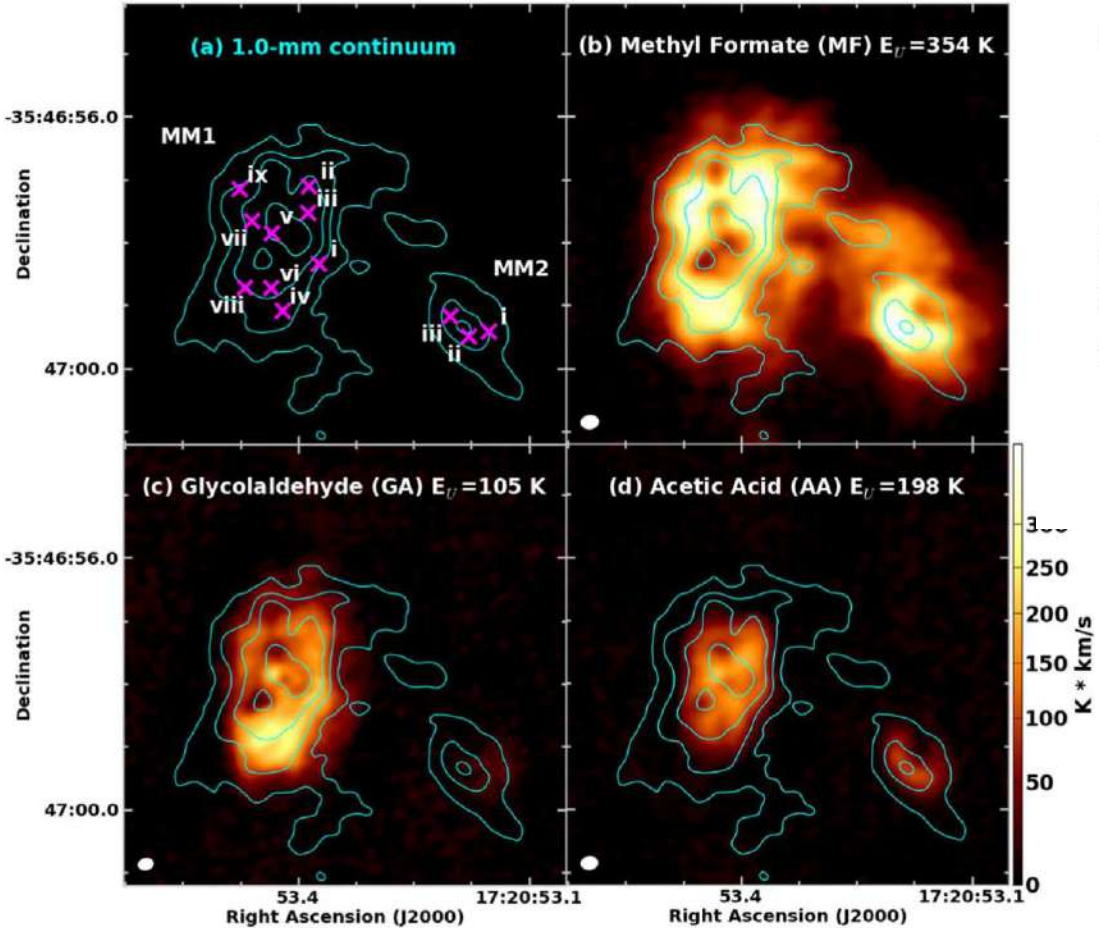
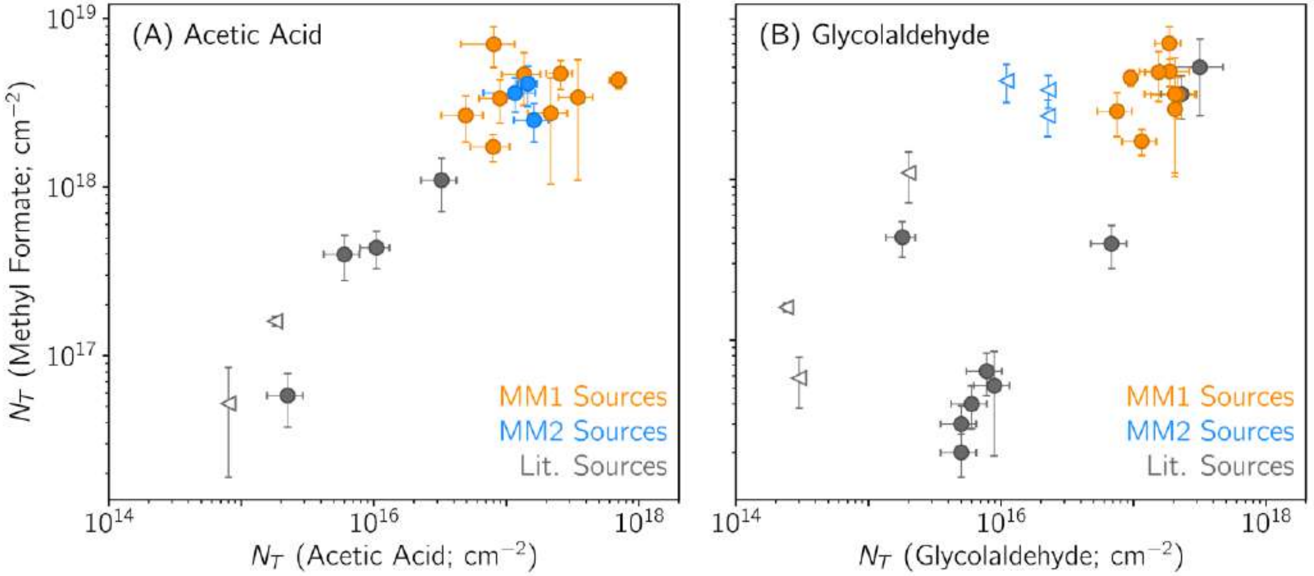
Laboratory Future

<u>Sergio Ioppolo</u>

InterCat, Department of Physics and Astronomy, Aarhus University

COMs in Hot Cores

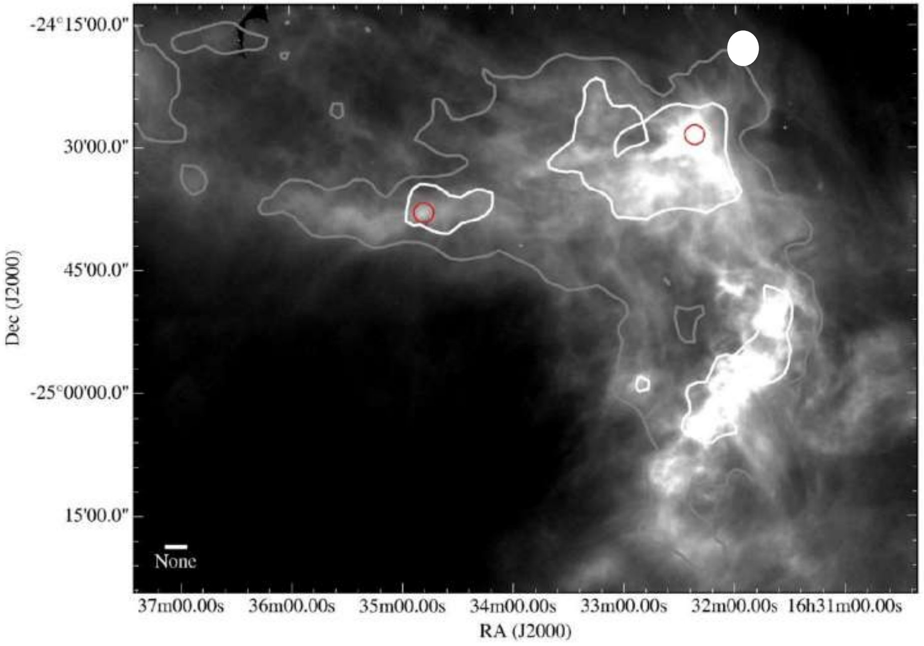




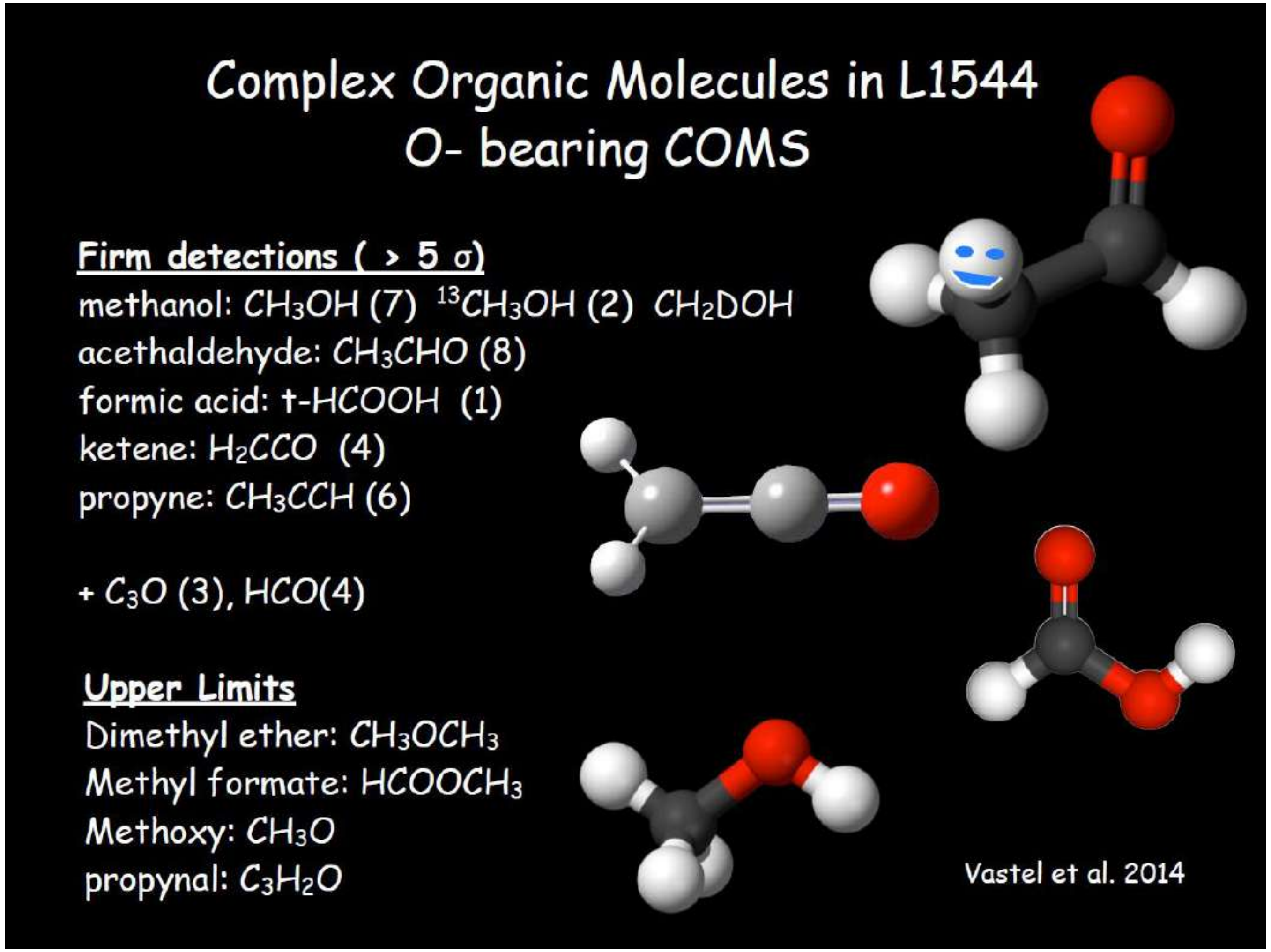
El-Abd *et al.*, ApJ (2019)

COMs in Prestellar Cores

(L1689B)



Bacmann *et al.*, *A&A* (2012)



