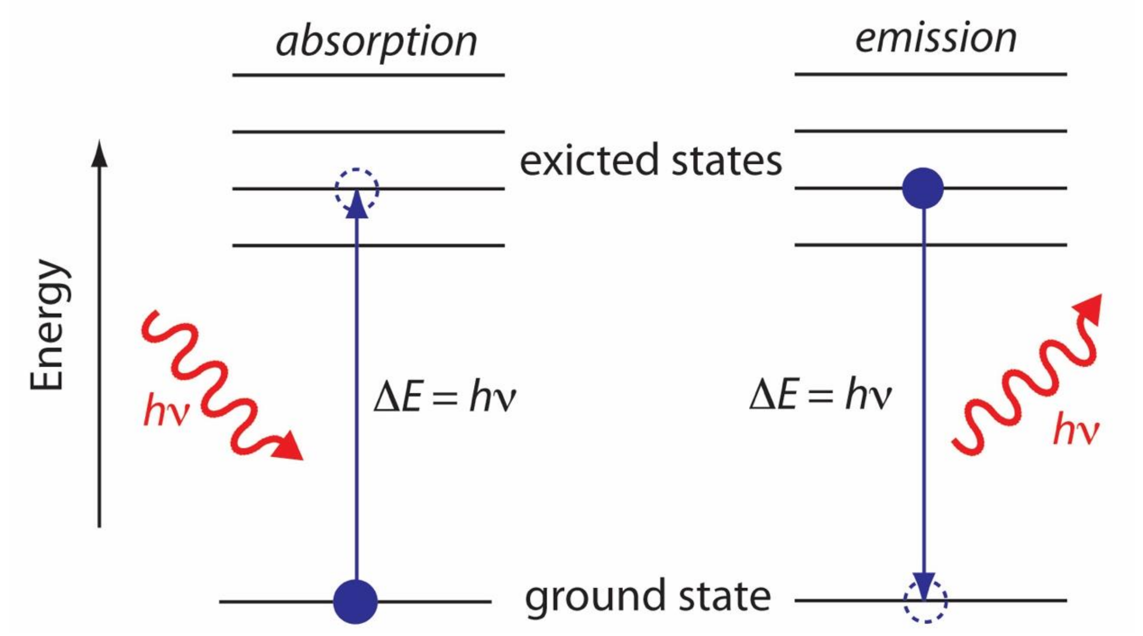


- Energy levels:
  - An electron receives photon, it transits from ground state to excited state → ?
  - An electron transits from excited state to ground state, it emits a photon → ?

Interstellar Medium: Physical processes

❑ Molecular clouds: Absorption and emission



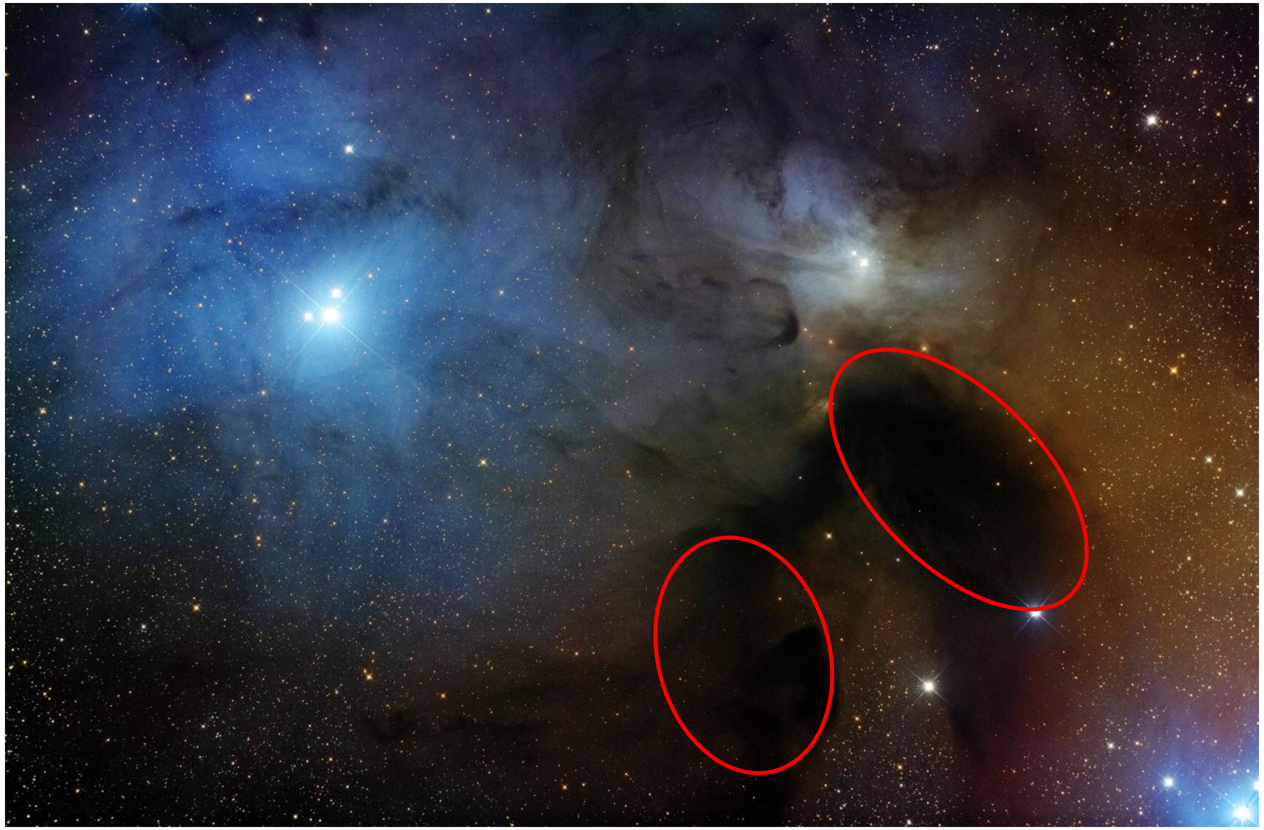


- Energy levels:
  - An electron receives photon, it transits from ground state to excited state → absorption
  - An electron transits from excited state to ground state, it emits a photon → emission

➢ Detect or analyze the components of MCs by using the UV/ radio telescopes.

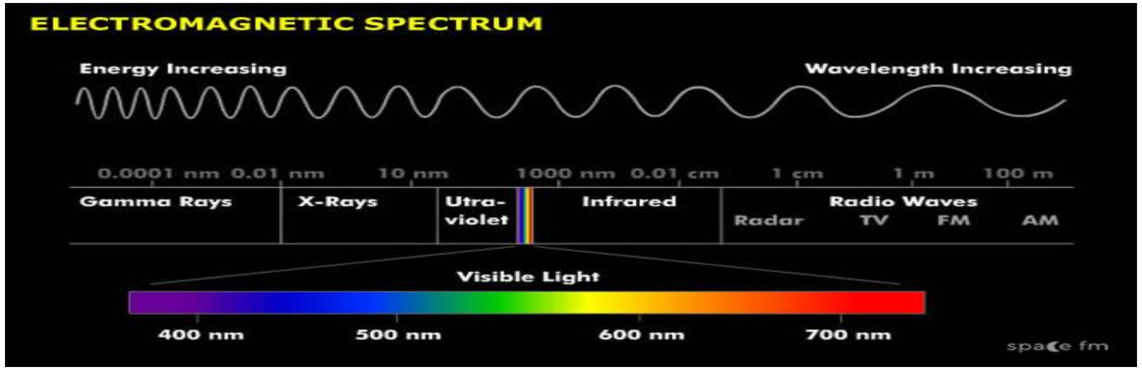
Interstellar Medium: Physical processes

❑ Molecular clouds: Absorption



Rho Ophiuchi region.
Image by Phil Hart, Ross Hortin, Mark Justice, Gavan Salter and Craig Davison using the ASV LMDSS dome and equipment. Processing by James McHugh.

- ➢ Dark patch is where light emitted from the close stars is absorbed by atoms and molecules inside.
- ➢ Any level in an atom can absorb light, but it requires light of the correct wavelength to make electron jump from ground state to excited states.



- ➢ **Example:** Energy of ionization of hydrogen is 13.6 eV → wavelength of 91 nm.

- ➢ The wavelength of UV is from 10 – 400 nm. Therefore, if the wavelength of UV < 90 nm, it cannot excite hydrogen for transition from ground state to excited states.

Interstellar medium: physical processes

❑ Dust

- Dust components include graphite, silicates, iron, ices…
- Typical size of a dust grain is about $\leq 10^{-7}$m smaller than the wavelength of visible light

▪ Scattering of light by dust:

- Particles have size smaller than the wavelengths of light being scattered .

➢ Meaning that the percentage of light that will be scattered is inversely proportional to the fourth power of the wavelength following by Rayleight law:

$$I = \frac{1}{\lambda^4} \qquad \text{(e.q 3)}$$

Where I is the probability of scattering.

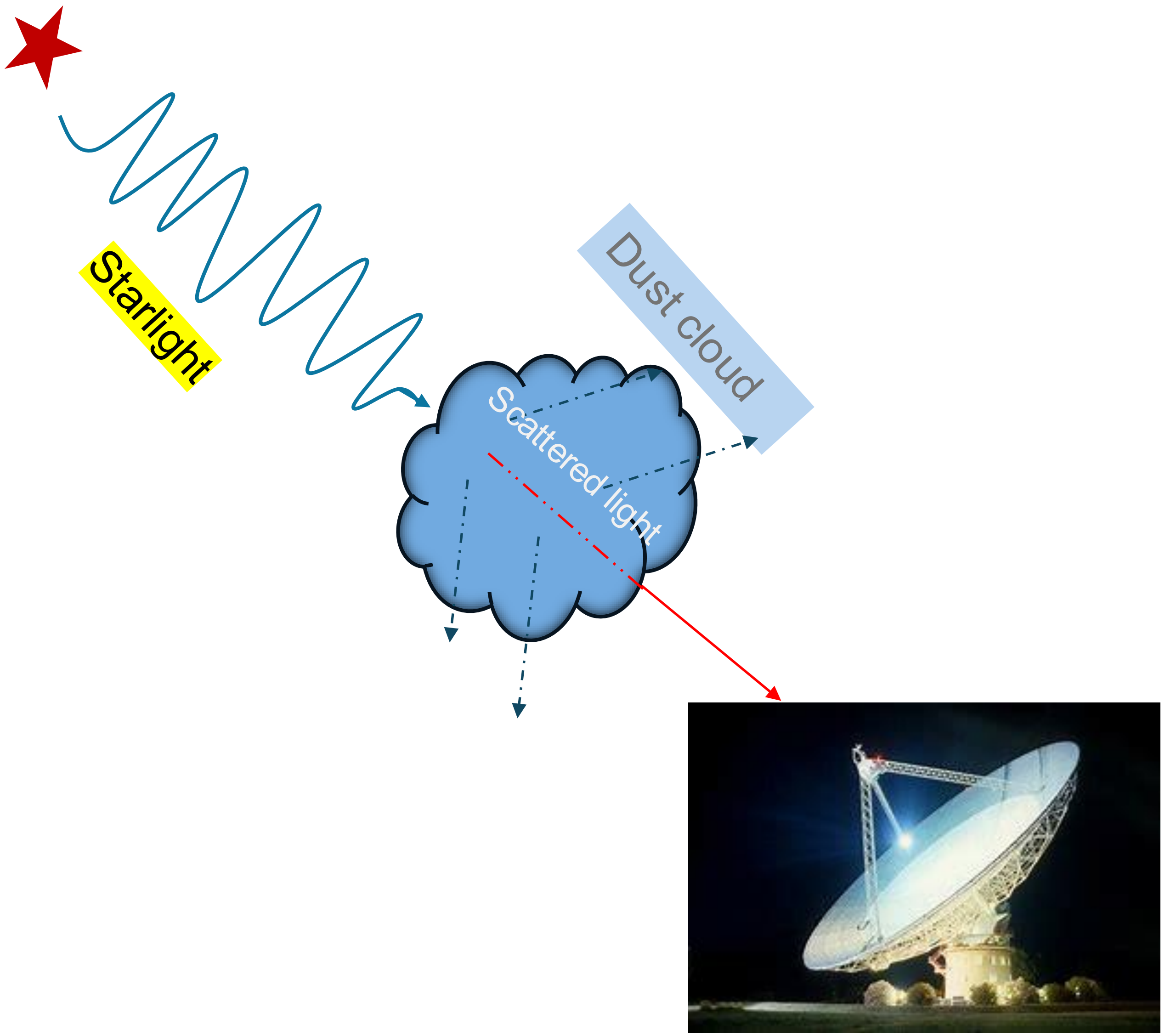
Interstellar medium: physical processes

❑ Dust

❖ Worked example:

- λ_{red} = 760 nm
- λ_{blue} = 450 nm

  ➔ ratio of I_{blue}/I_{red} ~ ?



Telescope

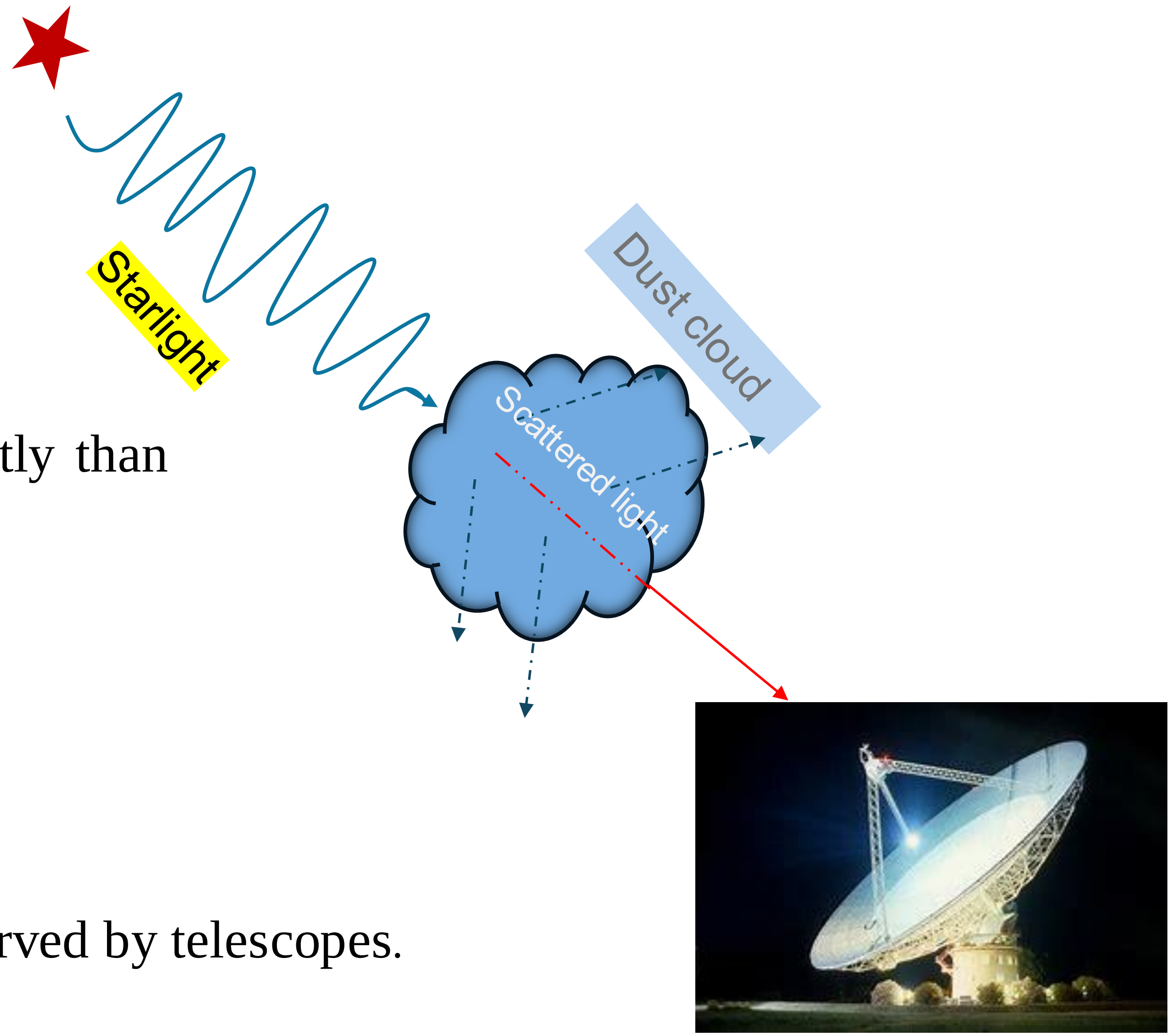
❑ Dust

❖ Worked example:

- λ_{red} = 760 nm
- λ_{blue} = 450 nm

➔ Ratio of I_{blue}/I_{red} ~ **8**

➔ the blue light is scattered more efficiently than the red light.