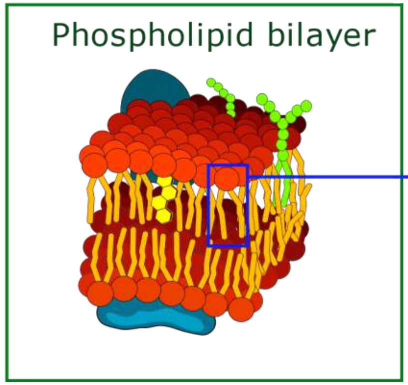
Credit: FORS Team, ESO

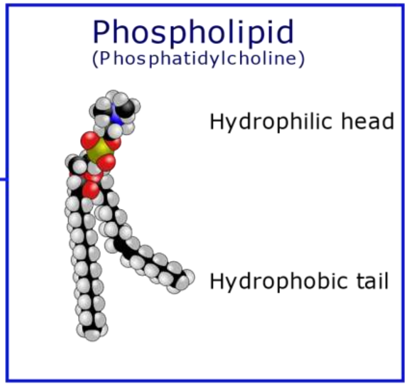
COMs in Molecular Clouds

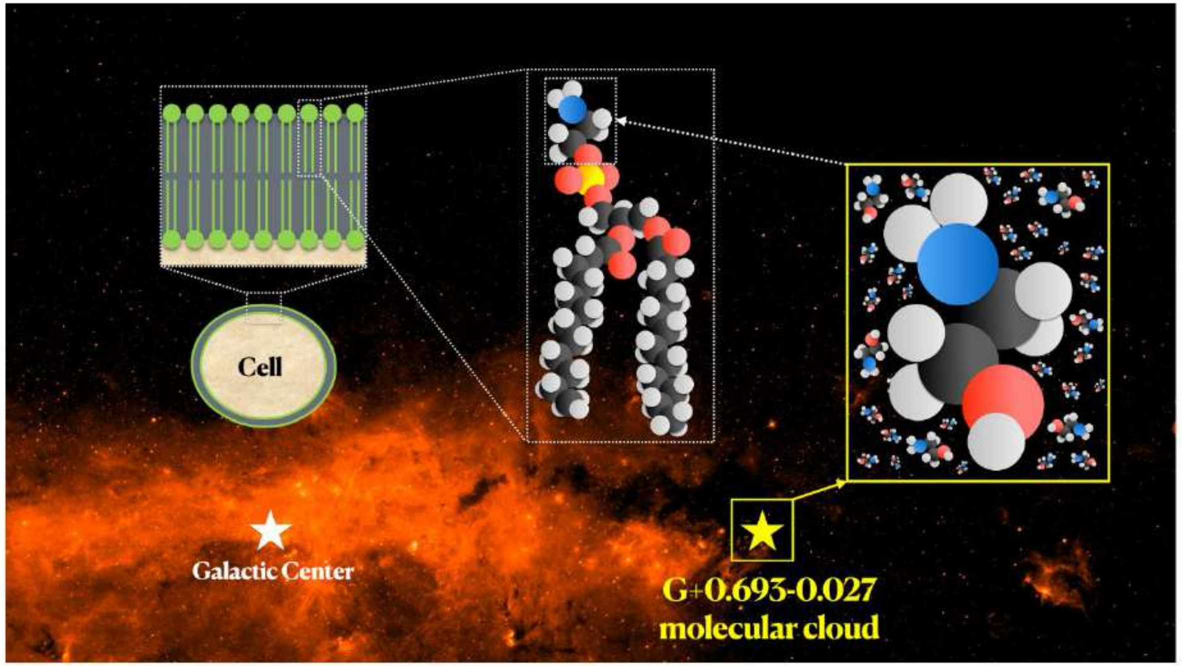
Discovery in space of ethanolamine, the simplest phospholipid head group

Víctor M. Rivilla[a,b,1], Izaskun Jiménez-Serra[a], Jesús Martín-Pintado[a], Carlos Briones[a], Lucas F. Rodríguez-Almeida[a], Fernando Rico-Villas[a], Belén Tercero[c], Shaoshan Zeng[d], Laura Colzi[a,b], Pablo de Vicente[c], Sergio Martín[e,f], and Miguel A. Requena-Torres[g,h]

[a]Centro de Astrobiología, Consejo Superior de Investigaciones Científicas–Instituto Nacional de Técnica Aeroespacial "Esteban Terradas", 28850 Madrid, Spain; [b]Osservatorio Astrofisico di Arcetri, Istituto Nazionale de Astrofisica, 50125 Florence, Italy; [c]Observatorio Astronómico Nacional, Instituto Geográfico Nacional, 28014 Madrid, Spain; [d]Star and Planet Formation Laboratory, Cluster for Pioneering Research, RIKEN, Wako 351-0198, Japan; [e]ALMA Department of Science, European Southern Observatory, Santiago 763-0355, Chile; [f]Department of Science Operations, Joint Atacama Large Millimeter/Submillimeter Array Observatory, Santiago 763-0355, Chile; [g]Department of Astronomy, University of Maryland, College Park, MD 20742; and [h]Department of Physics, Astronomy and Geosciences, Towson University, Towson, MD 21252

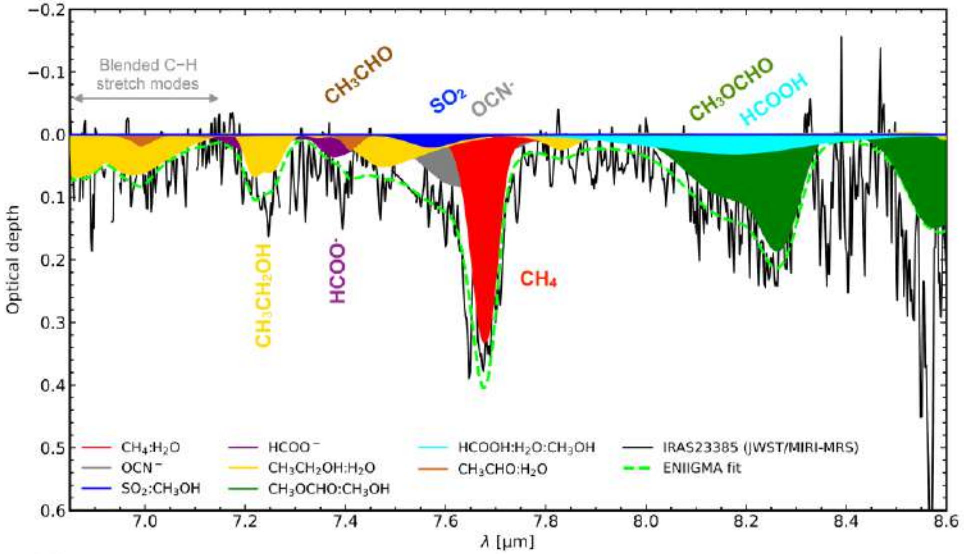


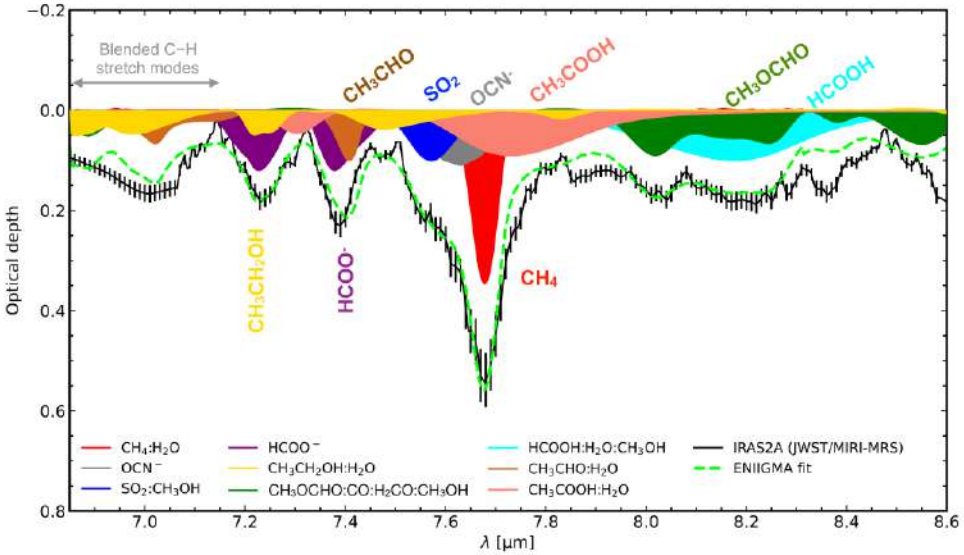


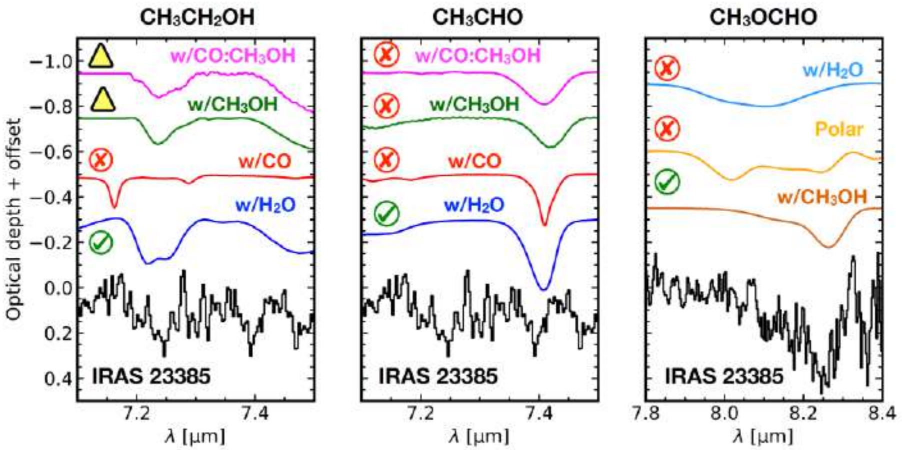


Discovery of ethanolamine, the simplest head of phospholipids (building blocks of cell membranes) towards the molecular cloud G+0.693–0.027 located in the center of our Galaxy. Credits: Víctor M. Rivilla & Carlos Briones (Centro de Astrobiología, CSIC–INTA) / NASA Spitzer Space Telescope, IRAC4 camera (8 microns).