Telescope

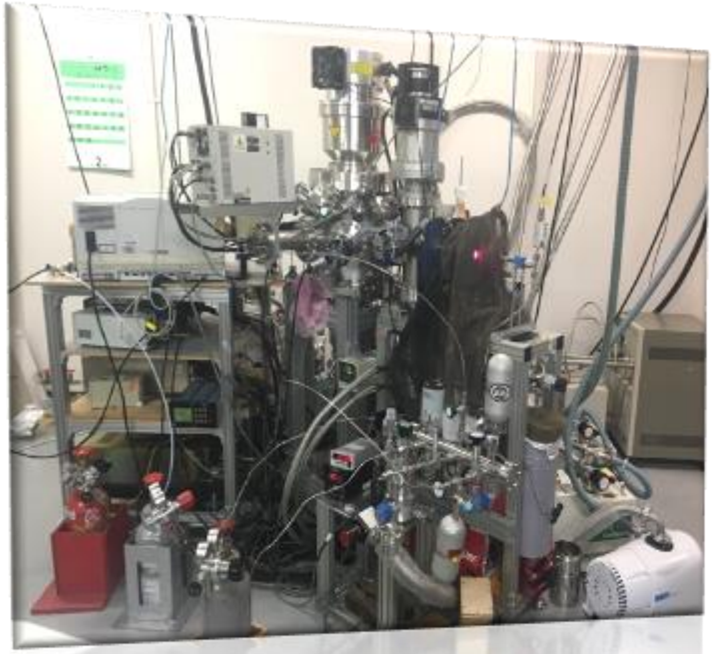
➢ Scattering of light by dust:

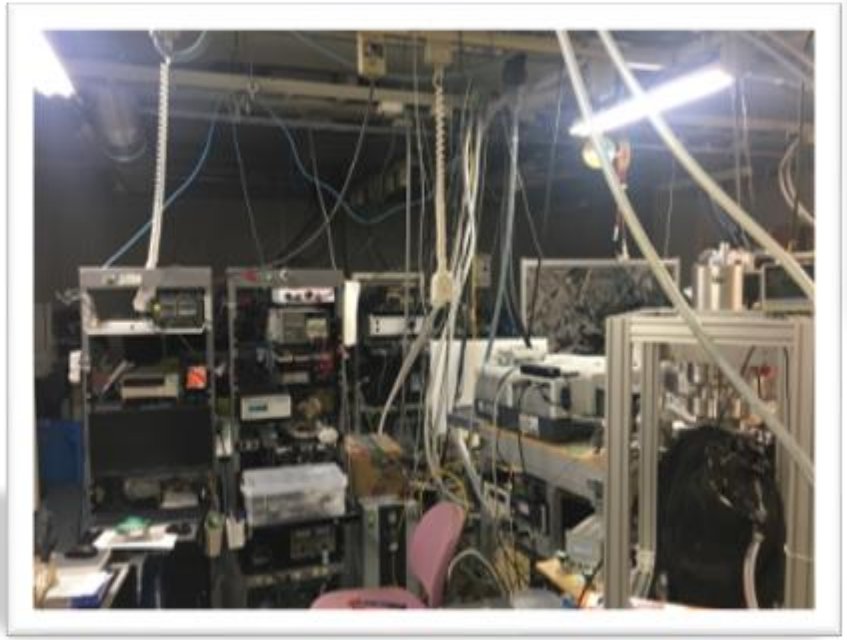
- The blue light is strongly scattered
- The red light is directly transmitted and observed by telescopes.

Astrophysical Chemistry/Ice and Planetary Science group

❑ Research areas:

- ✓ Atomic and molecular physics, Astrochemistry, Surface chemistry
- ✓ Elucidates fundamental processes of nano-particle formation and material evolution in the universe based on singularity in nano-scale

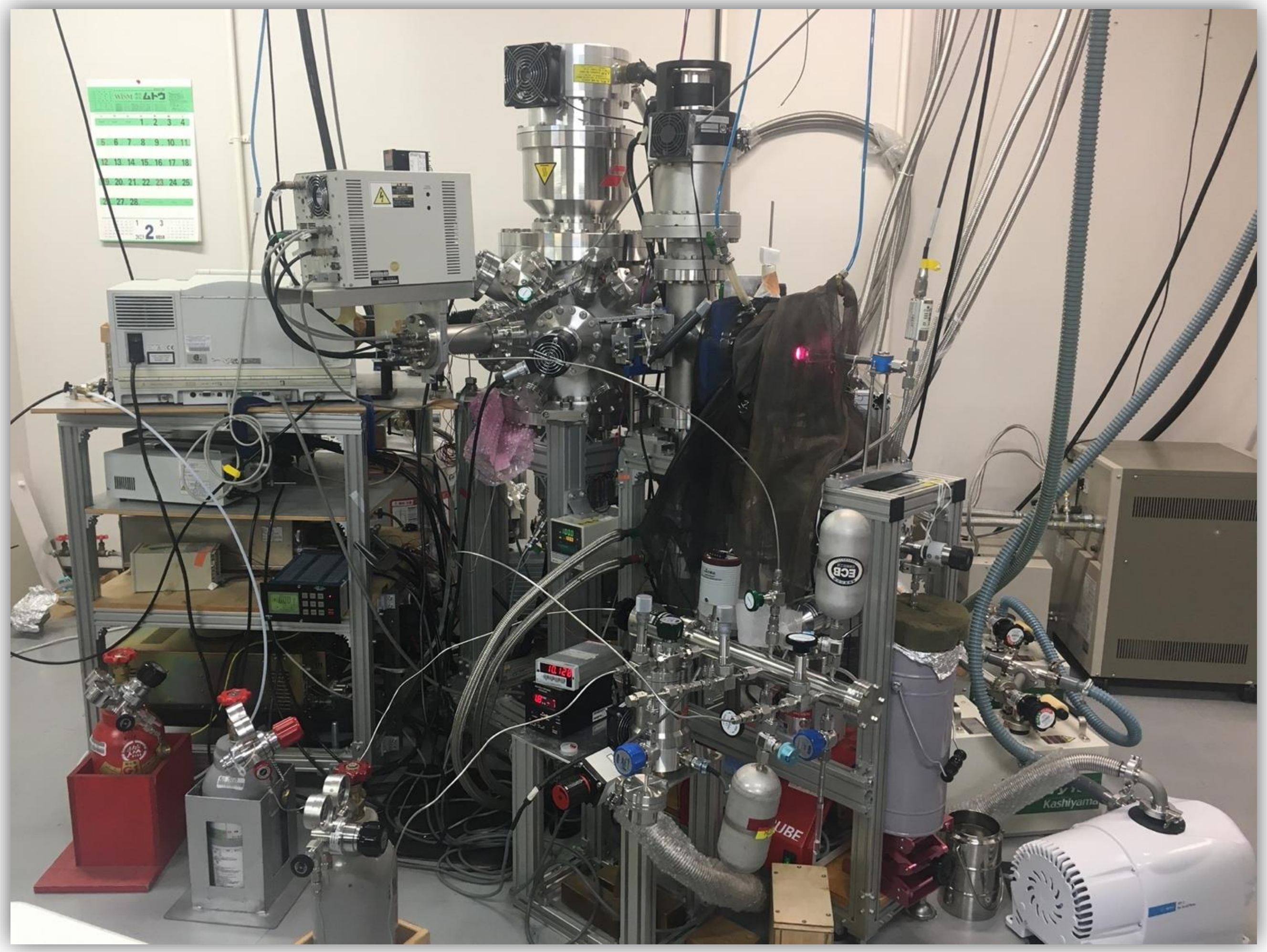




Astrophysical Chemistry/Ice and Planetary Science group

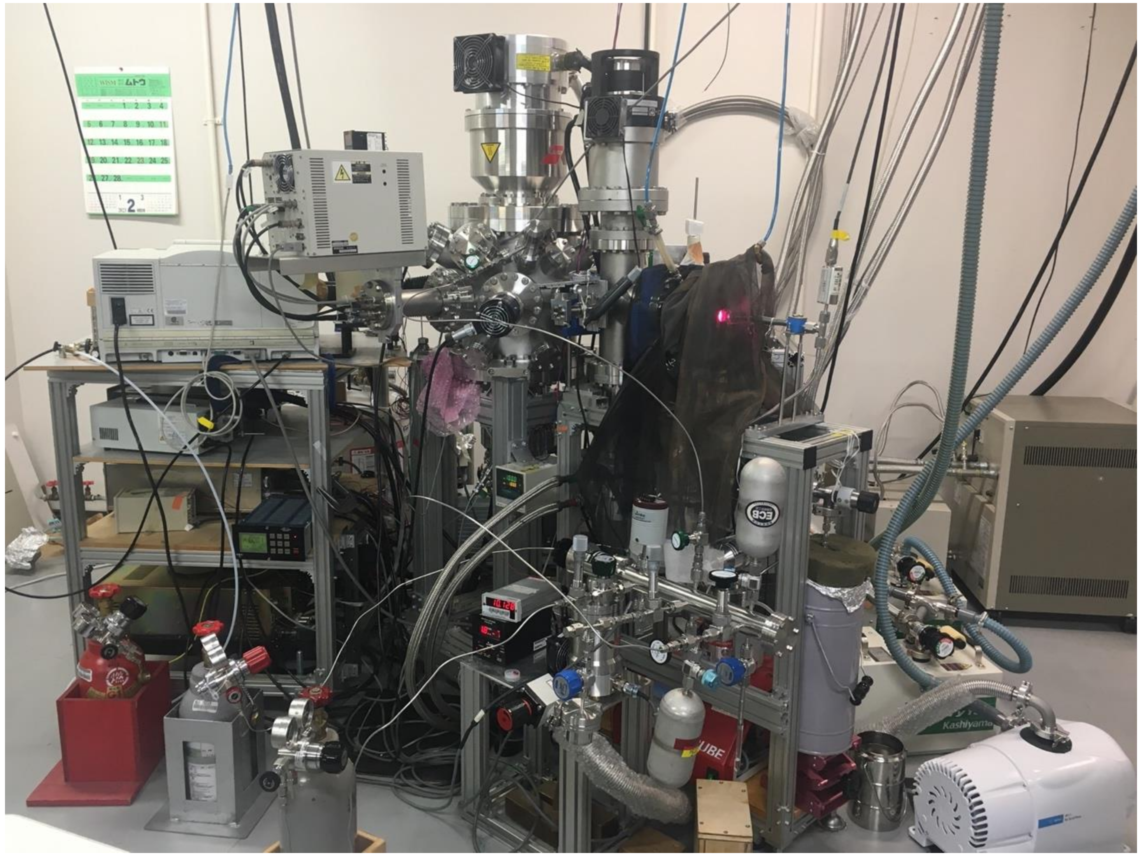
❖ Apparatus (ASURA)

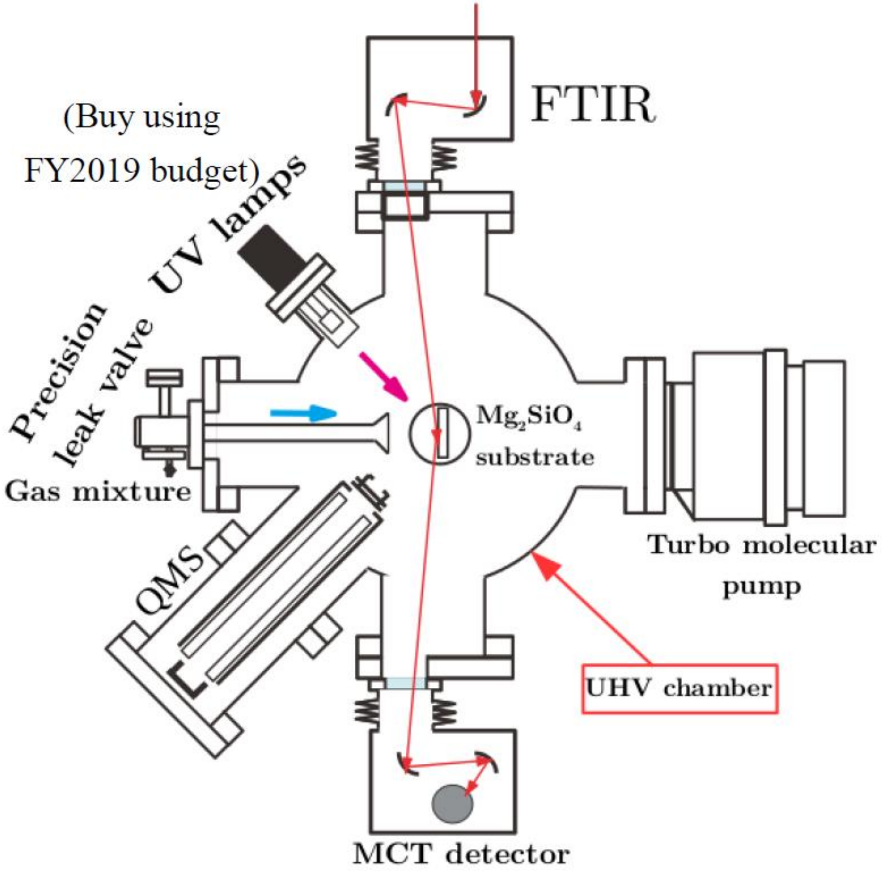
- Using Apparatus for Surface Reaction in Astrophysics (ASURA) to study the complex chemical reactions



Laboratory and Research Processing

❖ Apparatus (ASURA) setup

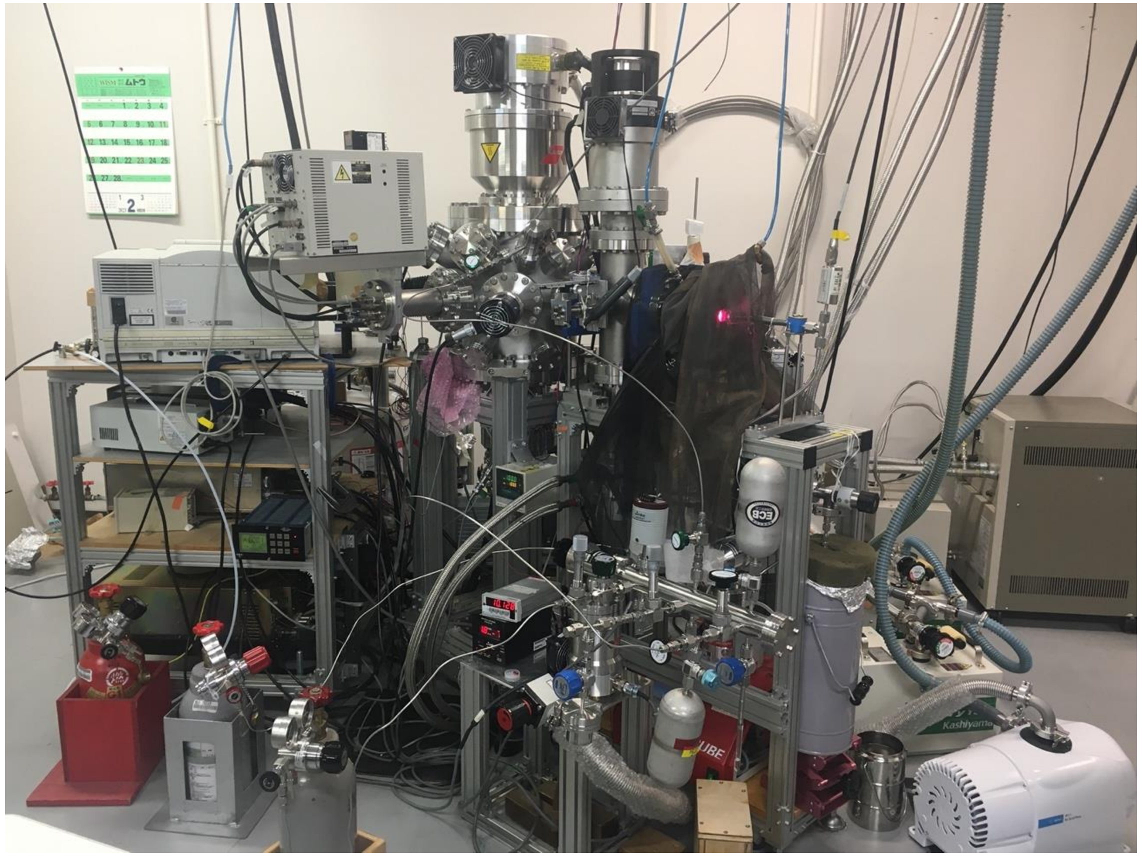


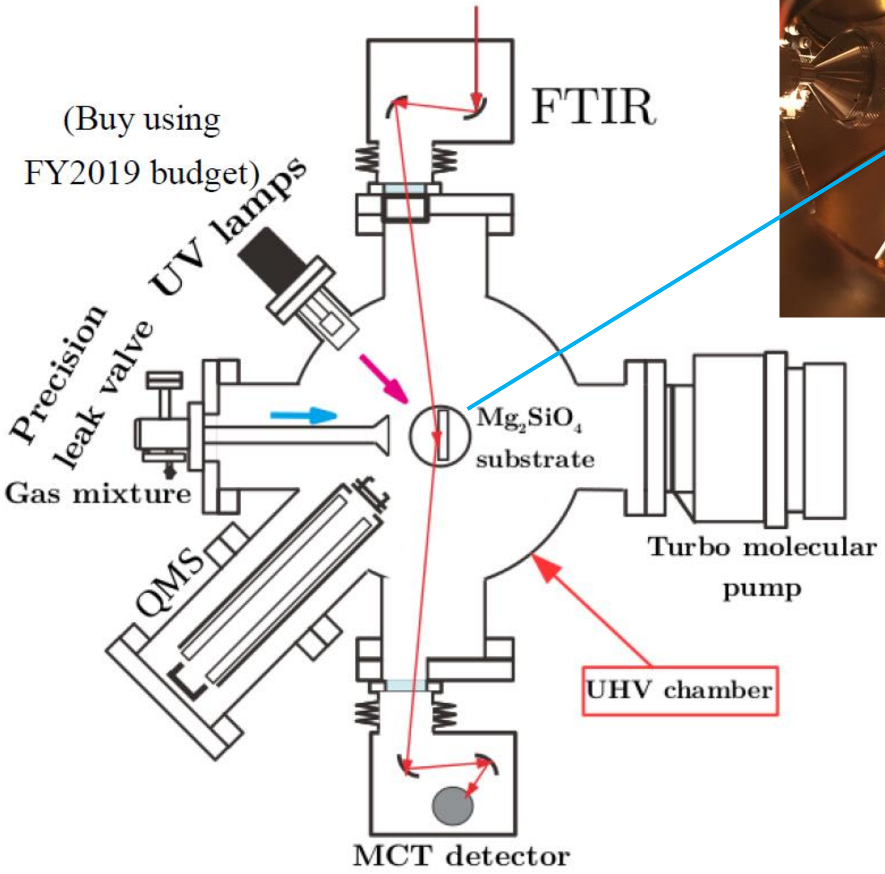


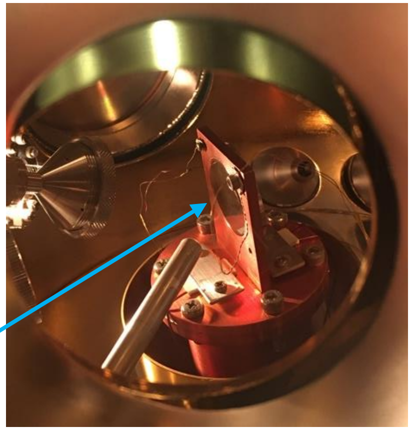
- A vacuum chamber with the basic pressure of 1.3×10^{-13} atm

Laboratory and Research Processing

❖ Apparatus (ASURA) setup



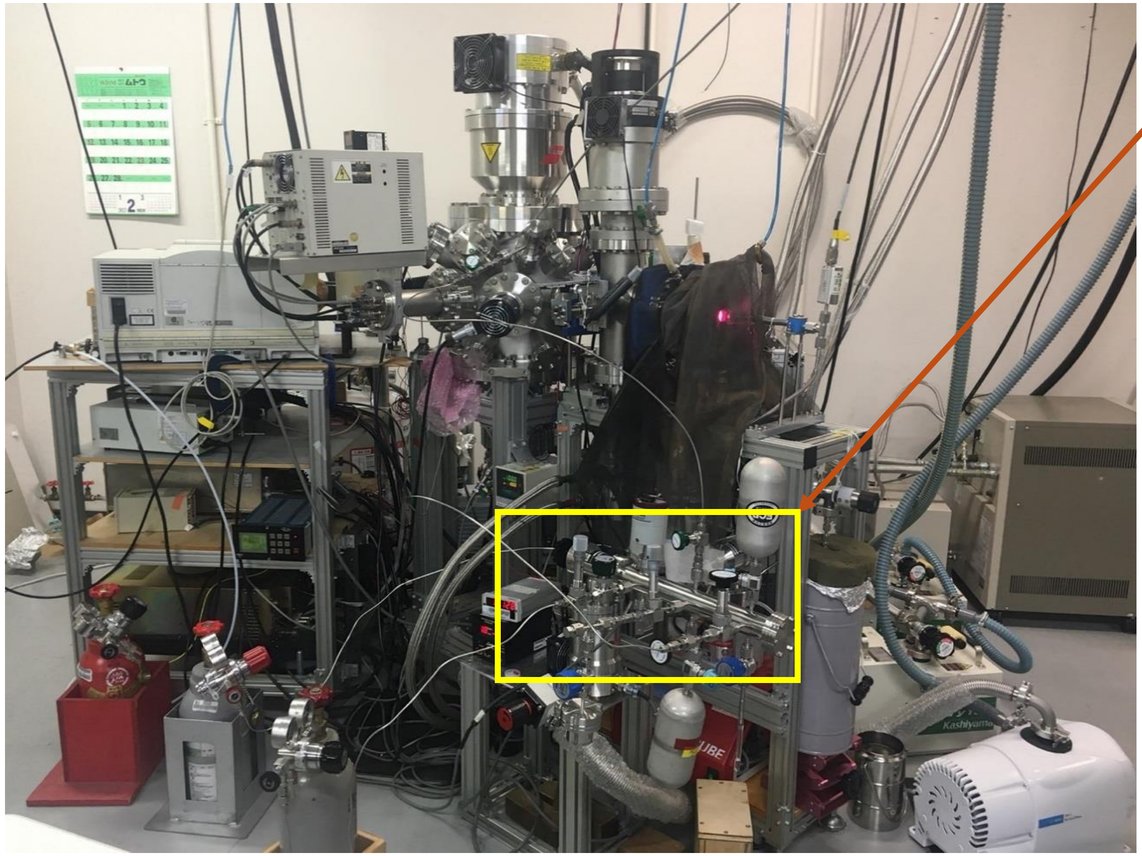


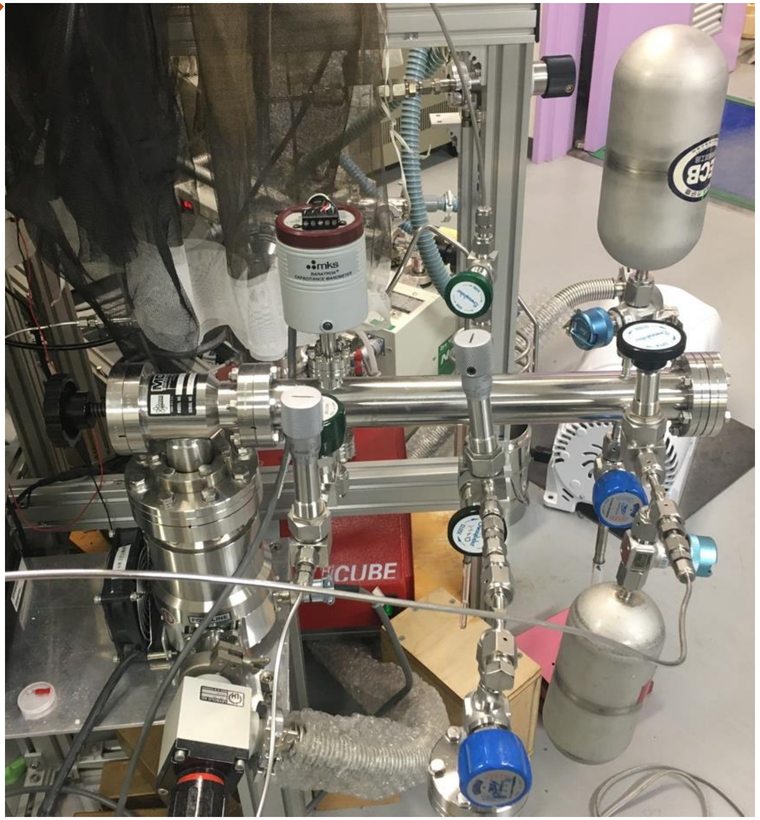


- A vacuum chamber with the basic pressure of 10^{-10} torr
- A substrate inside the vacuum chamber, where chemical processes occur on

Laboratory and Research Processing

❖ Apparatus (ASURA) setup



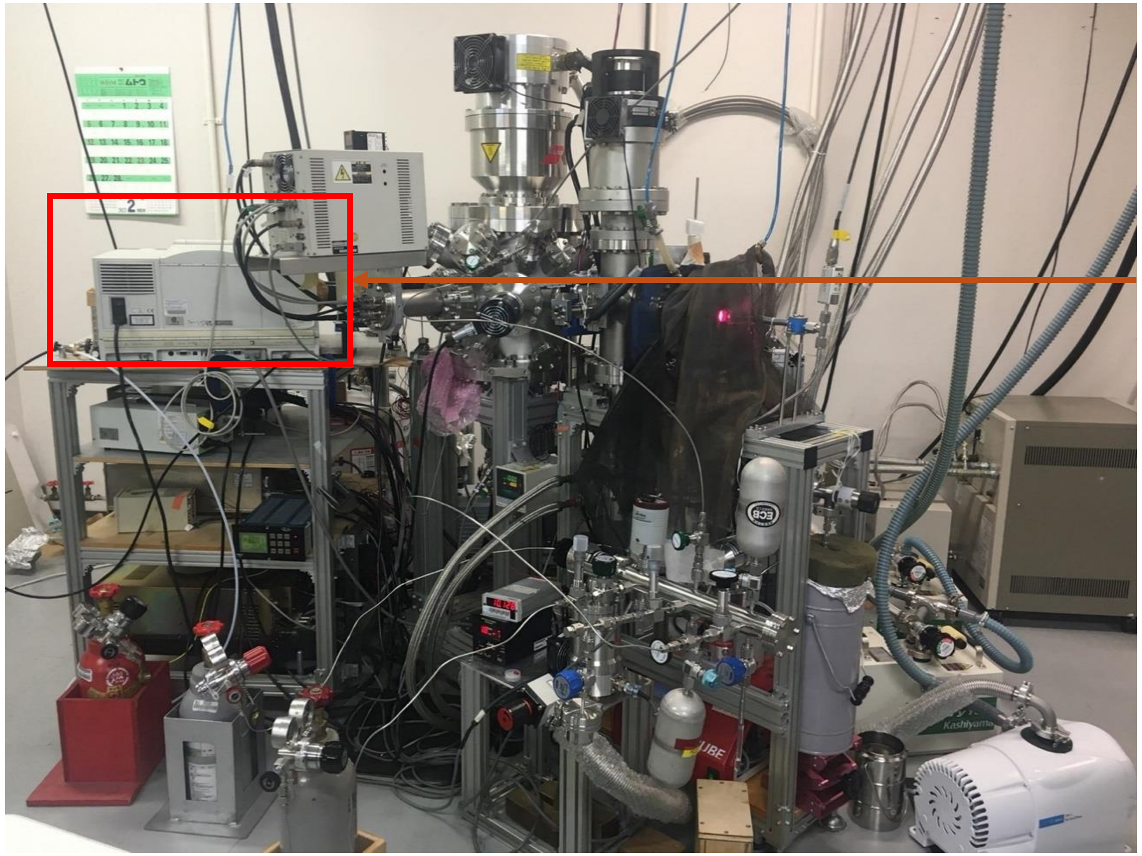


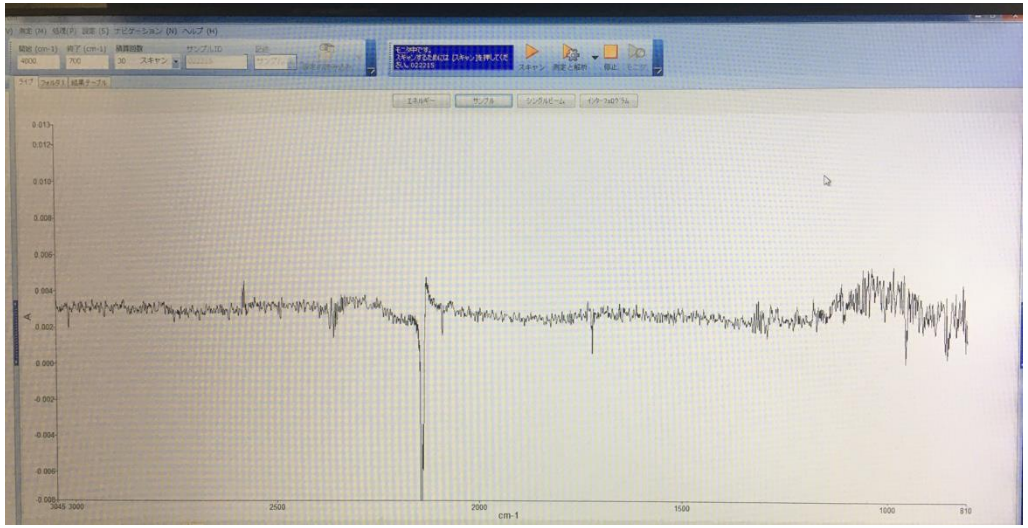
❑ A beam line system

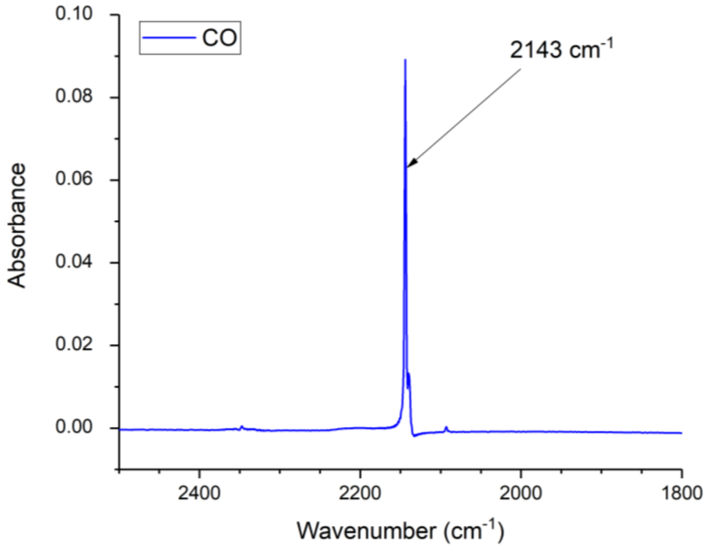
- Materials (H_2O, CO, CO_2,…) are introduced into the chamber via the beam line