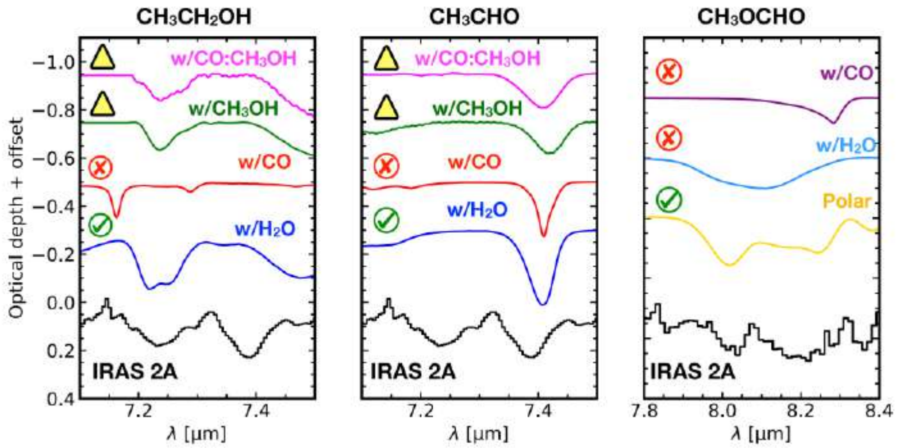
COMs in Ices toward YSO & MC





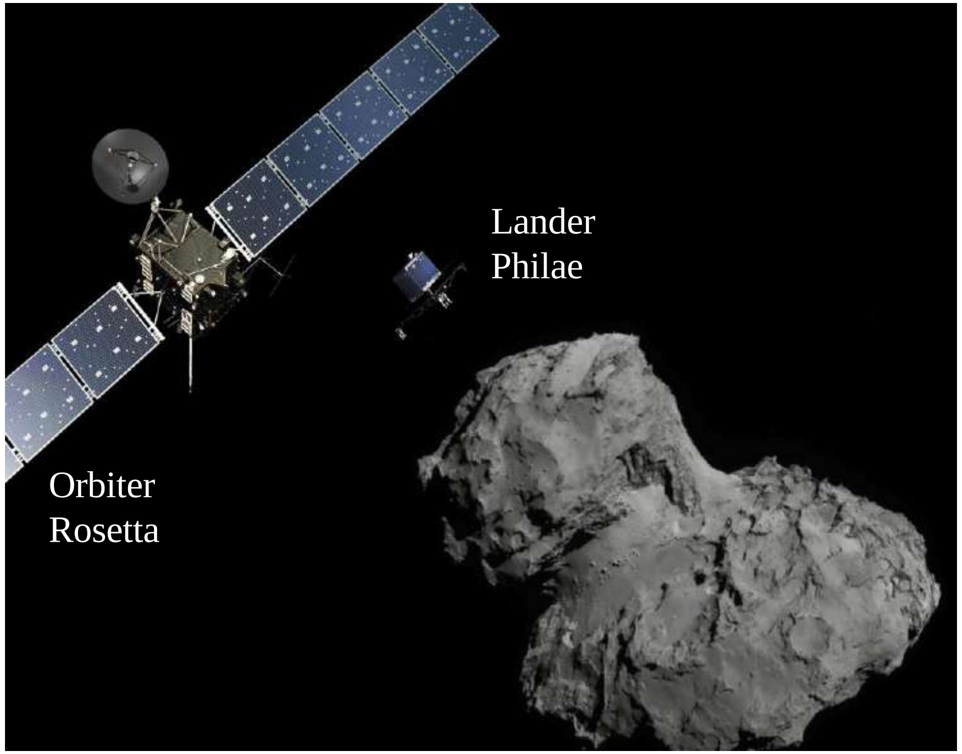


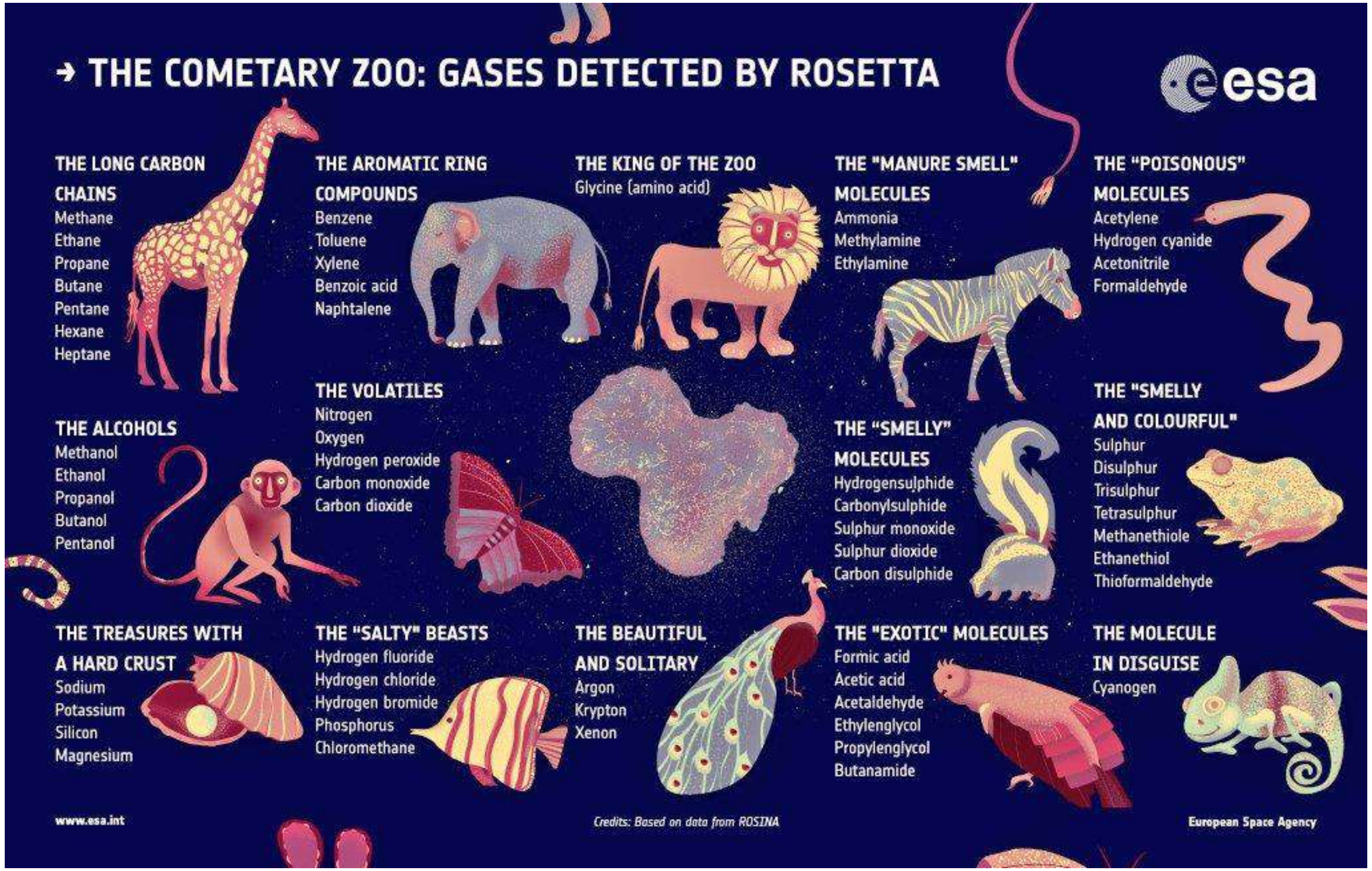
Ethanol **Acetaldehyde** **Methyl Formate**



Rocha *et al.* (2024)

COMs in the Solar System

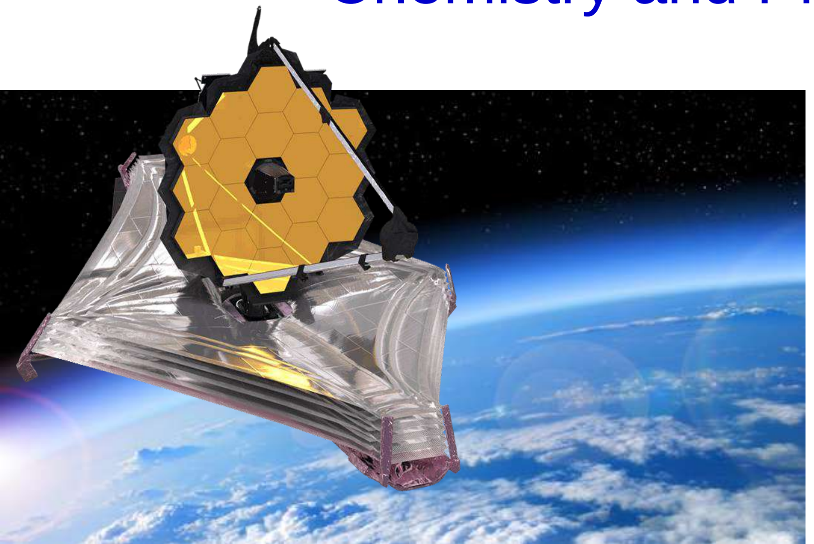


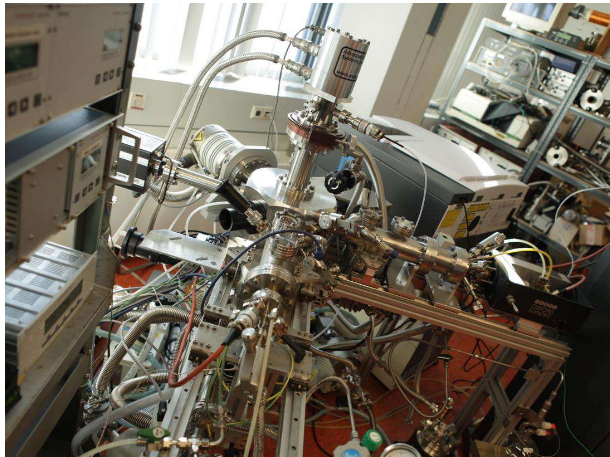


Altwegg *et al.*, Sci. Adv. (2016)

Future Needs

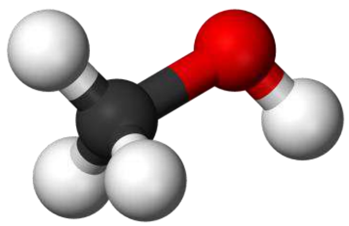
- Observations with ALMA, JWST, JUICE
  - More complex (prebiotic) species **(LAB SPECTRA)**
- Spatial distribution
  - Resolve relevant physicochemical scales **(LAB TECHNIQUES)**
- New processes simulated in Laboratory/Theory
  - Chemistry and Physics at the gas-ice interplay **(LAB METHODS)**

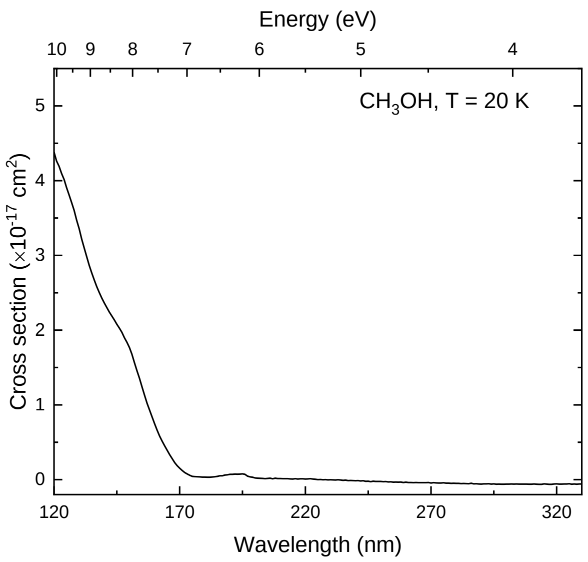




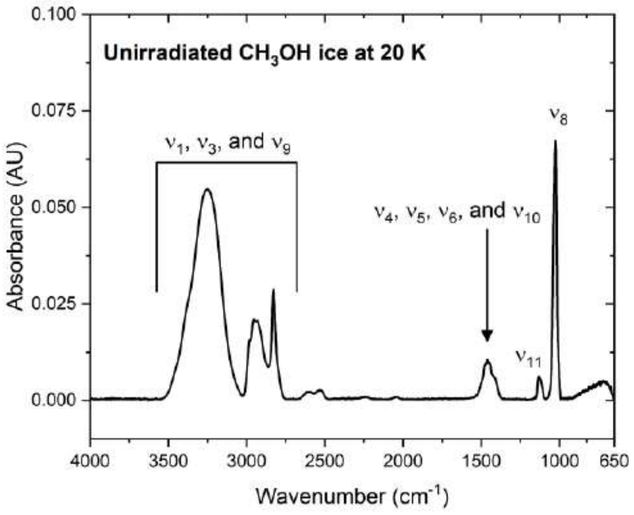
I. Fundamental properties of ices:

VUV/UV-vis/IR/THz (0.1 - 3000 μm) Ice Database

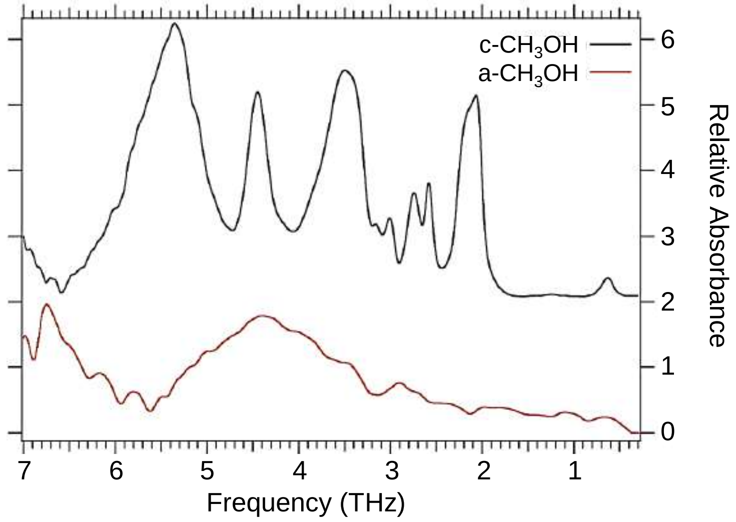




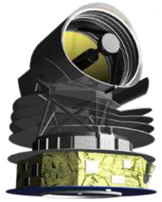
VUV



IR



THz



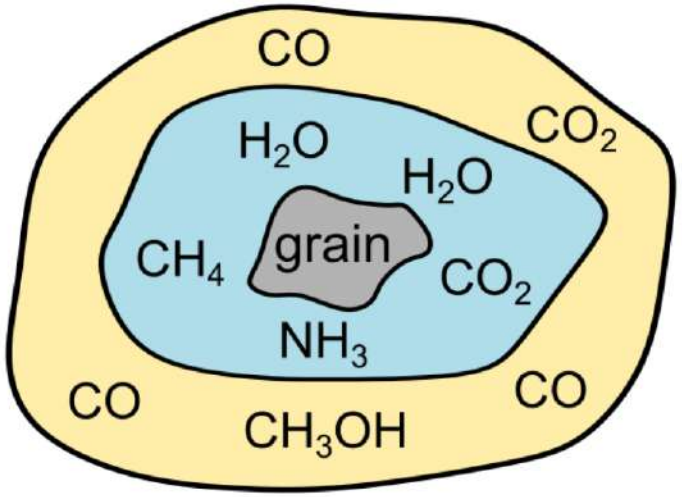
II. Bridging the gas-grain gap:
Linking Physics and Chemistry of Star Forming Regions

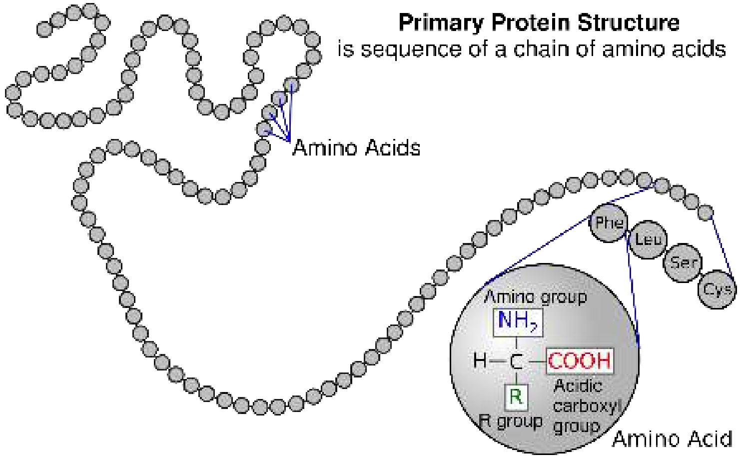
Better characterization of fundamental mechanisms:

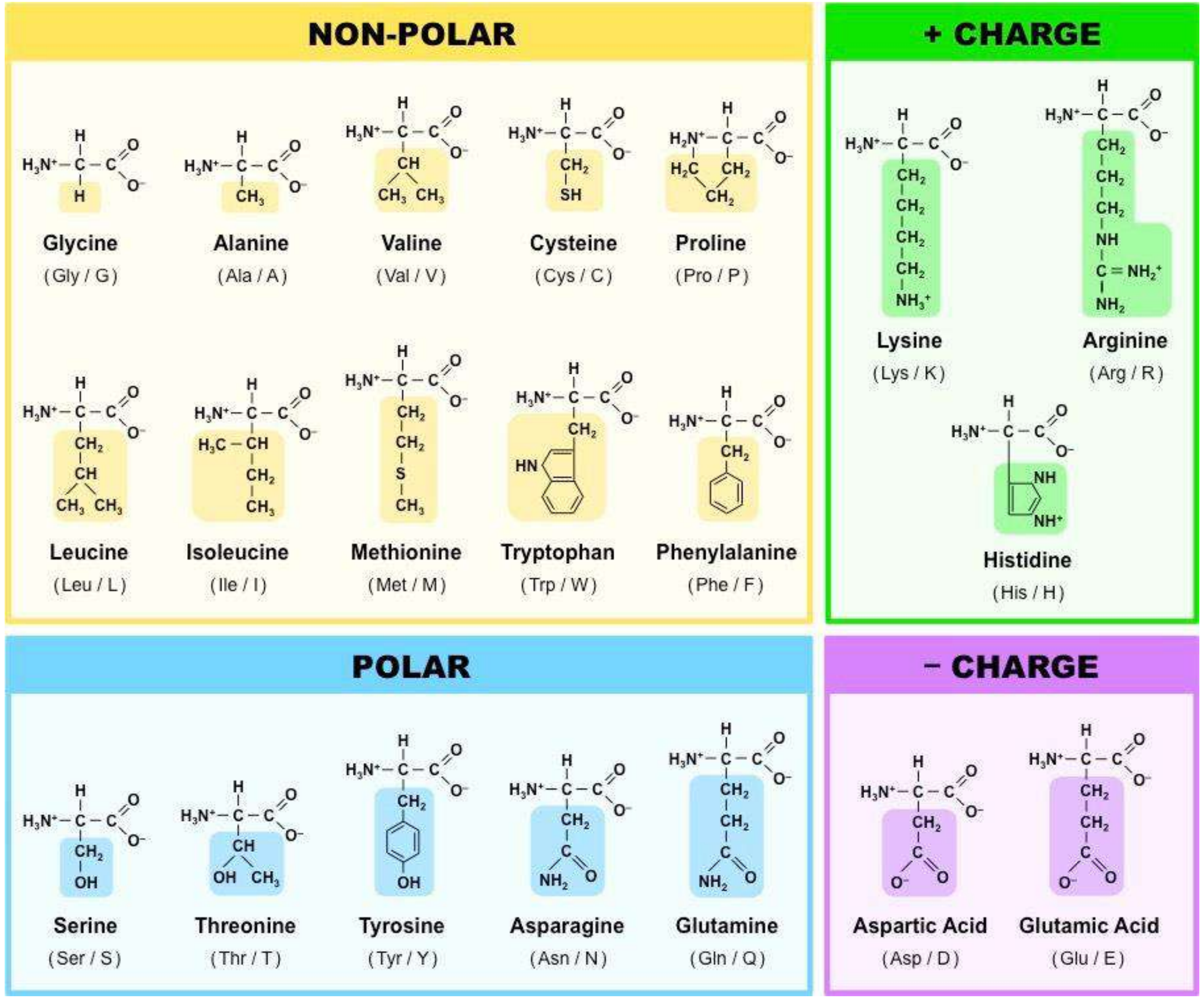
- Surface reaction
- Diffusion of molecules and radicals
- Trapping
- Segregation
- Desorption

III. From Astrochemistry to Astrobiology:

Surface Formation of the Building Blocks of Life in Space





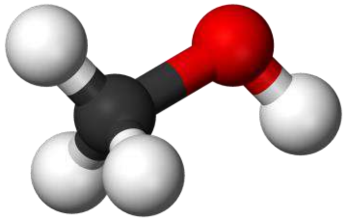


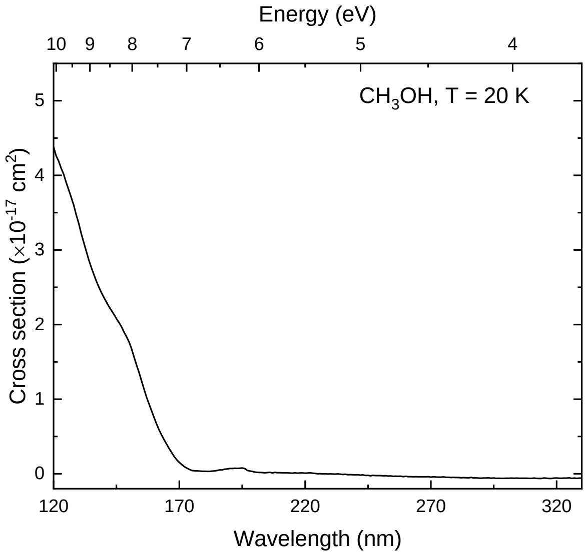
Laboratory Infrastructures

Credit: H. Linnartz

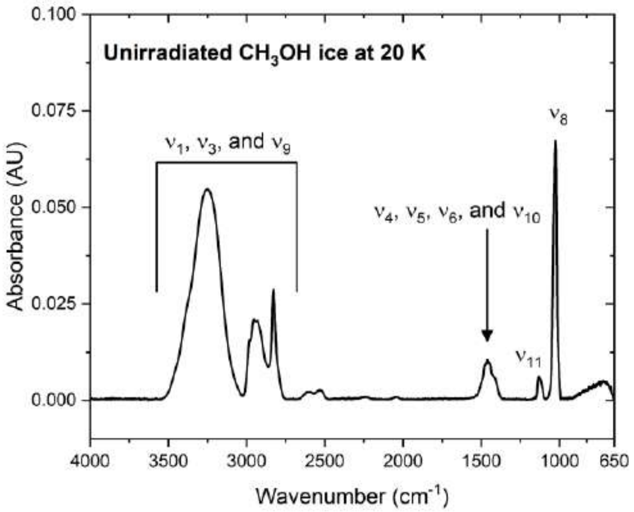
I. Fundamental properties of ices:

VUV/UV-vis/IR/THz (0.1 - 3000 μm) Ice Database

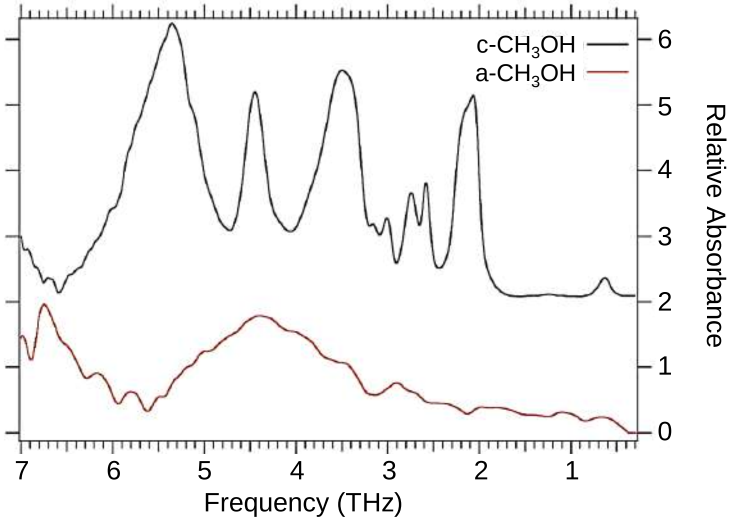




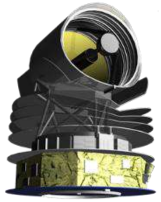
VUV



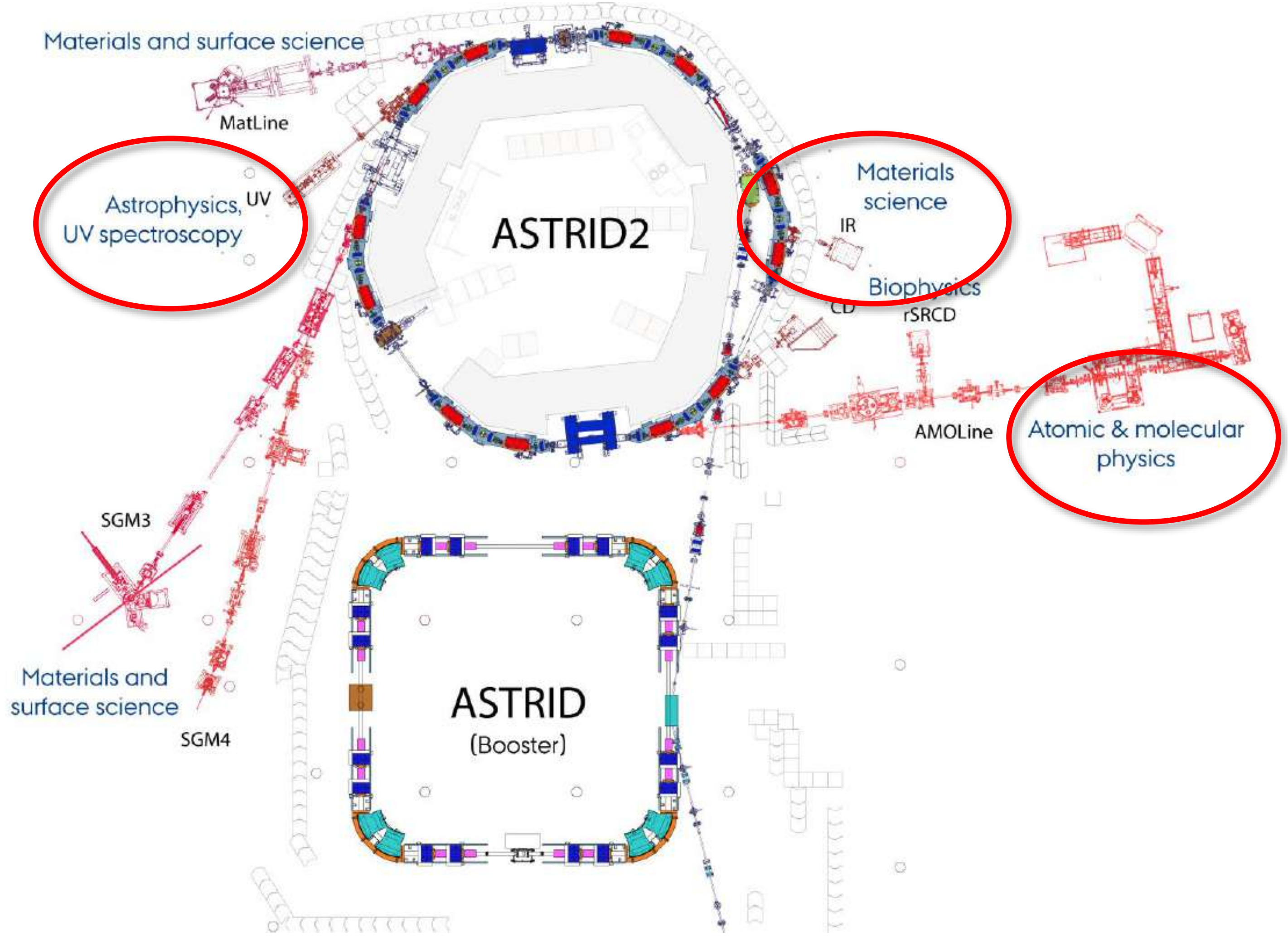
IR



THz

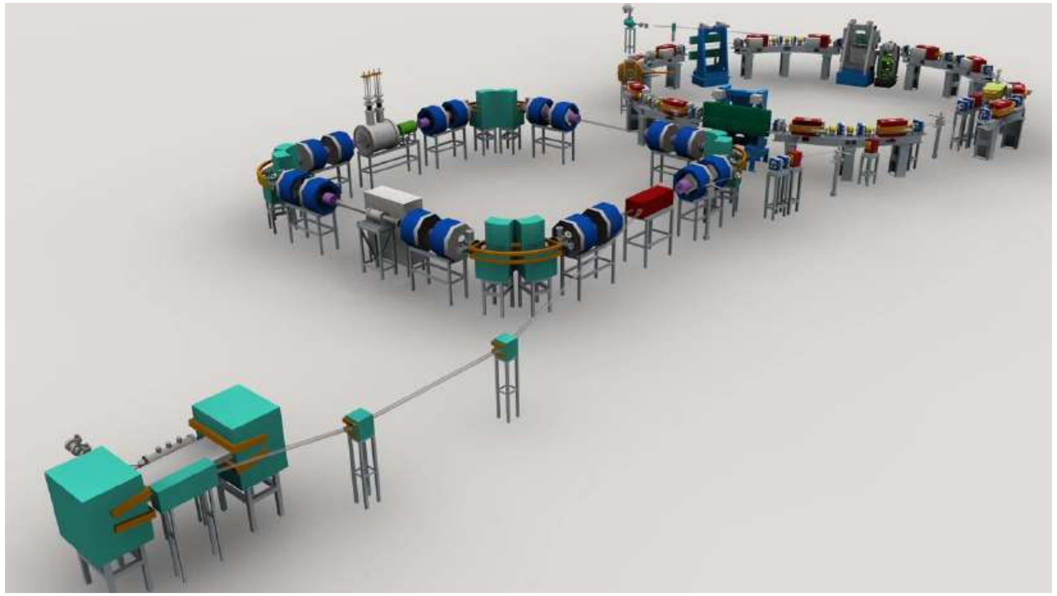


I. Fundamental properties of ices:
Spectra and Cross Sections (VUV/UV-vis)

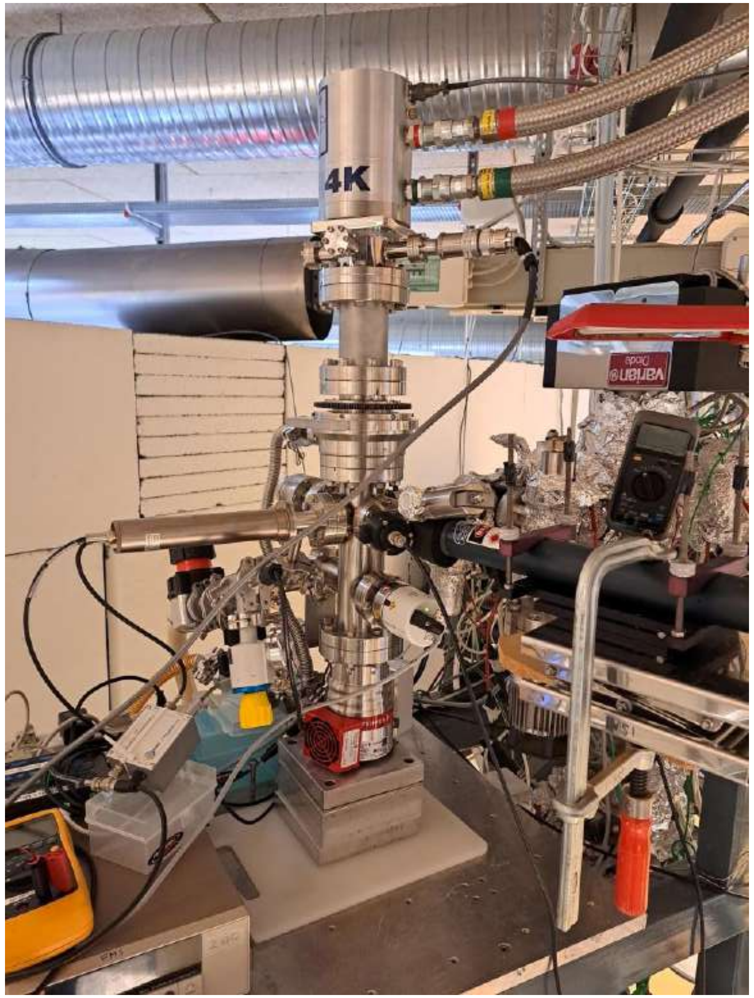


https://www.isa.au.dk/animations/animations.asp

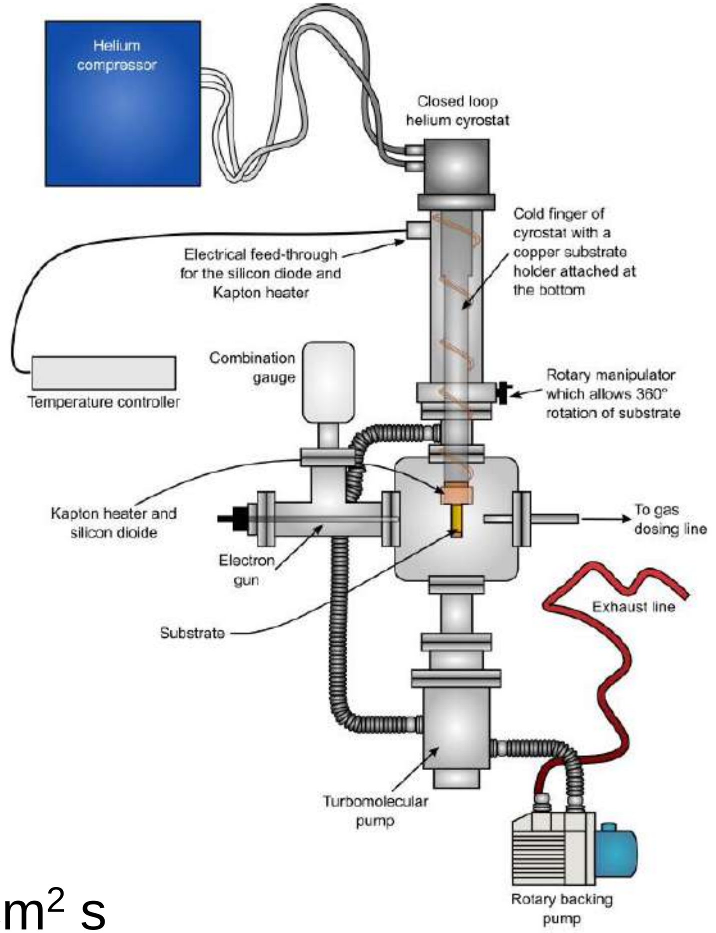
- *The energy of the circulating electrons in ASTRID2 is 580 MeV.*
- *The source is optimized to produce synchrotron radiation in the few eV to 1 keV energy range.*
- *Beam lifetime is infinite using top-up of the electron current with ASTRID.*
- *The diameter of ASTRID2 is 15 m.*



I. Fundamental properties of ices:
Spectra and Cross Sections (VUV/UV-vis)



UV Ice Camber (UVIC)

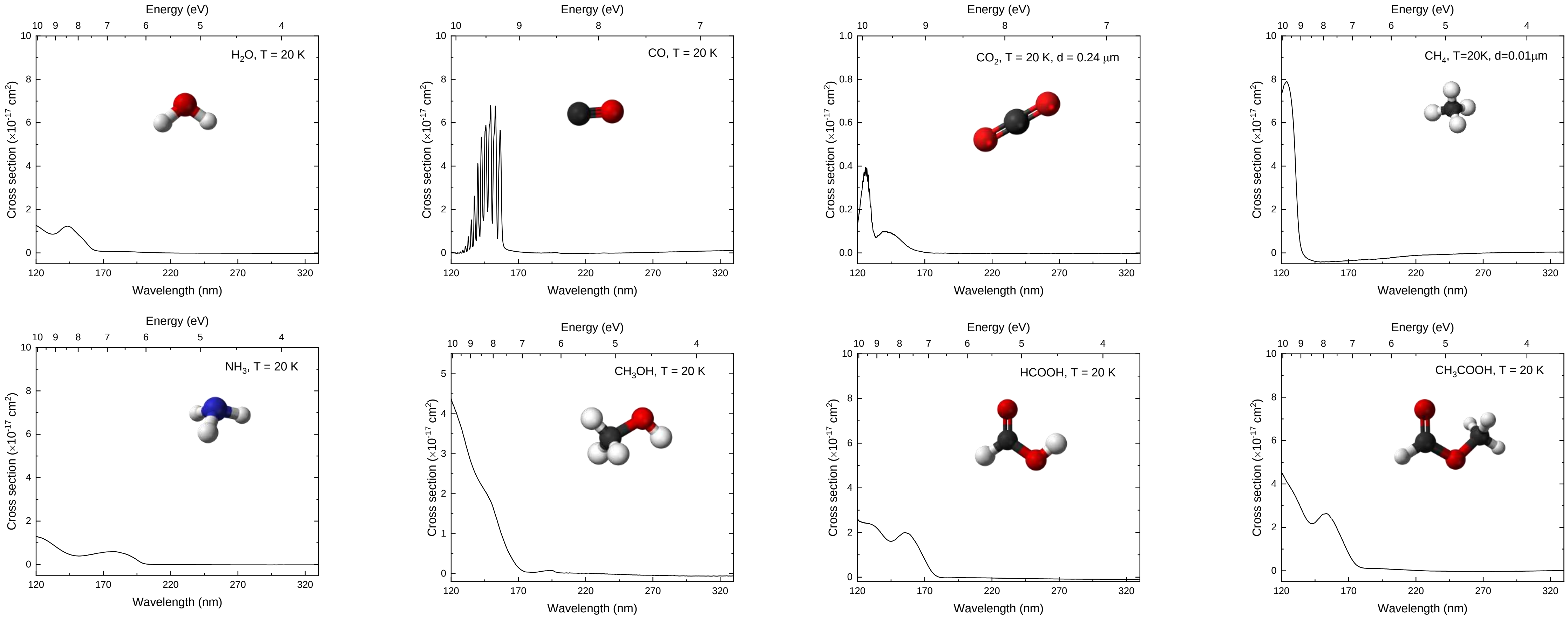


P < 1×10^{-9} mbar

$\boldsymbol{T}_{\mathbf{surf}}$ = 20 - 300 K

Flux (1 keV) = 2×10^{13} e^-/cm^2 s

I. Fundamental properties of ices:
Spectra and Cross Sections (VUV/UV-vis)



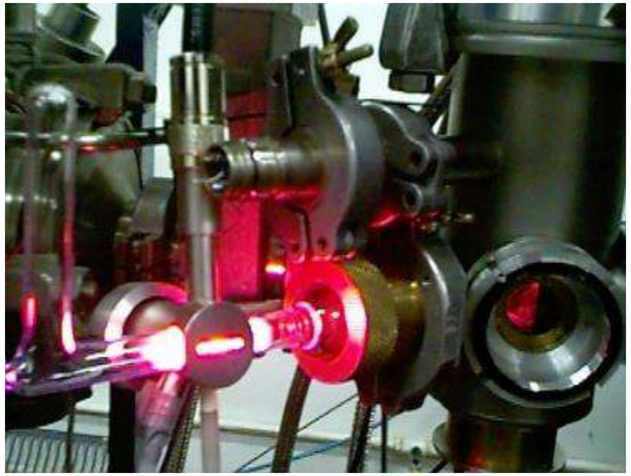
Traspas Muiña *et al.*, in prep.

I. Fundamental properties of ices:
Spectra and Cross Sections (VUV/UV-vis)

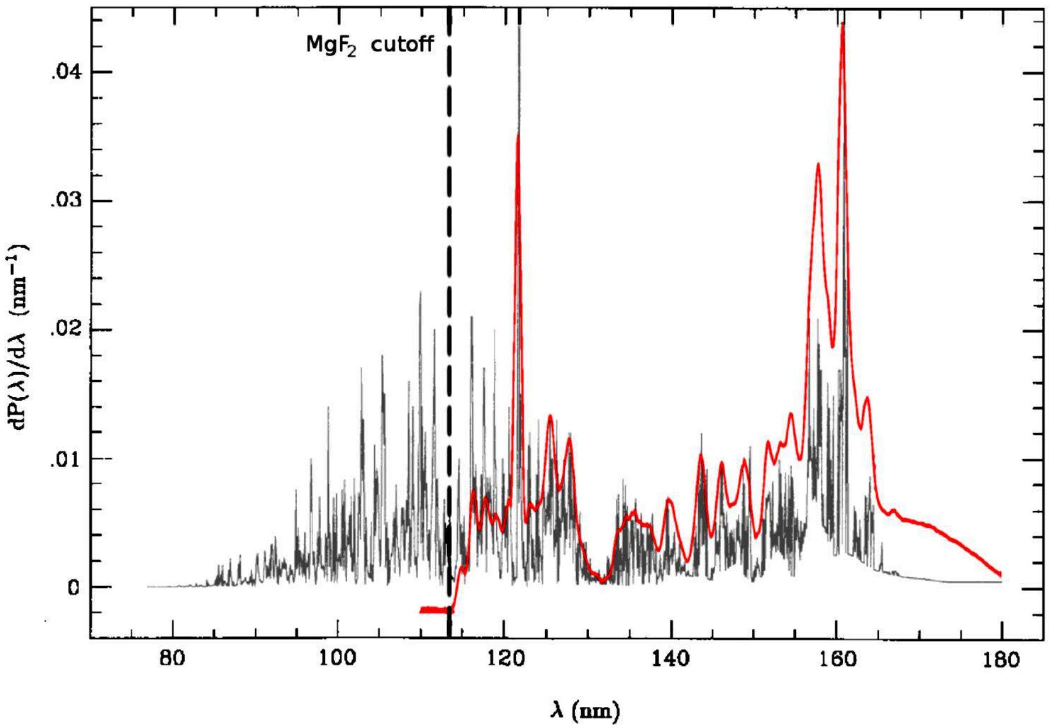
CURRENT WORK:

A comprehensive large VUV/UV-vis ice database to

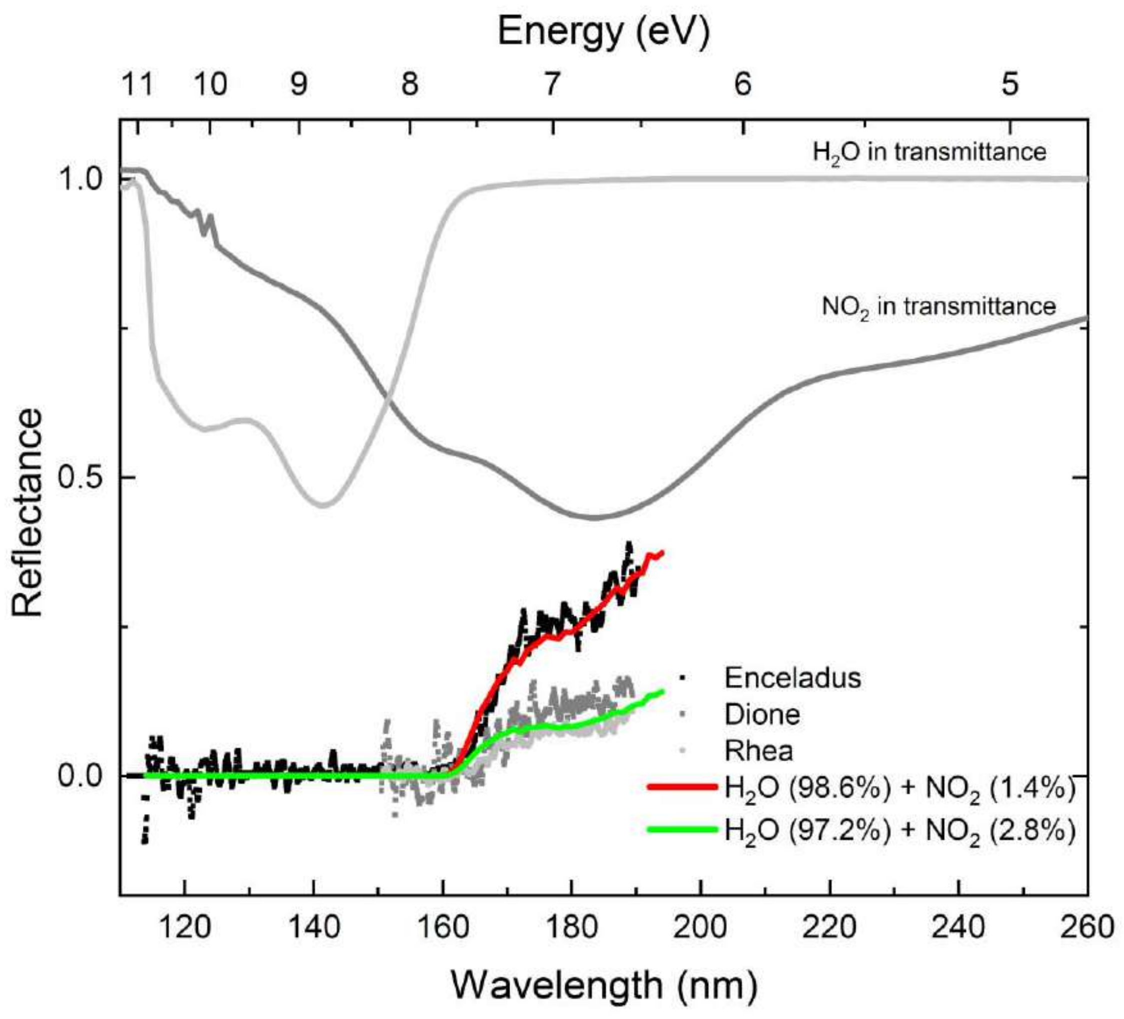
1. Identify simple & complex molecules (e.g., prebiotic species) in Space.
2. Aid the study of UV photoprocesses.
3. Complement MIR measurements.

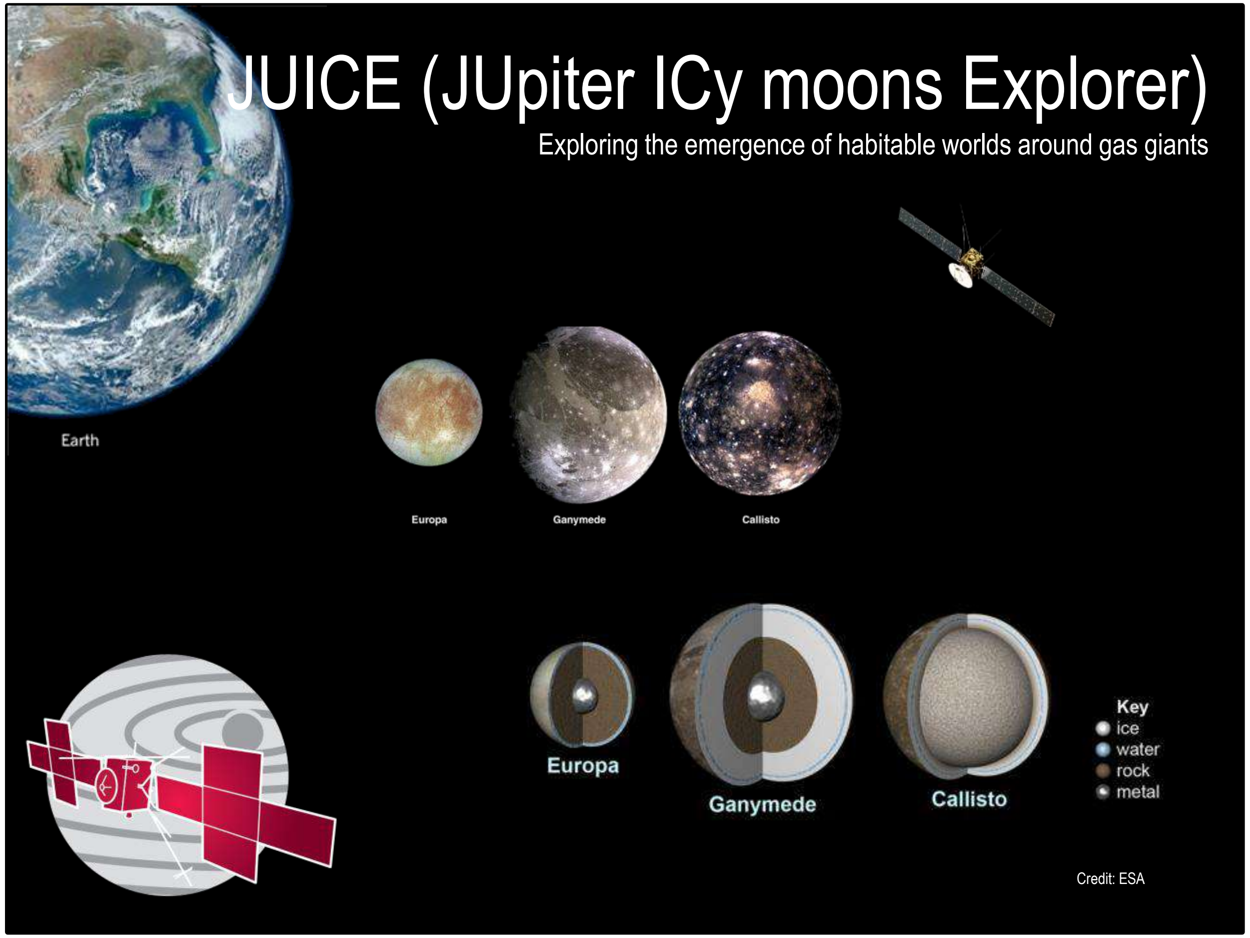


LASP INAF-Catania



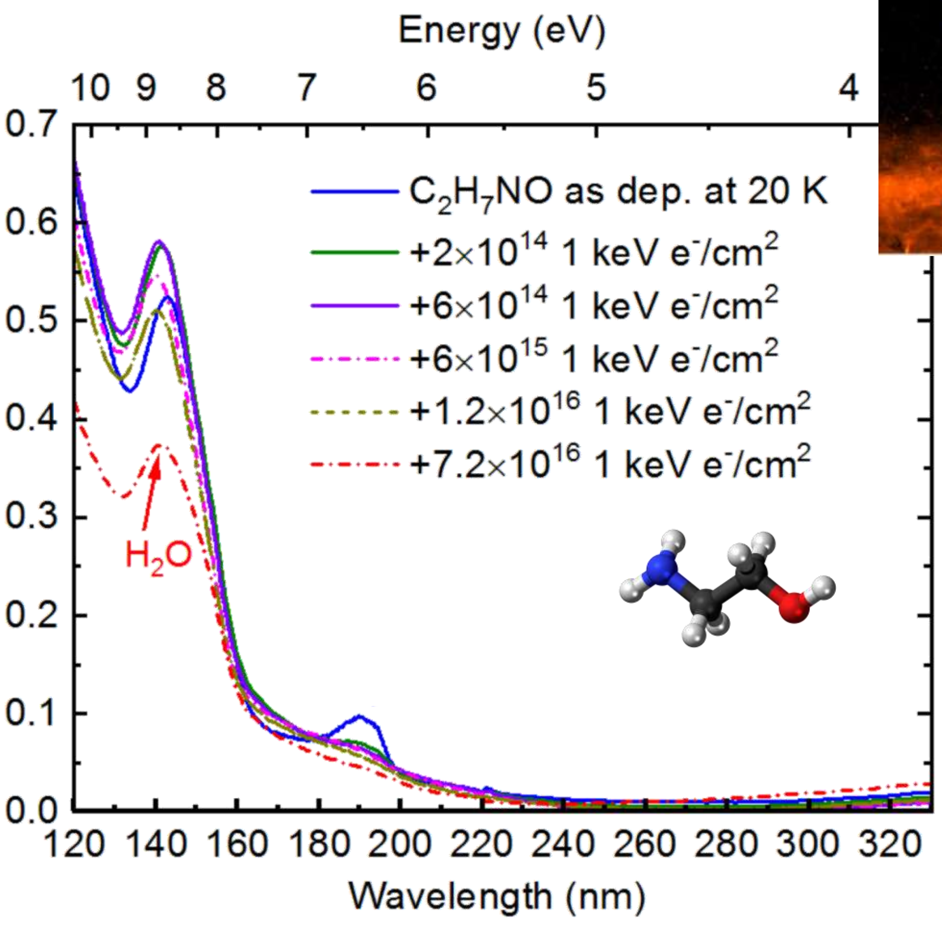
I. Fundamental properties of ices:
I. Molecules in Space



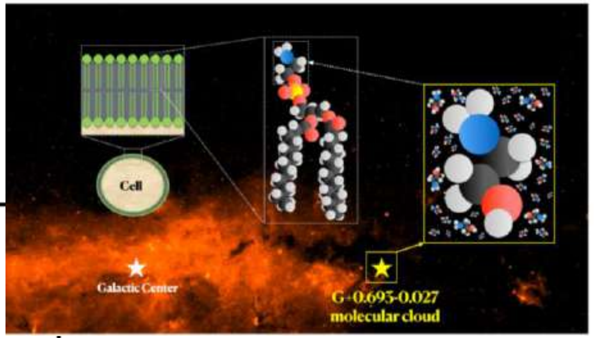


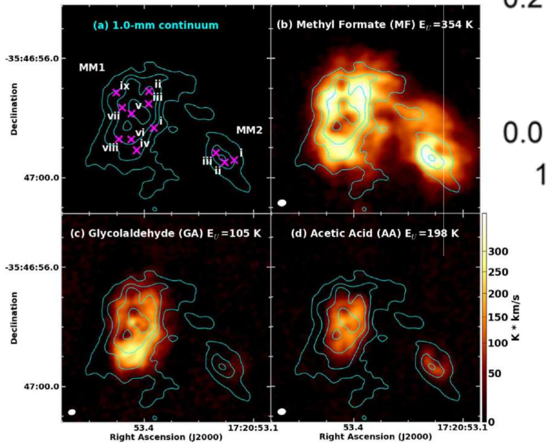
Ioppolo et al., *A&A* (2020)

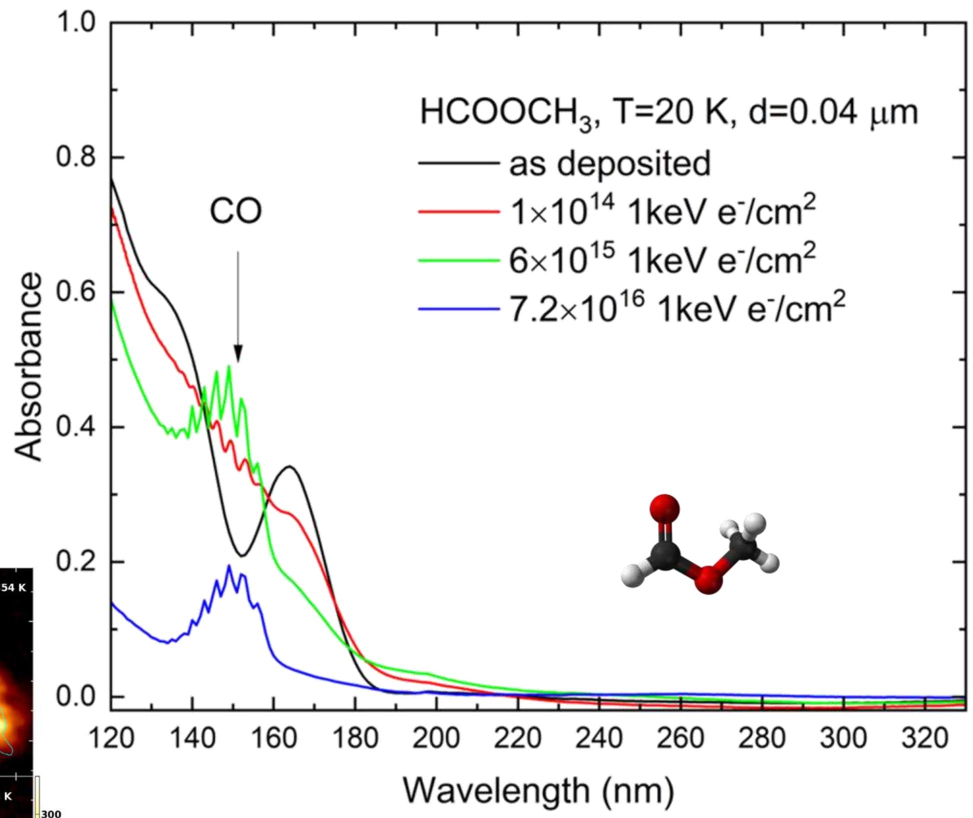
I. Fundamental properties of ices:
2. Formation & Survivability of Molecules