Laboratory and Research Processing

❖ Apparatus (ASURA) setup



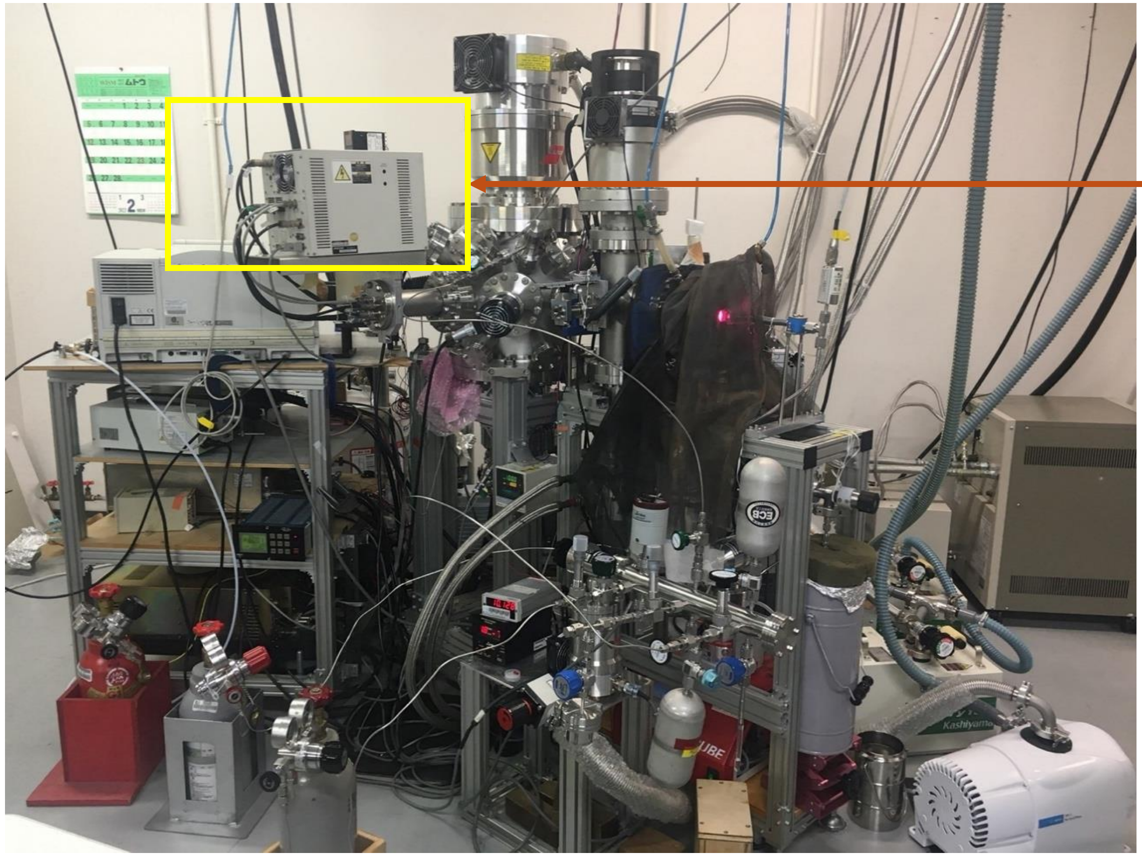


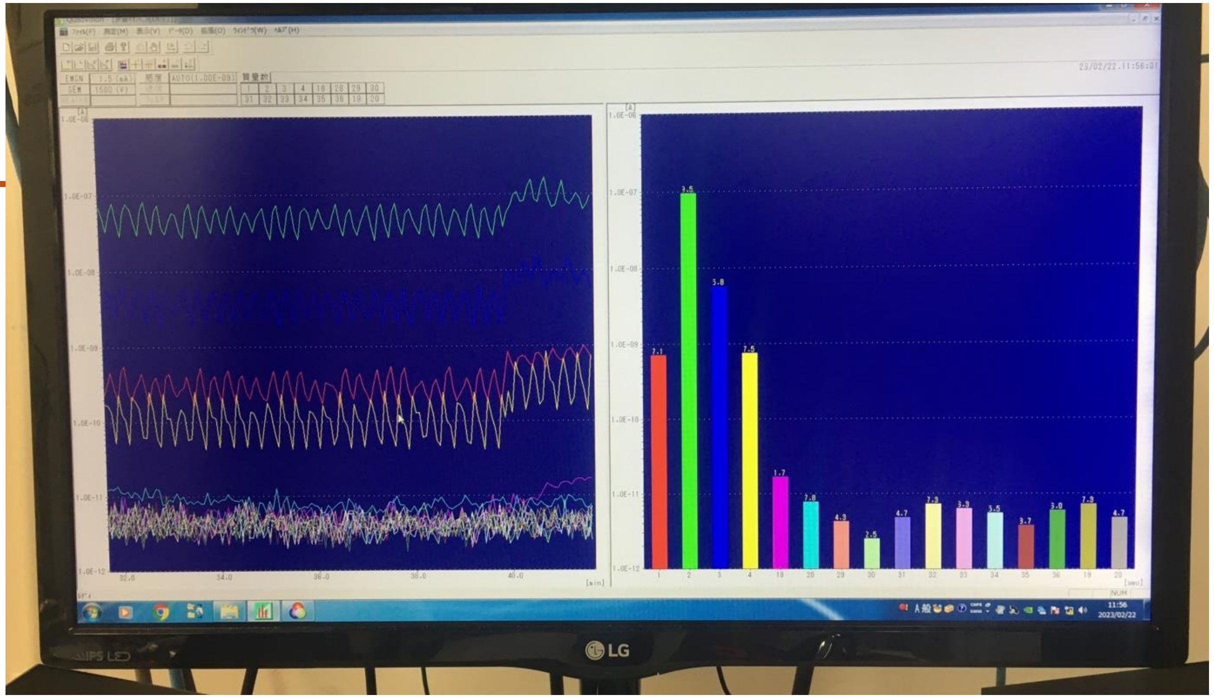


❑ Infrared Spectrometer to record the spectrum of molecules

Laboratory and Research Processing

❖ Apparatus (ASURA) setup



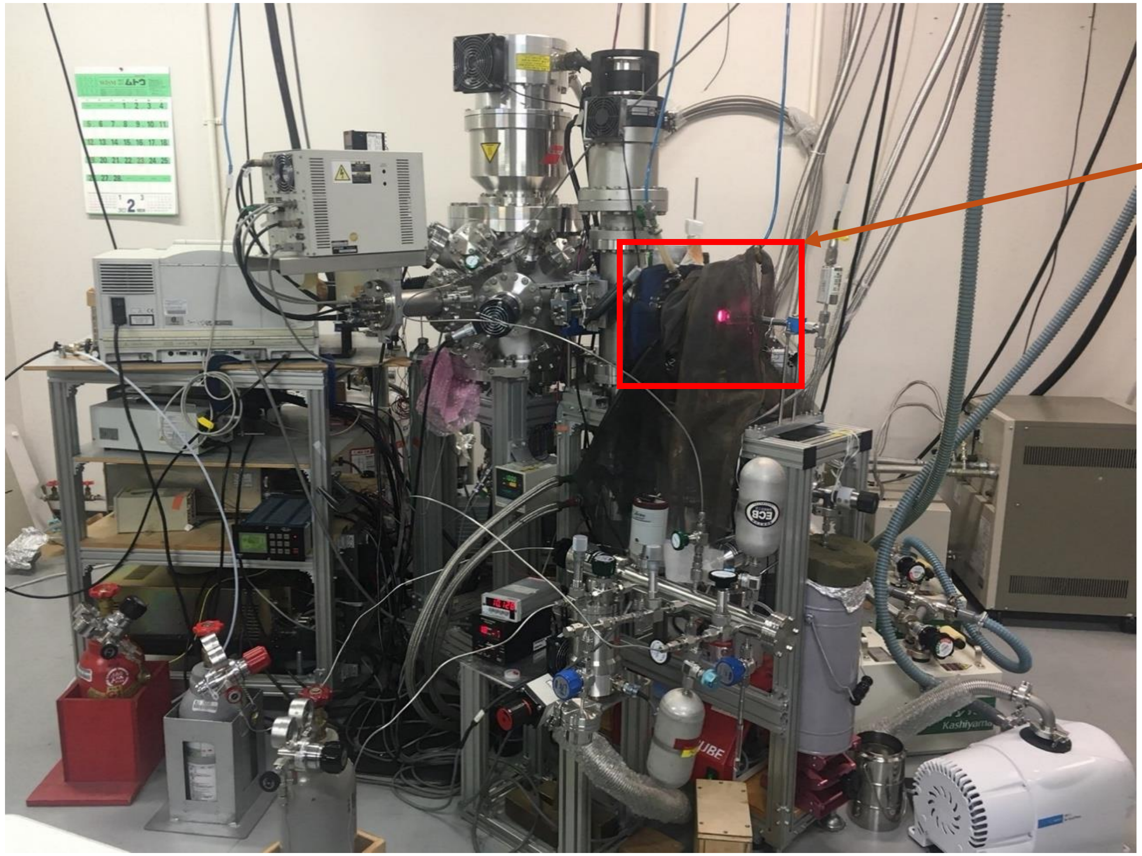


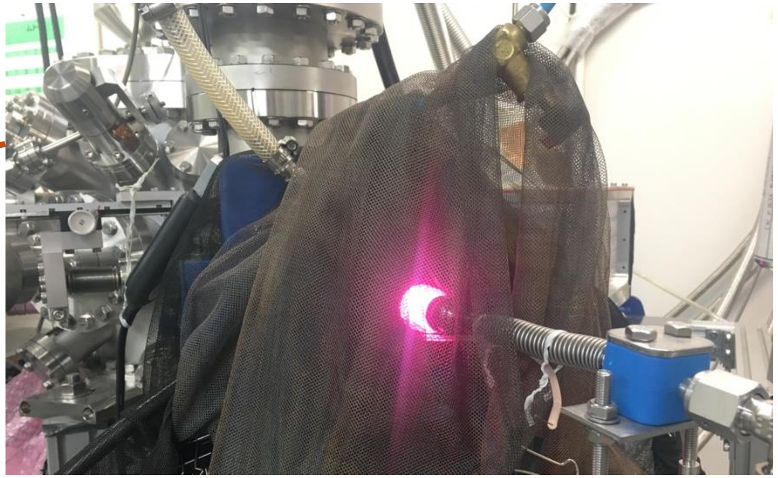
- ❑ Quadrupole mass spectrometer (QMS)

- Recording the presented molecules in the vacuum chamber
  - ✓ Hydrogen atoms (H – red column)
  - ✓ Hydrogen molecules and deuterium atoms (H_2 & D – green column)
  - ✓ Hydrogen deuteride molecules (HD – blue column)
  - ✓ Deuterium molecules (D_2 – yellow column)

Laboratory and Research Processing

❖ Apparatus (ASURA) setup



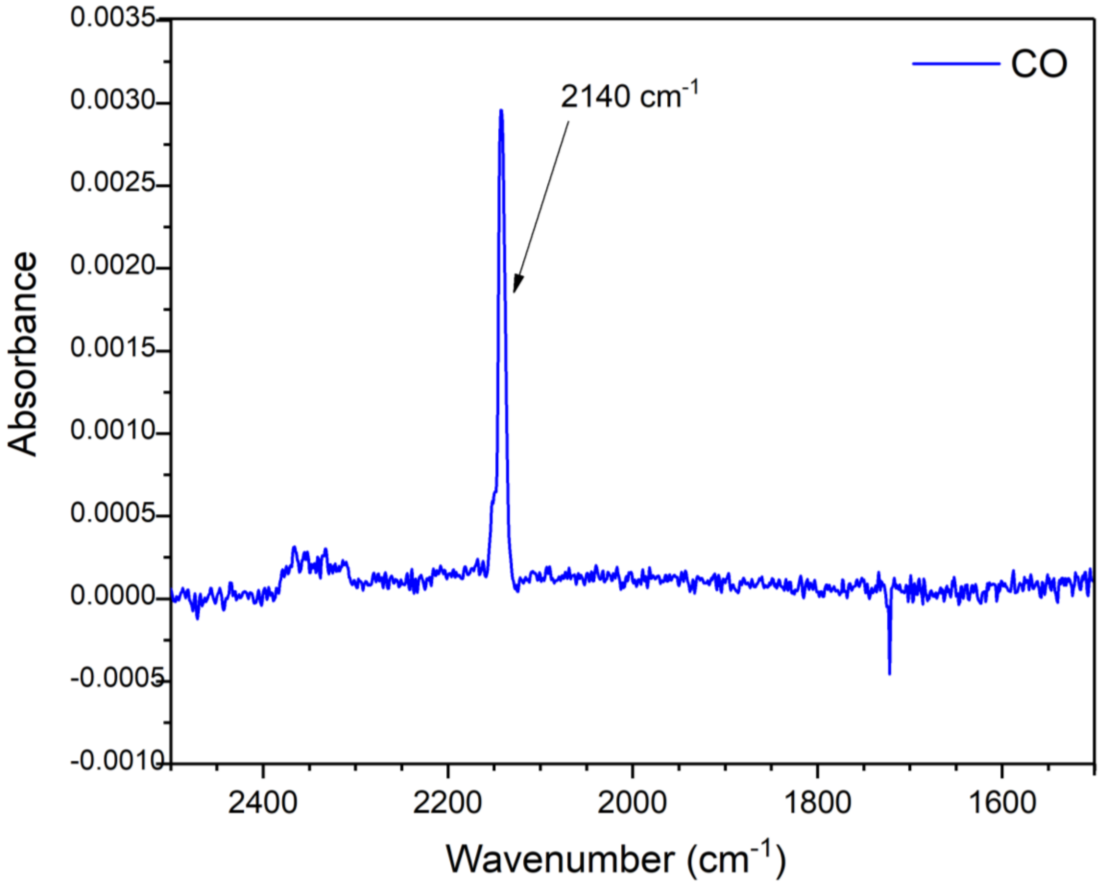


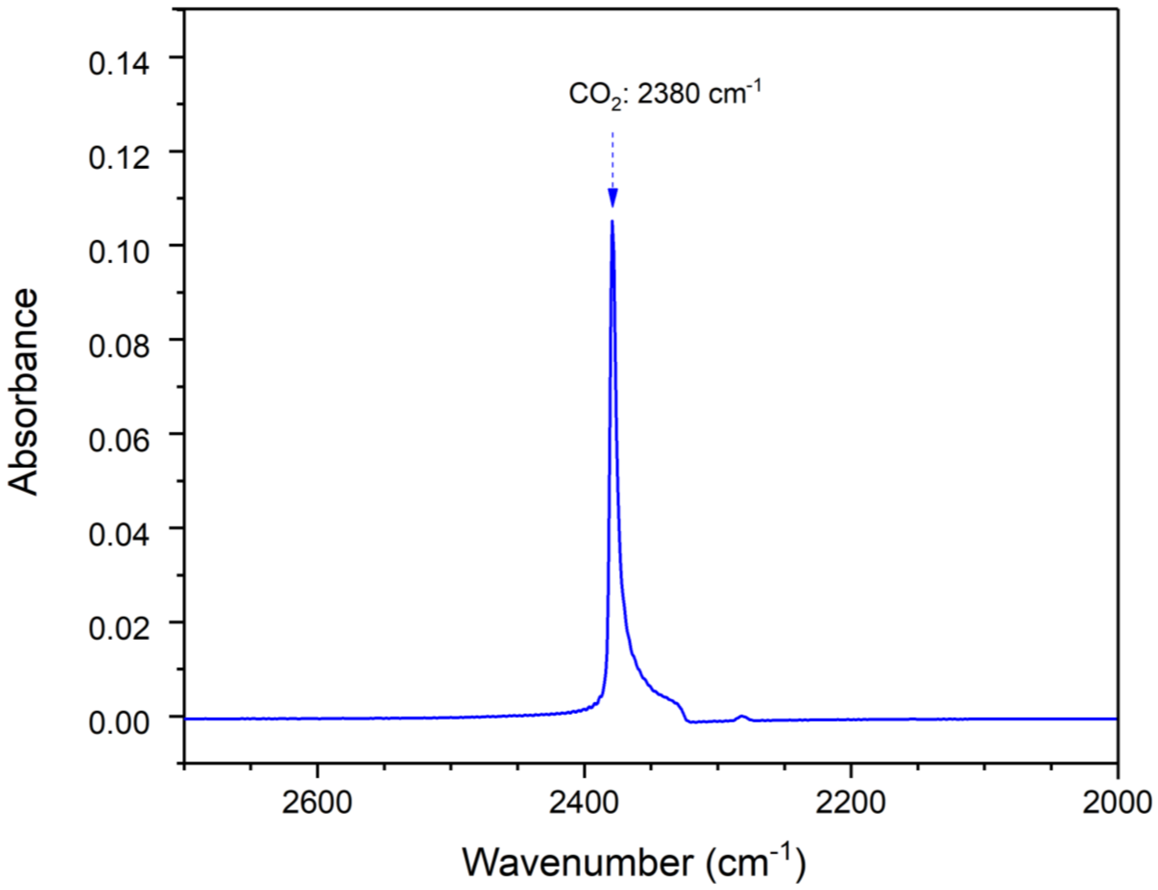
- ❑ Microwave-discharged plasma is used to dissociate H_2 molecules to generate H atoms

$$H_2 + hv \rightarrow H + H$$

Infrared spectra of some molecules

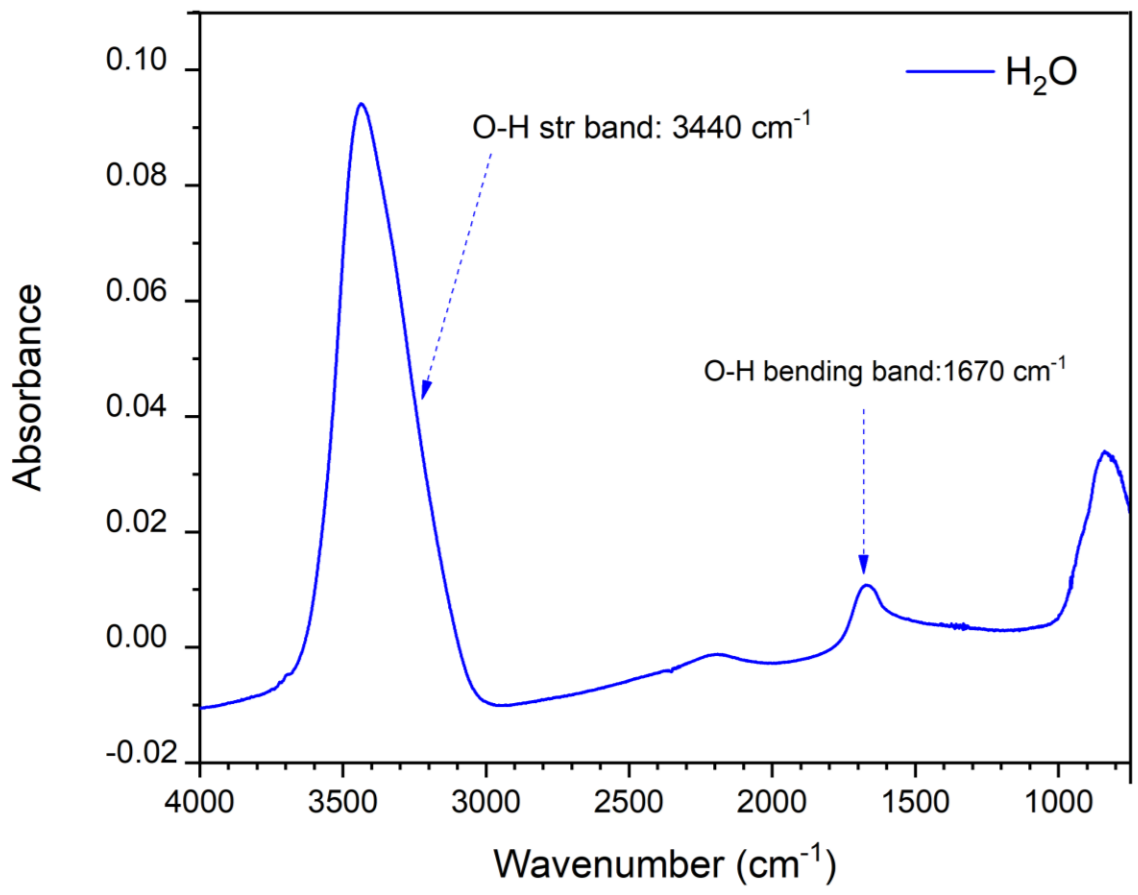
- Infrared spectrum of Carbon monoxide (CO) and Carbon dioxide (CO_2) on dust grains

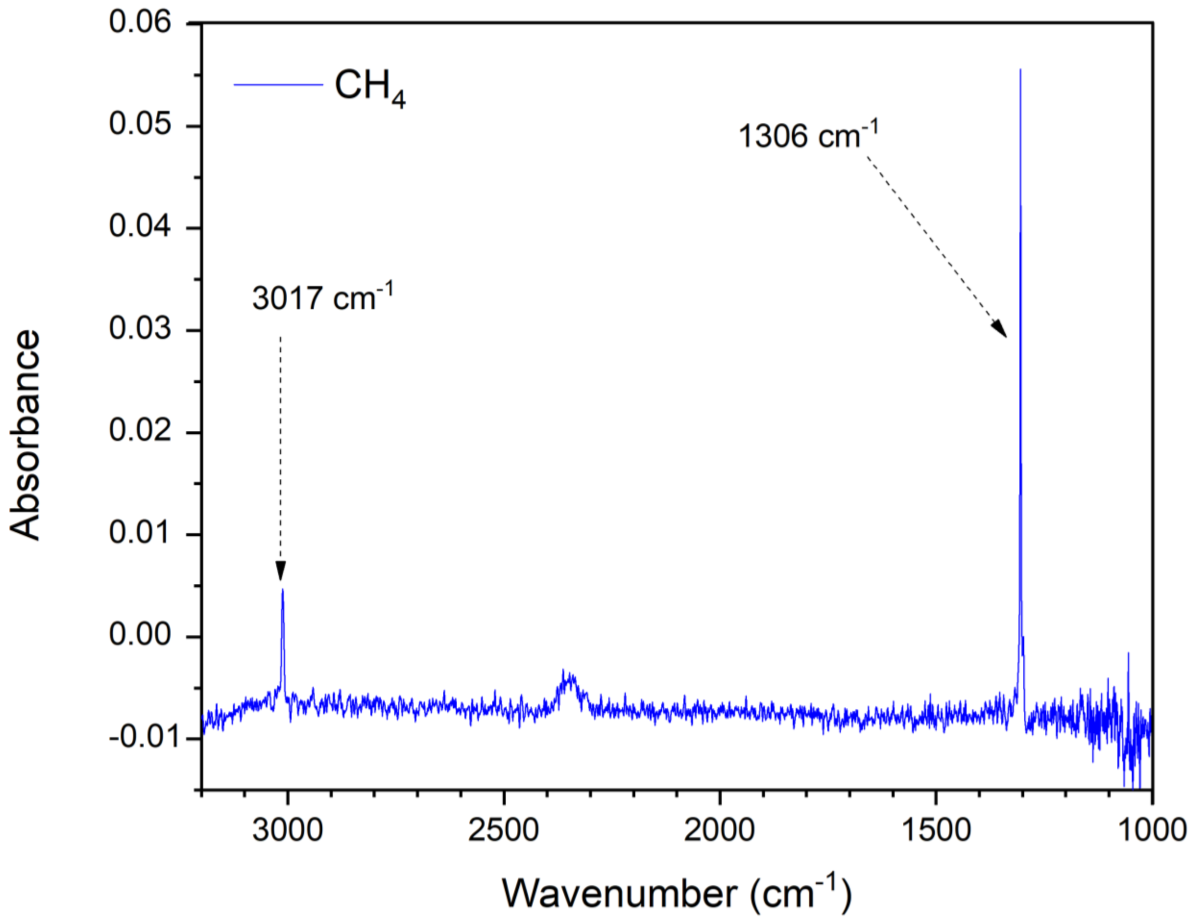




Infrared spectra of some molecules

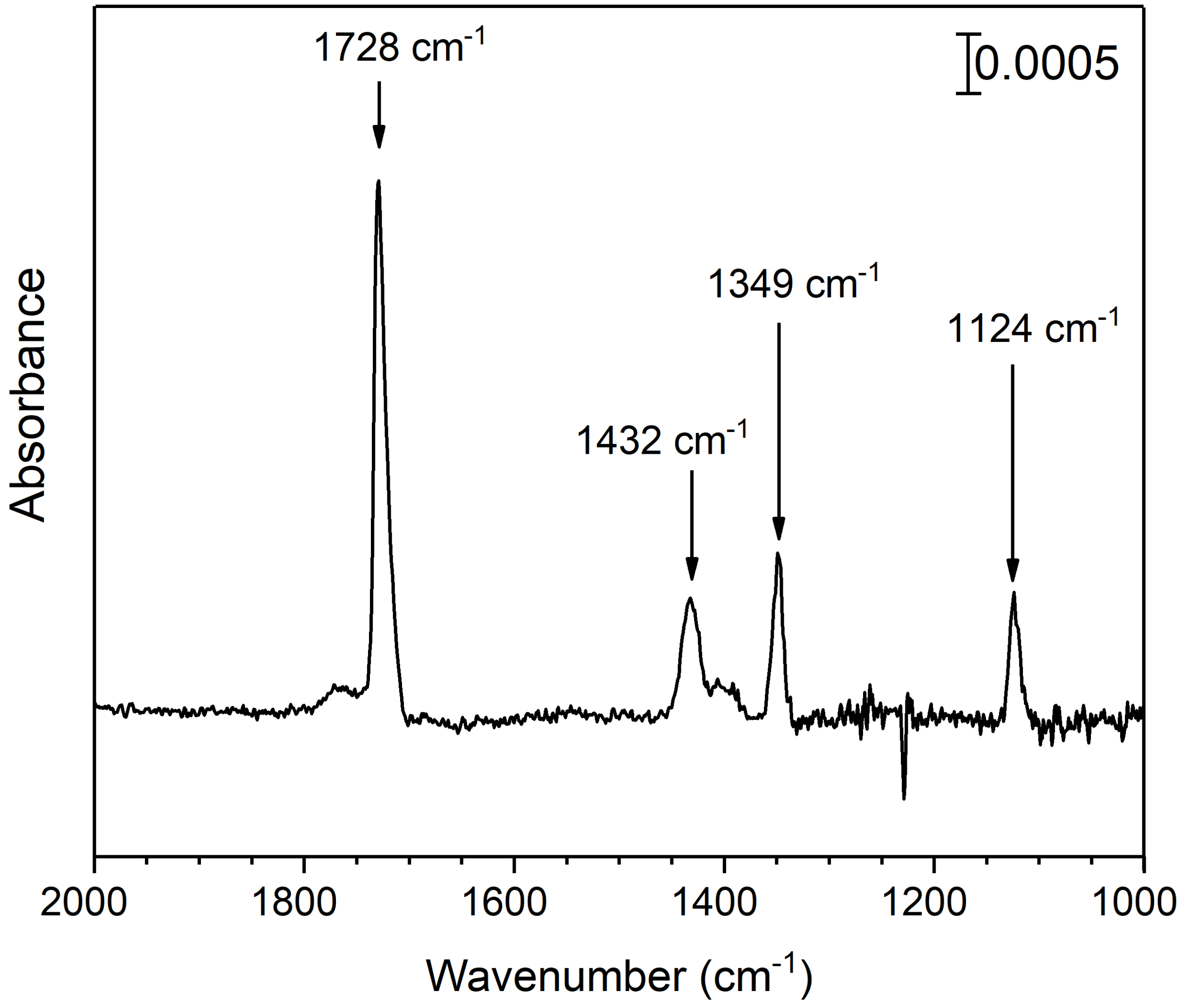
- Infrared spectrum of water (H_2O) and methane (CH_4) on dust grains