Zhang *et al.*, *MNRAS* (2024)

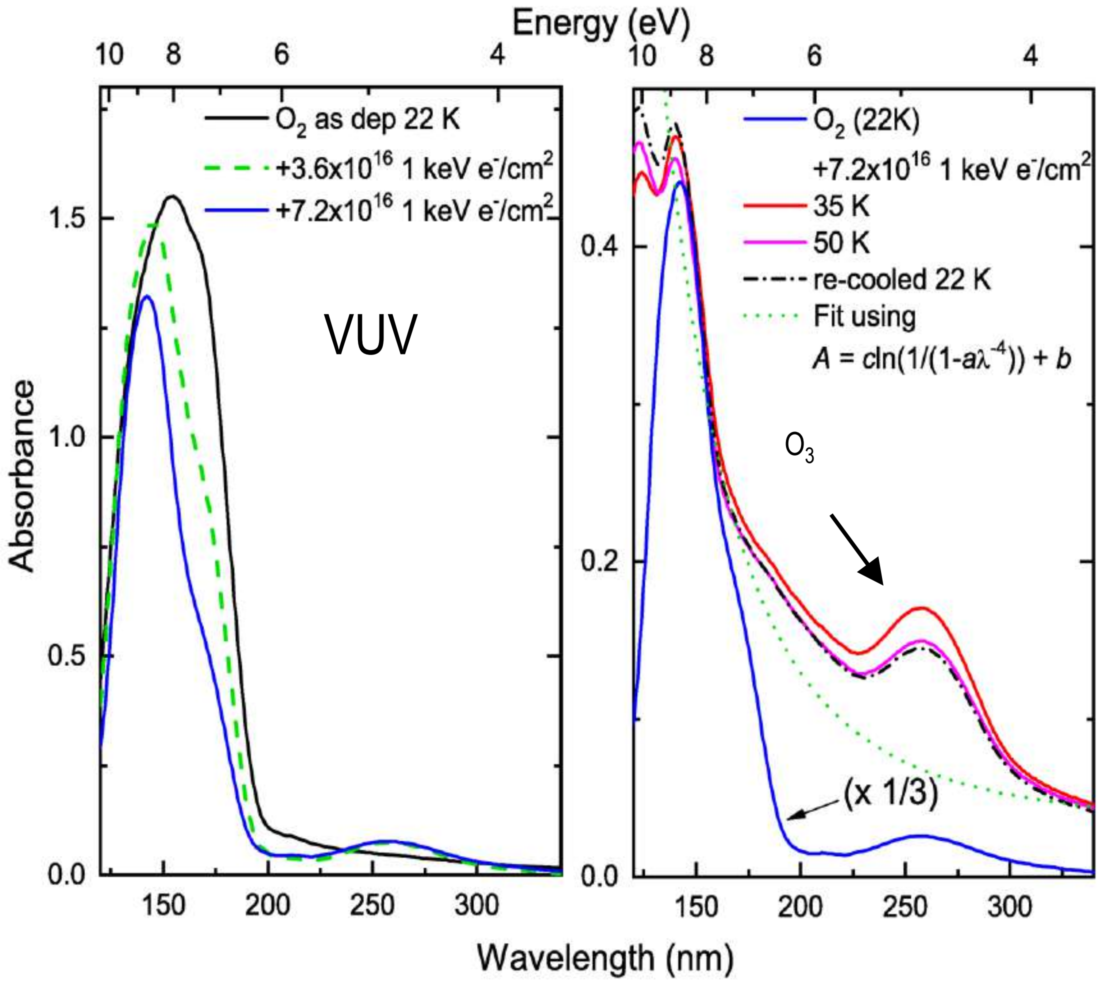


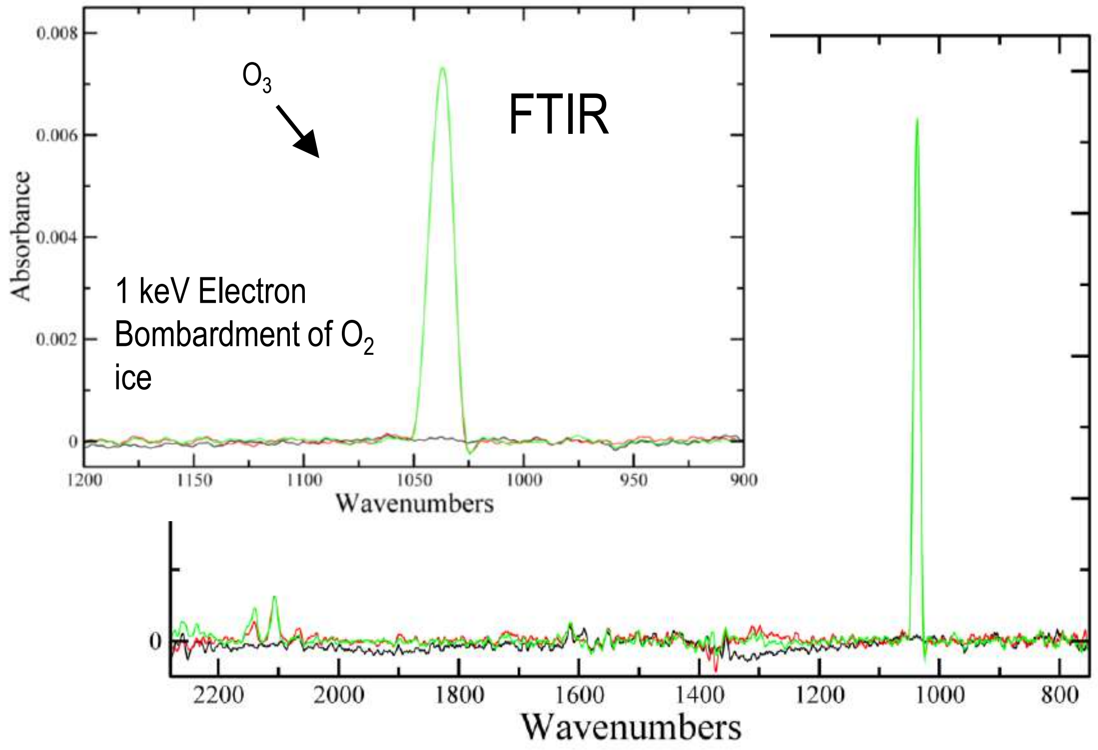




Traspas Muiña *et al.*, in prep.

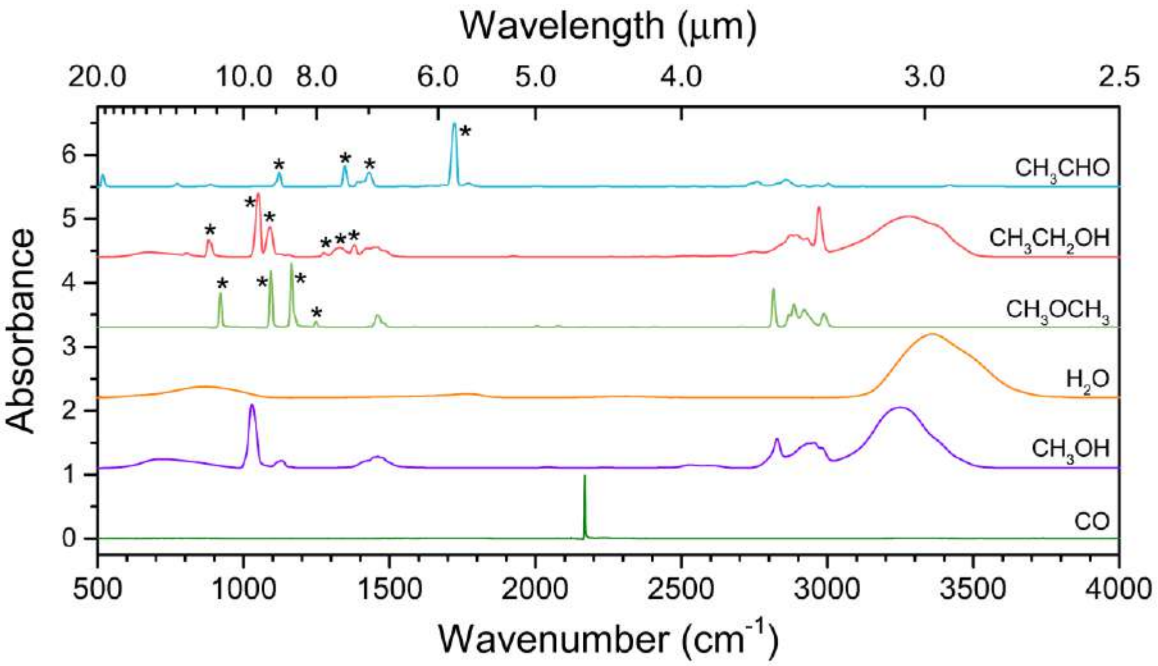
I. Fundamental properties of ices:
3. Complementary Information





Ioppolo et al., *A&A* (2020)

I. Fundamental properties of ices:
Spectra and Optical Constants (NIR, MIR & FIR)



Terwisscha van Scheltinga *et al.*, *A&A* (2018)

I. Fundamental properties of ices:
Spectra and Optical Constants (NIR, MIR & FIR)

ICE lab: ***Instituto de Estructura de la Materia, IEM-CSIC, Madrid, Spain***

Victor Herrero

Belén Maté

Paola Caselli

Michela Giuliano

CASICE lab @ MPE (Garching)