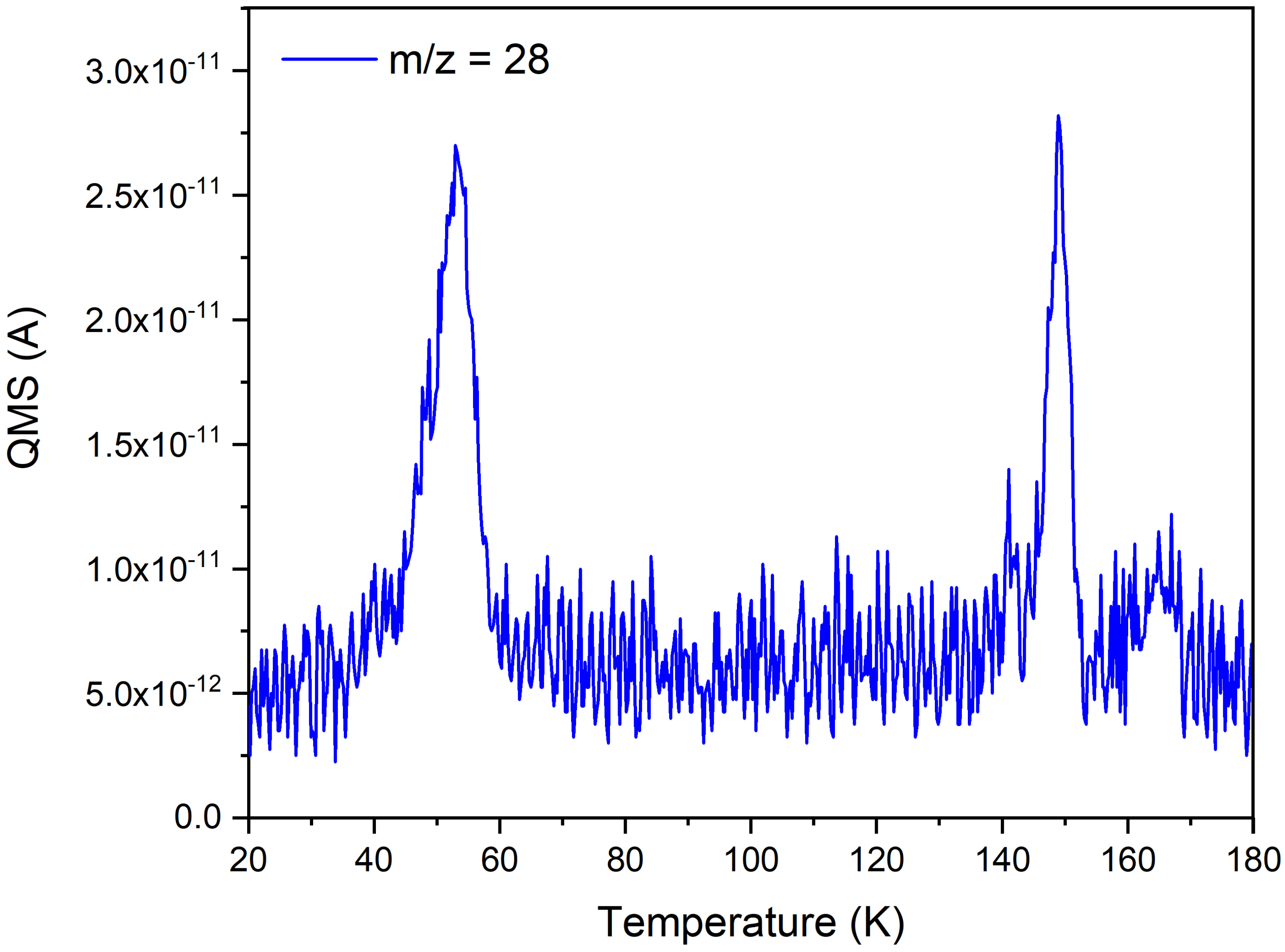
Infrared spectra of some molecules

- Infrared spectrum of Acetaldehyde (CH_3CHO) on dust grains



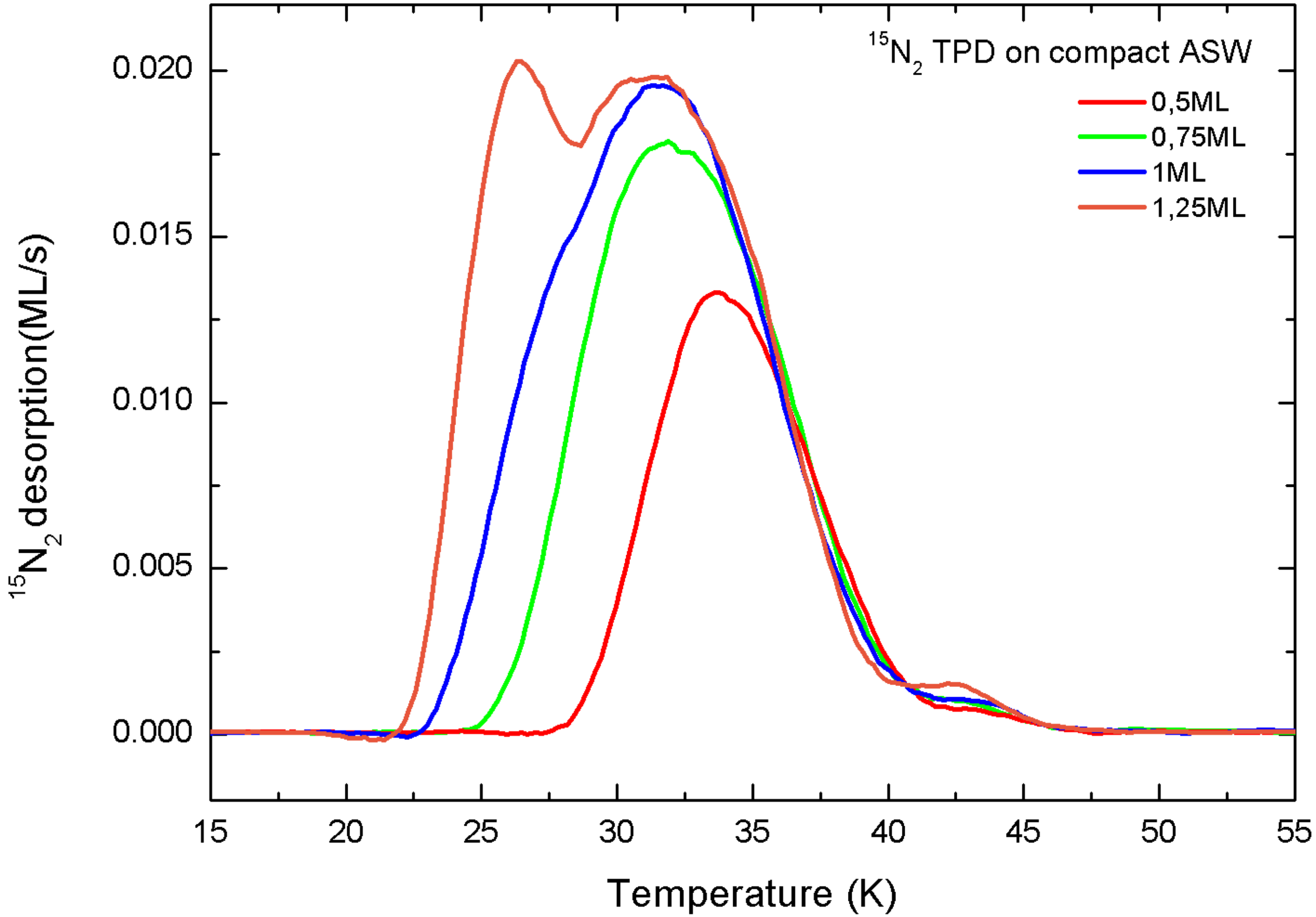
Mass spectrometer

- The major desorption peak of CO at m/z = 28 in range the temperature from 30 to 60 K.
- The minor peak desorbed from 130 to 155 K is attributed to CO.

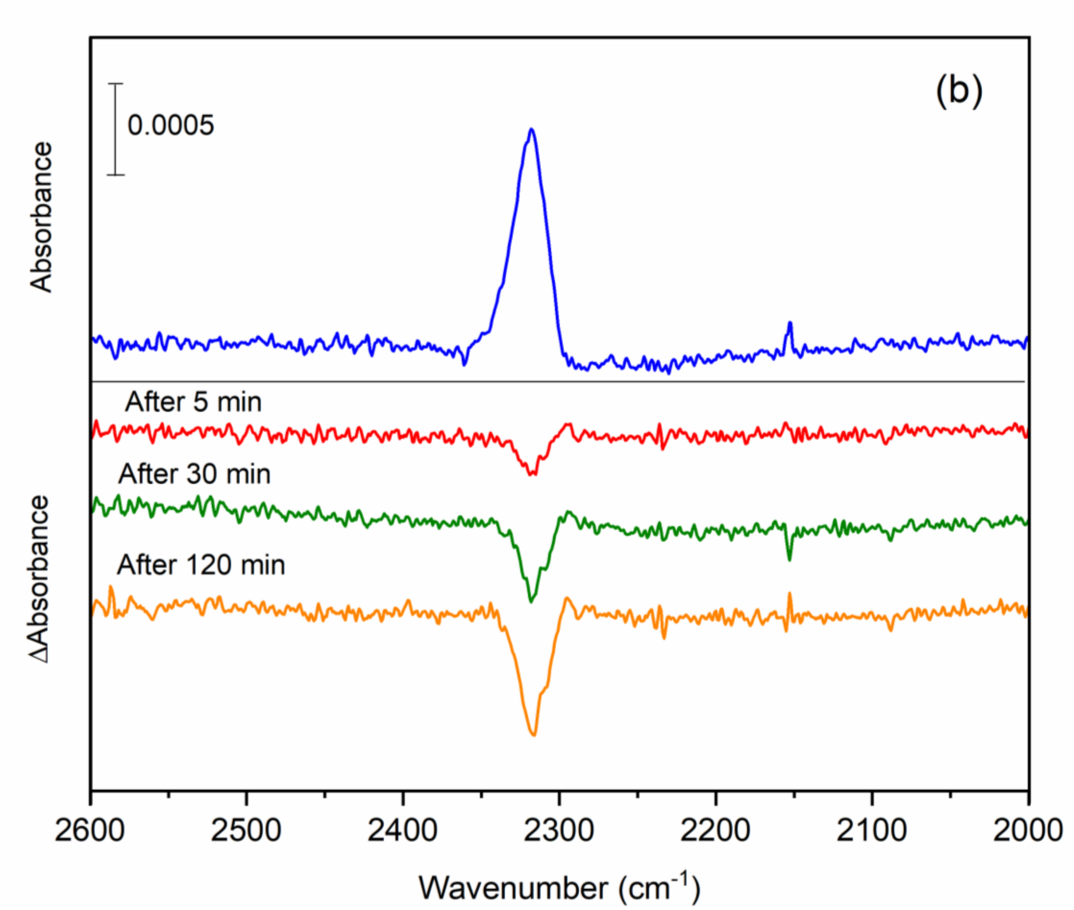


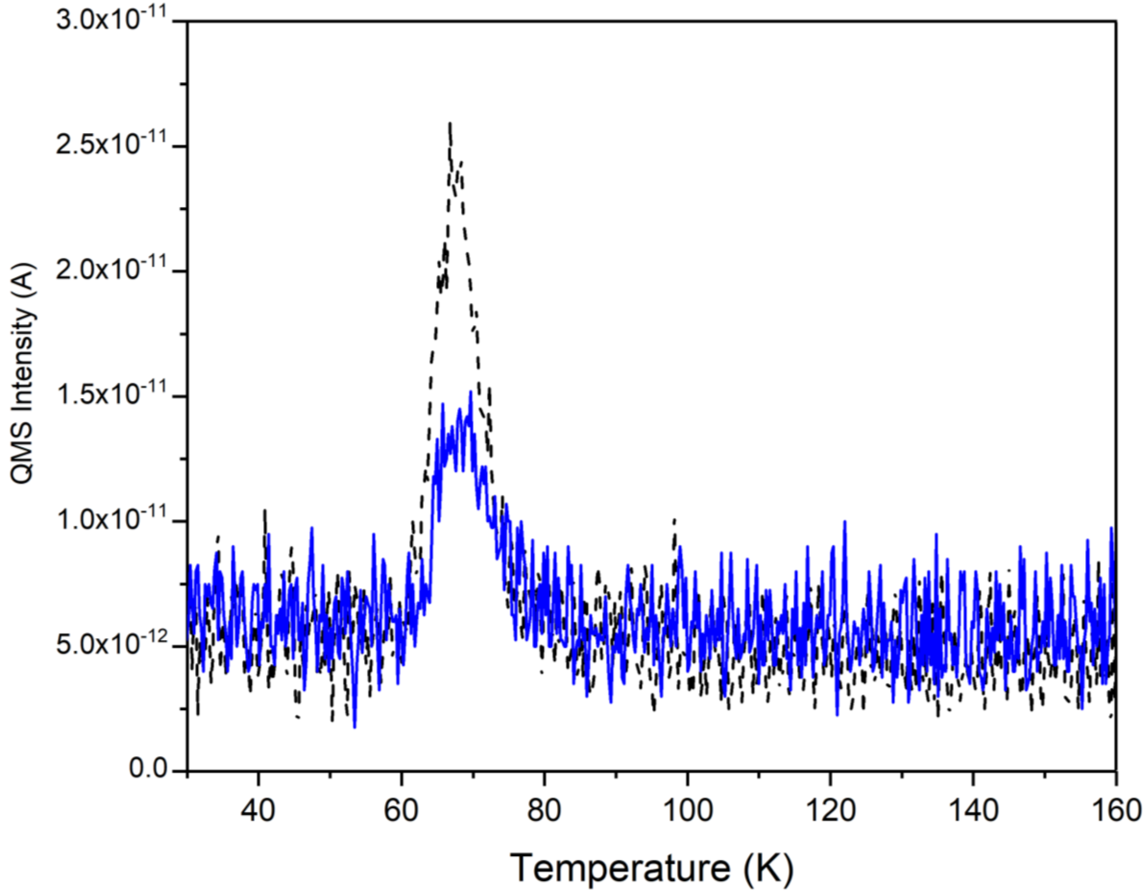
Mass spectrometer

- The major desorption peak of N_2 at m/z = 30 in range the temperature from 25 to 40 K.



Chemical pathways of phosphine (PH3) on dust grains

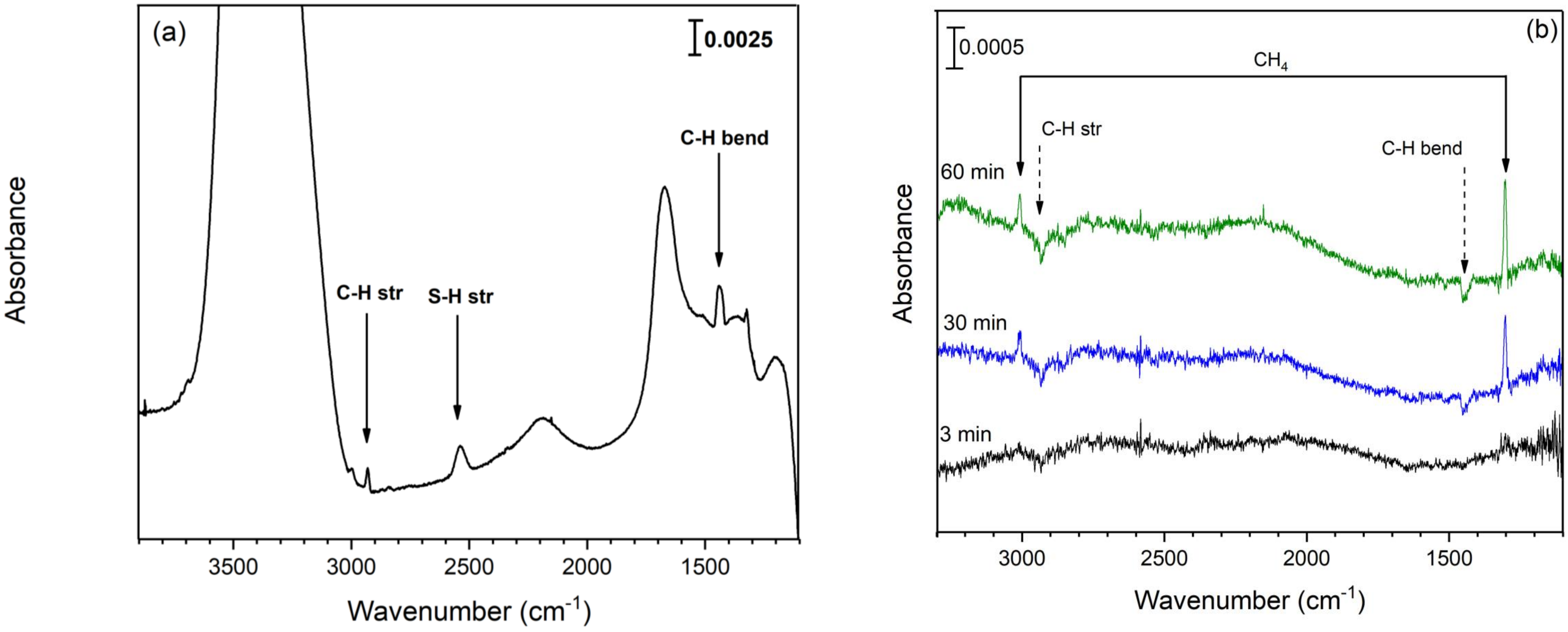




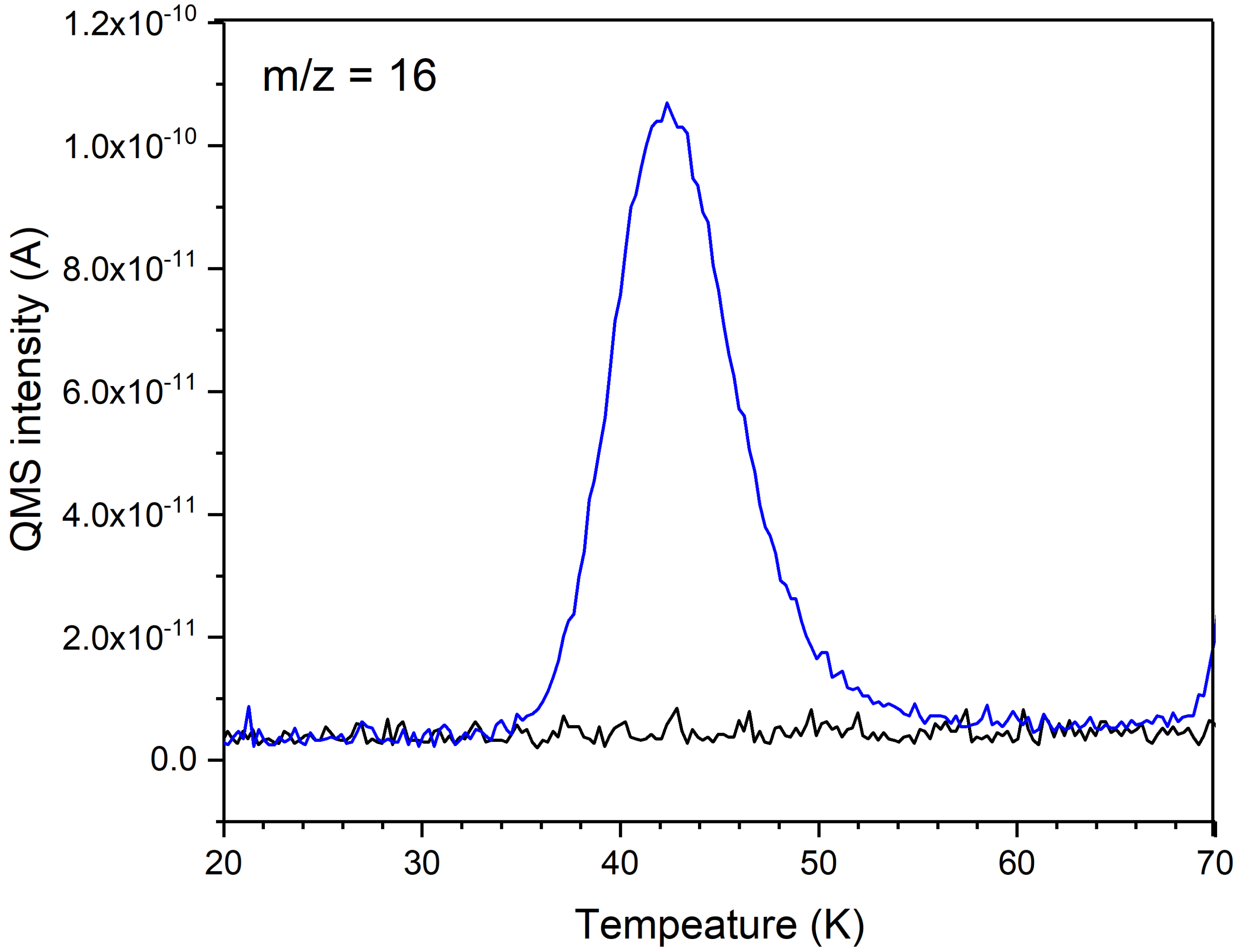
$PH_3 + H \rightarrow PH_2 + H_2$,

$PH_2 + H \rightarrow PH + H_2$.

Chemical pathways of Methyl Mercaptan (CH_3SH) on dust grains



Chemical pathways of Methyl Mercaptan (CH_3SH) on dust grains



- A desorption peak at m/z = 16 in range the temperature from 35 to 55K is attributed to CH_4

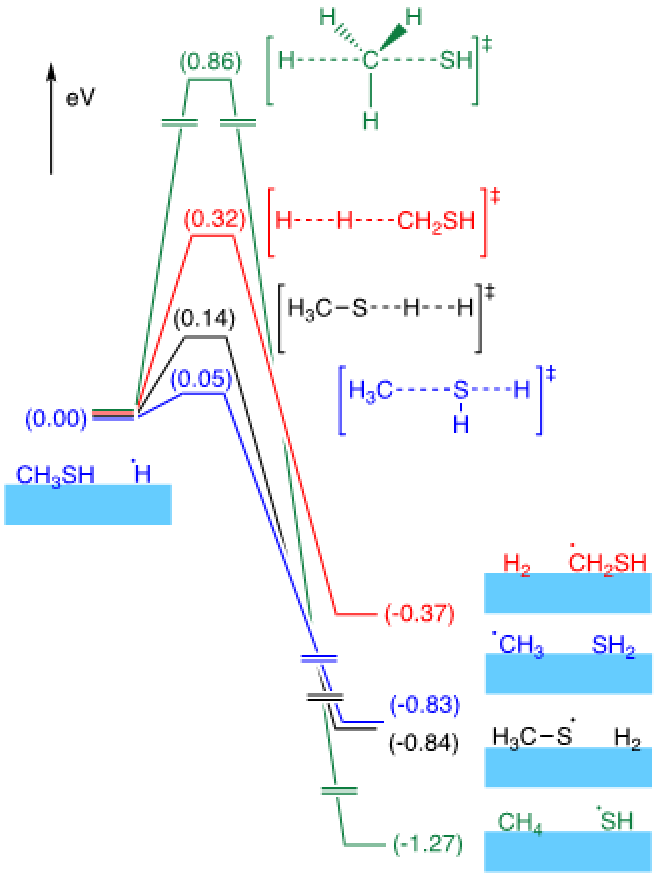
✓ CH_3SH was removed from the substrate because of the interaction with H atoms

✓ CH_4 was formed on the reaction surface

Thank you for your attention!

Possible chemical reactions of CH_3SH with H atoms on ASW at low temperatures

- Possible chemical pathways of CH_3SH with H atoms on ASW



Computed potential energy surfaces for the reactions between CH_3SH and H on ASW

1. $CH_3SH + H \rightarrow CH_4 + SH$, $\Delta E = 0.86$ eV
2. $CH_3SH + H \rightarrow CH_2SH + H_2$, $\Delta E = 0.32$ eV
3. $CH_3SH + H \rightarrow CH_3S + H_2$, $\Delta E = 0.14$ eV
4. $CH_3SH + H \rightarrow CH_3 + H_2S$. $\Delta E = 0.05$ eV

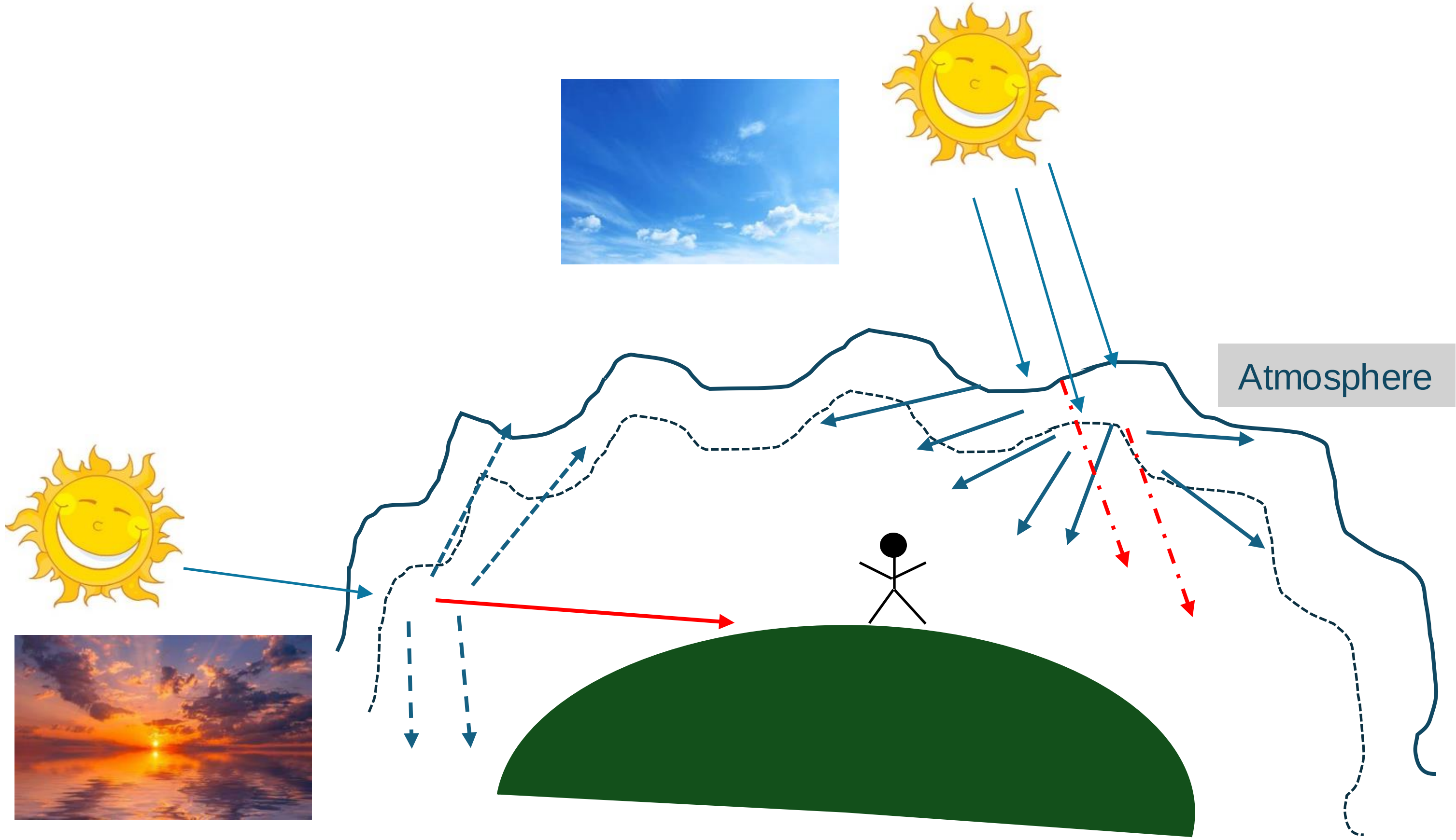
$+ H \rightarrow CH_4$: without activation barrier

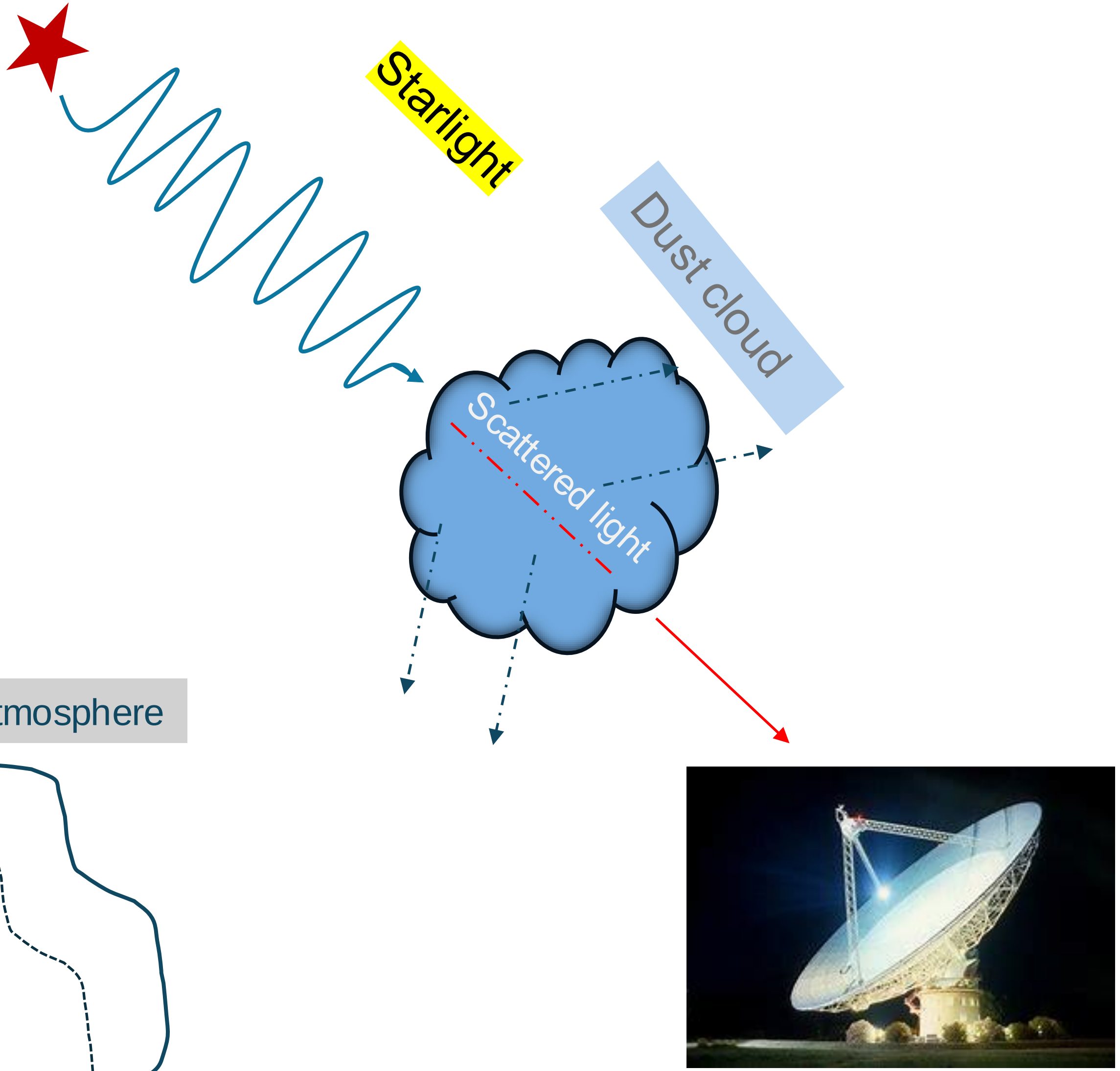
$+H \rightarrow HS + H_2$: chemical desorption (Oba et al.2018)

$HS + H \rightarrow H_2S$

Interstellar medium: physical processes

- Earth's atmosphere
  - Components: a lots of particles such as: dust, H_2O ice, H_2O droplets, N_2, O_2, etc.
- Question: Why is the sky blue?





Telescope

❑Reflection

M78 and Reflecting Dust Clouds
Image Credit & Copyright: Ian Sharp

- A nebula is a giant cloud of dust and gas what thrown out by the explosion of a dying star in space.

- Reflection nebula
  - Scatter starlight → the blue light is strongly scattered

- The blue patches = reflection nebulas
- The dark patches = dark clouds completely absorb starlight

Properties of ionized gas

Type	Number density (cm^{-3})	Temperature (K)	Major constituents	Main detection technique
Hot ionized medium	0.003	10^6 -10^7	H^+, C^{3+}, N^{4+}, O^{5+}	UV absorption, X-ray emission
Warm ionized medium	> 10	10^4	H^+, He^+, O^+, C^+, N^+	Optical, UV, IR, Hα
H II regions	0.1 - 10^4	8 x 10^3	H^+, He^+, O^+, C^+, N^+	Hα emission

- Goals: To understand how these phases are observed and how they are heated and ionized.

Interstellar medium: physical processes

❑ Properties of neutral gas

Type	Number density (cm^{-3})	Temperature (K)	Major constituents	Main detection technique
Warm neutral medium	0.2 - 0.5	6 – 10 x10^3	H, He	21 cm emission
Atomic cold neutral medium	10 - 100	100	$H^0 + H_2$	21 cm absorption, 3.4 μm, UV absorption
Molecular hot cores (protostellar cores)	> 10^6	100 - 300	H_2	Rovibrational emission CH_3CN, CH_3OH, NH_3

❖ Goals: To understand how these properties are determined, what the relevant thermal and ionization processes are, how atomic and molecular clouds are related, and how the latter lead to star formation.

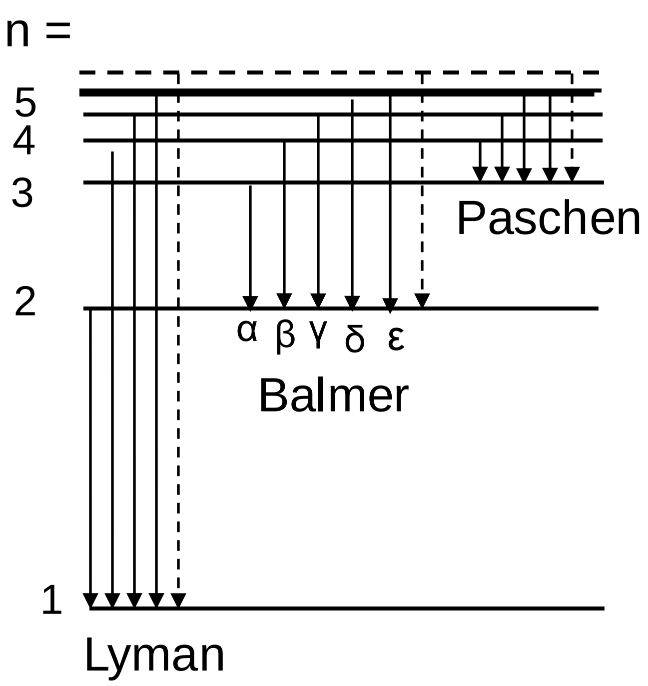
The formation and life cycle of stars

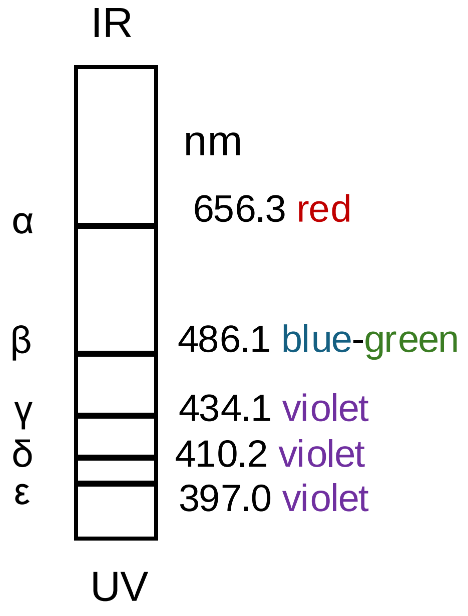
- Difference between stars and planets

	Stars	Planets
Meaning	Stars are the astronomical objects, that emit their own light, produced due to thermonuclear fusion, occurring at its core	Planets refers to the celestial object that has a fixed path (orbit), in which it moves around the star
Light	They have their own light	They do not have their own light
Temperature	High	Low
Size	Big	Small
Matter	Hydrogen, helium, and other light elements	Solid, liquid, or gas, and a combination thereon

❑ Molecular clouds: Emission

Nebula IC 434 in the constellation Orion





- Hα emission at 656.46 nm in the red part of the visible light and responsible for the reddish of molecular cloud

=> Observe the reddened clouds in the ISM.

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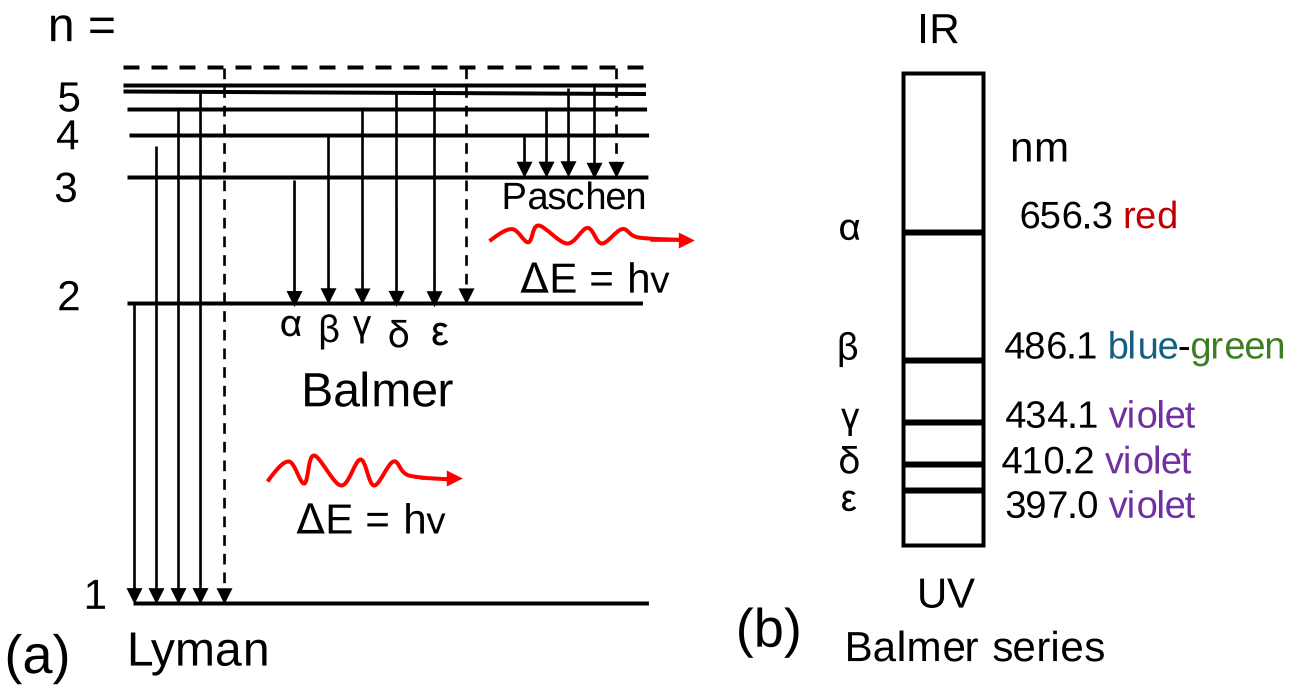
- Hydrogen occupies 90 % of the total components in interstellar gas.

=> There are five hydrogen species present in interstellar clouds: H^+, H^-, H, H_2, H_3^+

- $H^+ + e^- \rightarrow \{H^*\} \rightarrow H + h\upsilon$ (e.q 1)



(a) Graphical representation of the electronic transitions between excited states and the ground state (n = 1, Lyman series) of the hydrogen atoms, and electronic transitions ending on the levels n = 2 (Balmer series), and n = 3 (Paschen series).

(b) Projection of the Balmer series into an optical spectrum.

- Balmer series lines are most the studied H atom lines since they are in the visible.
- The Lyman series is expected to be ultraviolet continua.

Interstellar medium: physical processes

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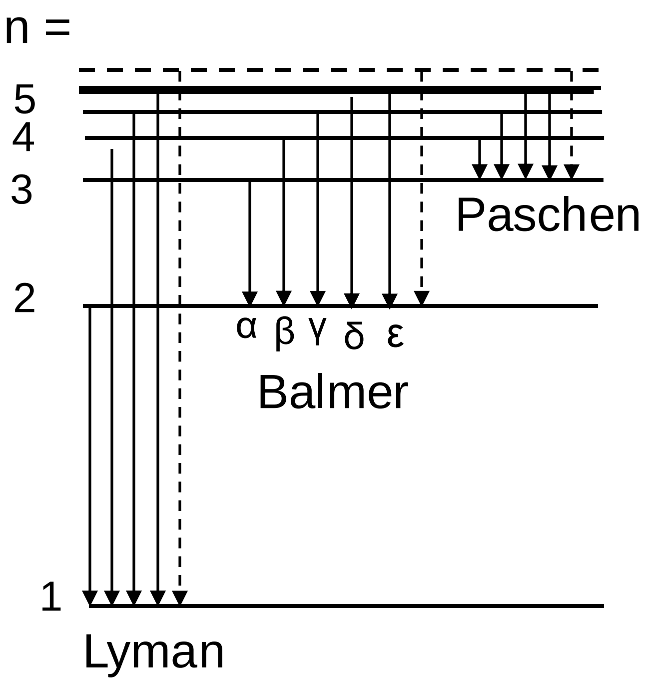

- The wavelengths, for these transitions, are given by the Rydberg formula:

$$\frac{1}{\lambda} = \frac{1}{hc}\left(E_{n1} - E_{n2}\right) = R_H\left(\frac{1}{n_1^2} - \frac{1}{n_2^2}\right),\ n_1 < n_2 \quad \text{(e.q.2)}$$

Where: R_H = 109677.581 cm^{-1}: Rydberg constant

n is the principal quantum number (n = 1, 2, 3, ….∞)

- The range of each H atom series is given by the lowest frequency transition, between n_1 and $n_2 = n_1 + 1$; $n_2 = n_1 + 2$, $n_2 = n_1 + 3$ …

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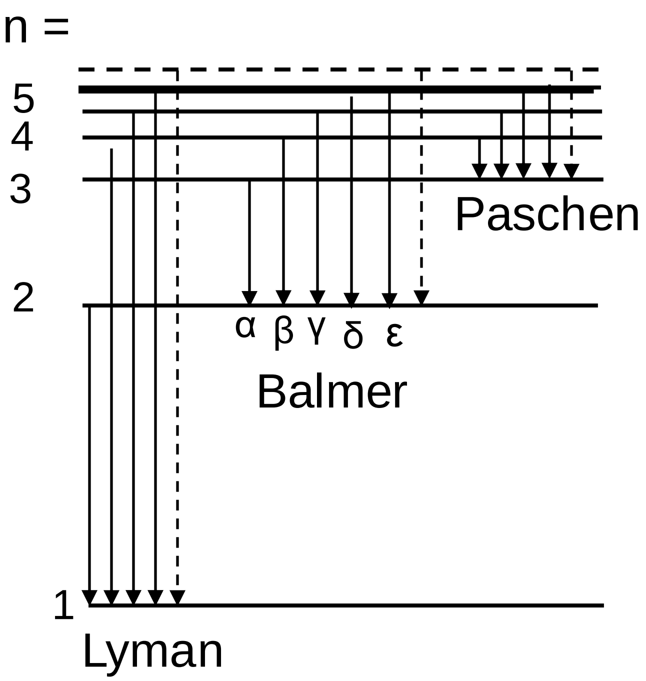

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- n_1; $n_2 = n_1 + 1$; $n_2 = n_1 + 2$, $n_2 = n_1 + 3$ …

❑ Worked Example:

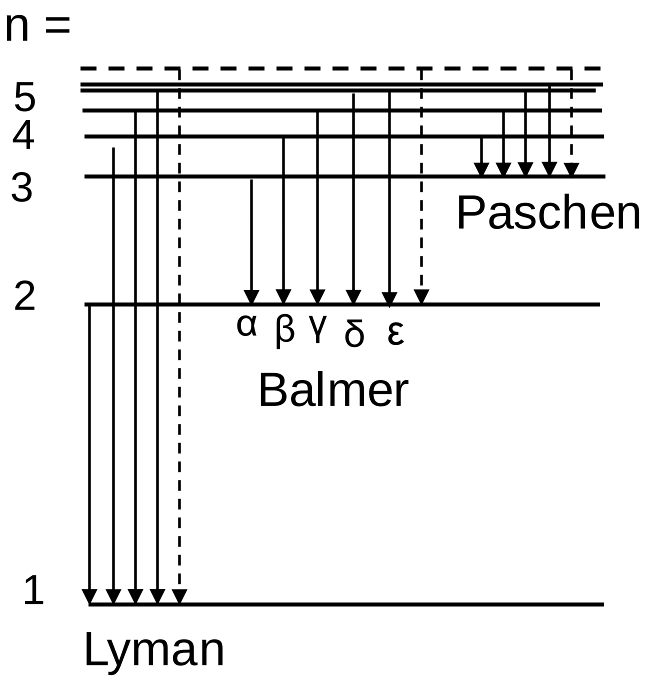
➢ Lyα: $n_1 = 1$ and $n_2 = 2$, using e.q.1: $\frac{1}{\lambda} = R_H\left(1 - \frac{1}{4}\right) = \frac{3}{4}R_H = 82258.2\ cm^{-1}$

$\Rightarrow \lambda = 1.21568 \times 10^{-5}$ cm = 121.568 nm: UV

➢ The transition of Hα: n_1 = ?, n_2 = ?, λ = ???

➢ The transition of Hγ: n_1 = ?, n_2 = ?, λ = ???

❑ Molecular clouds: Emission



- The wavelengths, for these transitions, are given by the Rydberg formula:

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Where $R_H = 109677.581\ \text{cm}^{-1}$; n is the principal quantum number (n = 1, 2, 3, ….∞)

- n_1; $n_2 = n_1 + 1$; $n_2 = n_1 + 2$, $n_2 = n_1 + 3$ …

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➢ The transition of Hα: n_1 = **2**, n_2 = **3**, λα = **656.46** nm

➢ The transition of Hγ: n_1 = **2**, n_2 = **5**, λγ = **434.173** nm