The Cosmic Ice Laboratory - People

Perry A. Gerakines

Reggie L. Hudson

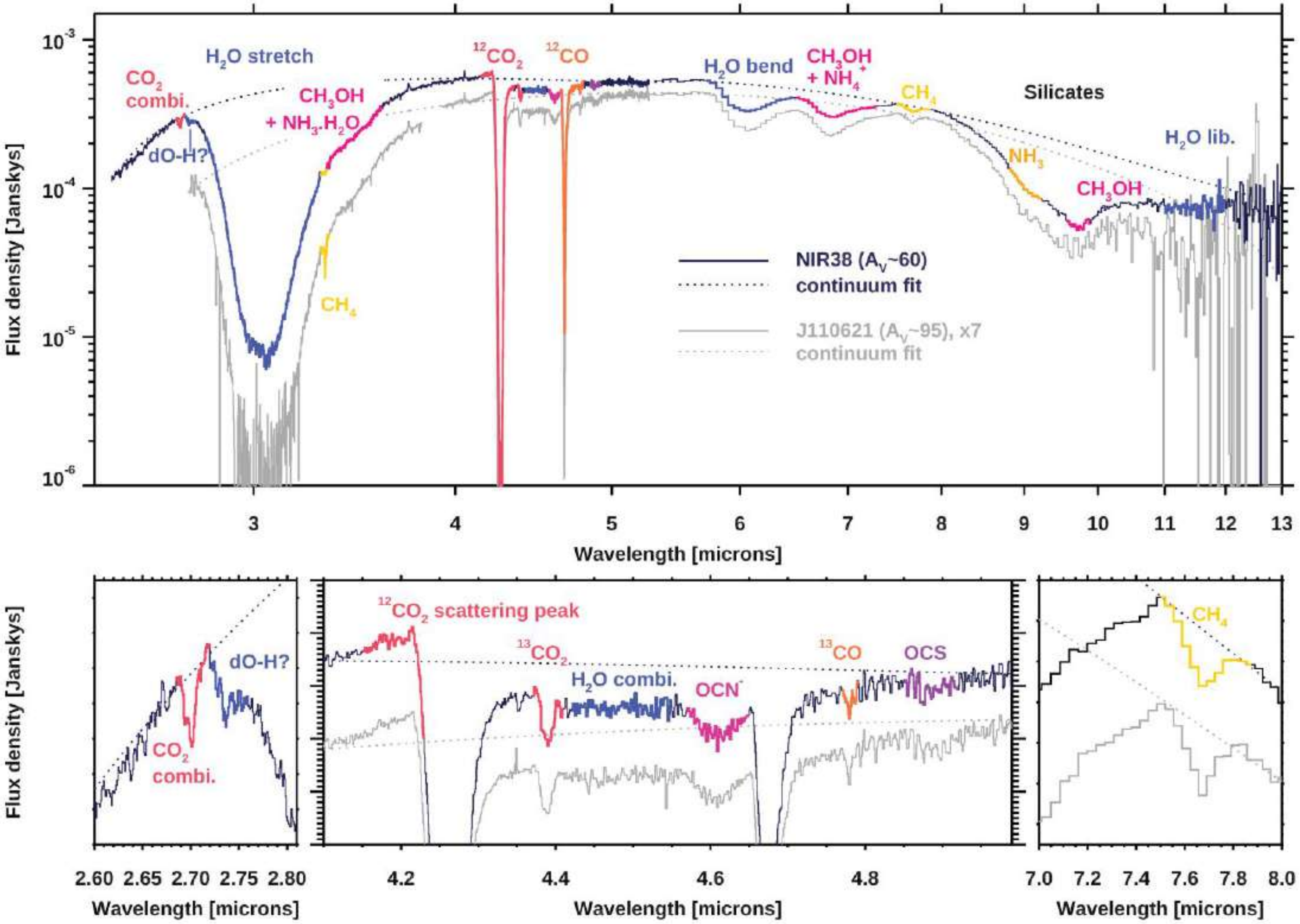
Christopher K. Materese

I. Fundamental properties of ices:
Spectra and Optical Constants (Ice Age program)

ERS: PI McClure, co-PI Boogert, co-PI Linnartz,
co-I Ioppolo + 46 co-Is

Cycle 1: **PI McClure, co-**I Ioppolo + 25 co-Is

400 hours of observational time in first year to study cosmic ices



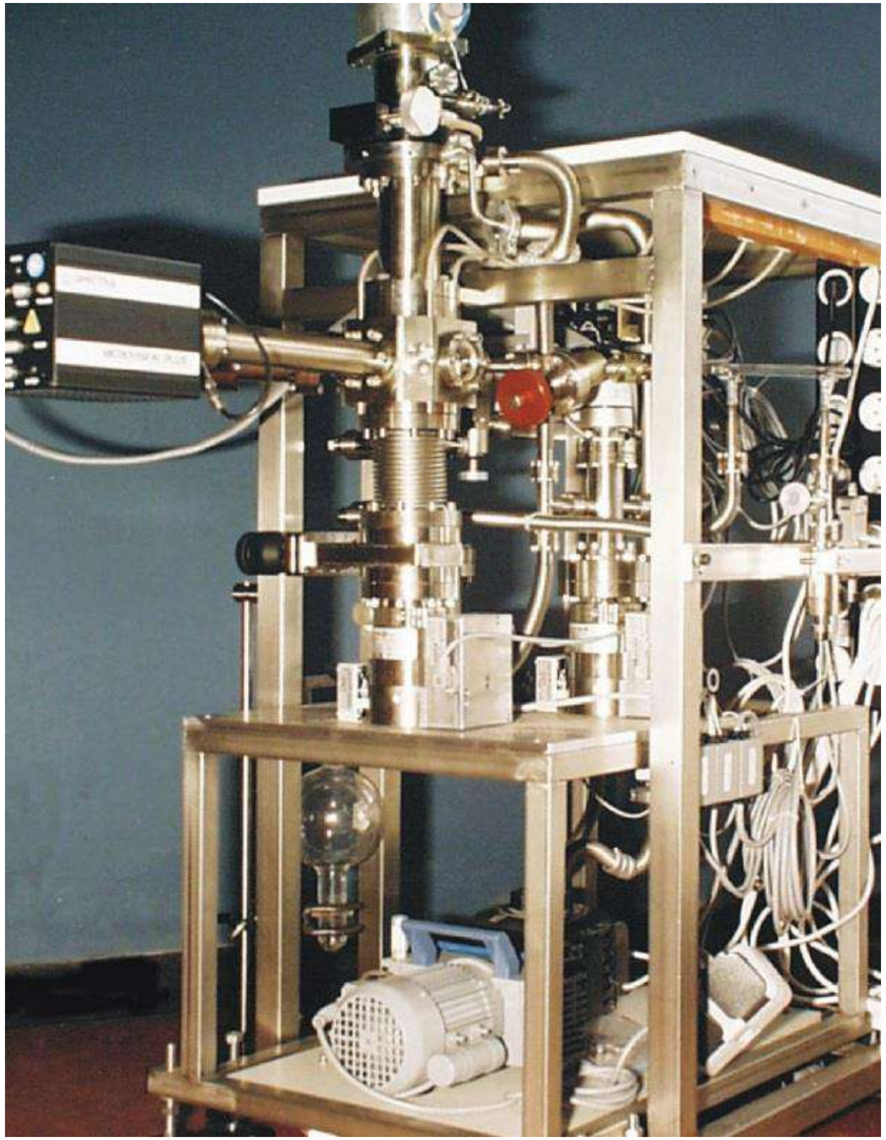
McClure et al. Nat. Astron. (2023)

II. Bridging the gas-grain gap:
Linking Physics and Chemistry of Star Forming Regions

Better characterization of fundamental mechanisms:

- Surface reaction
- Diffusion of molecules and radicals
- Trapping
- Segregation
- Desorption

II. Bridging the gas-grain gap:
Interaction of ice and free atoms (SURFRESIDE)



No Atom Source (QMS)

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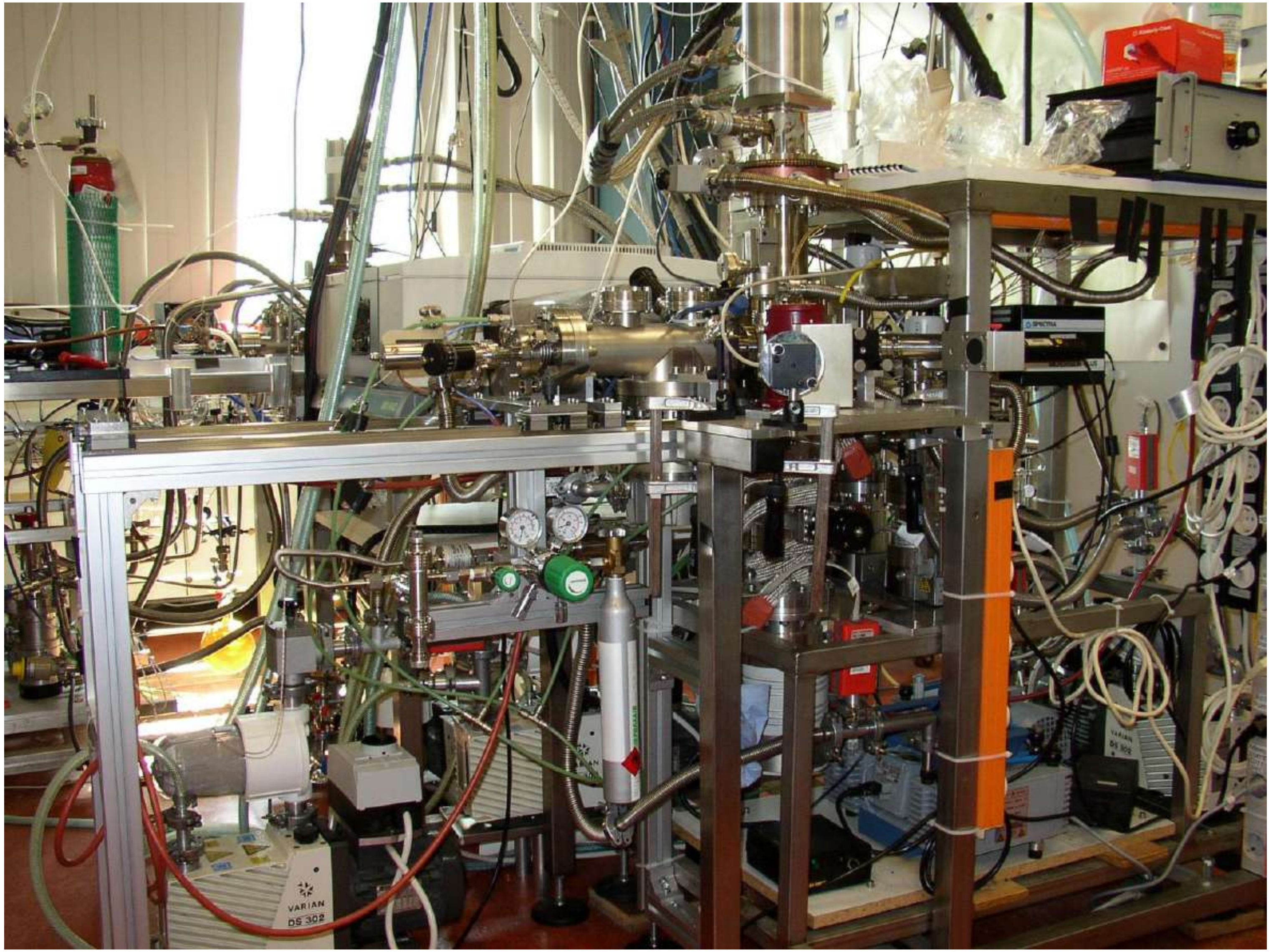
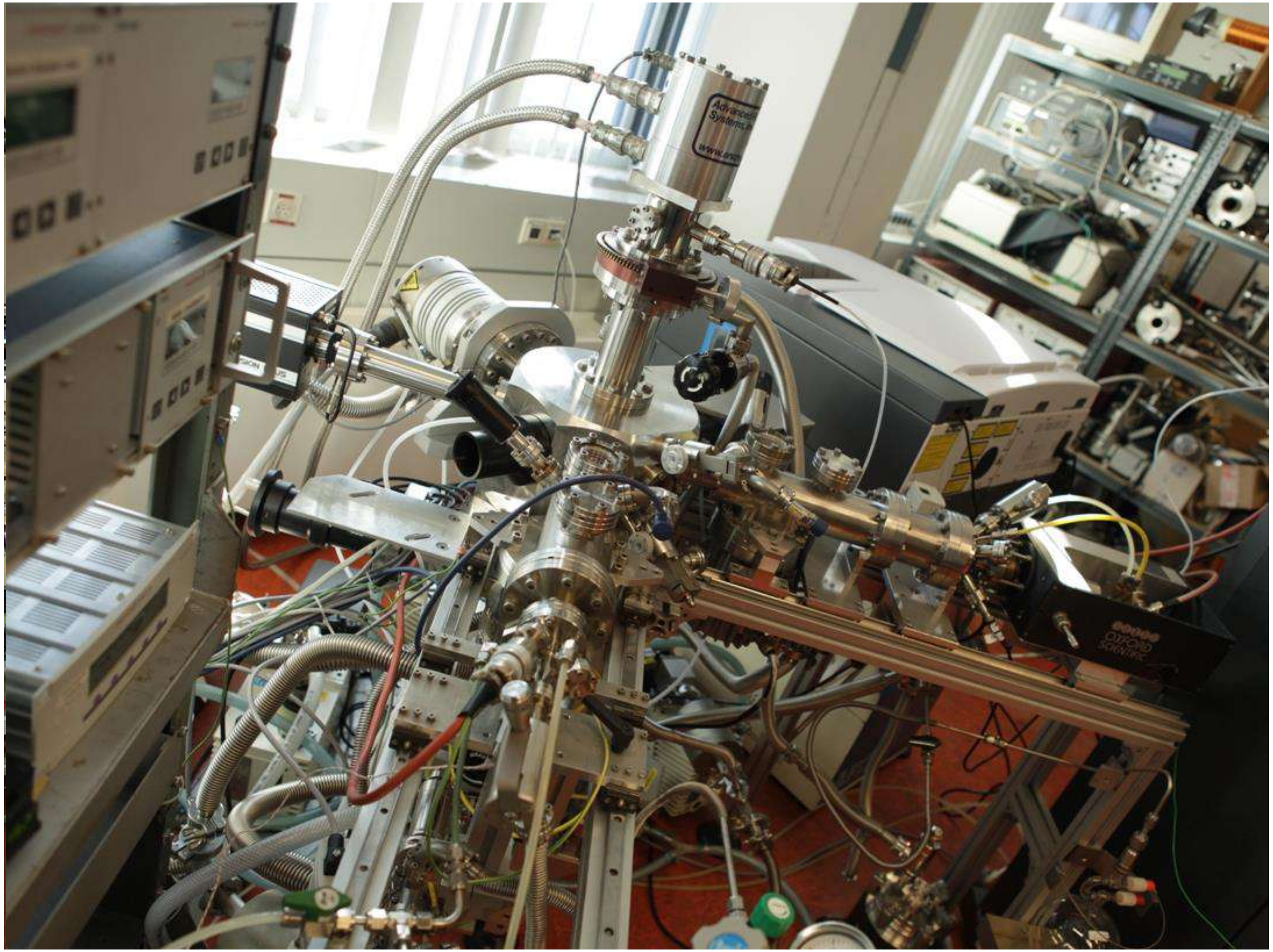
Interaction of ice and free atoms (SURFRESIDE)



No Atom Source (QMS)

H/D Atom Source (FTIR + QMS)

II. Bridging the gas-grain gap:
Interaction of ice and free atoms (SURFRESIDE)

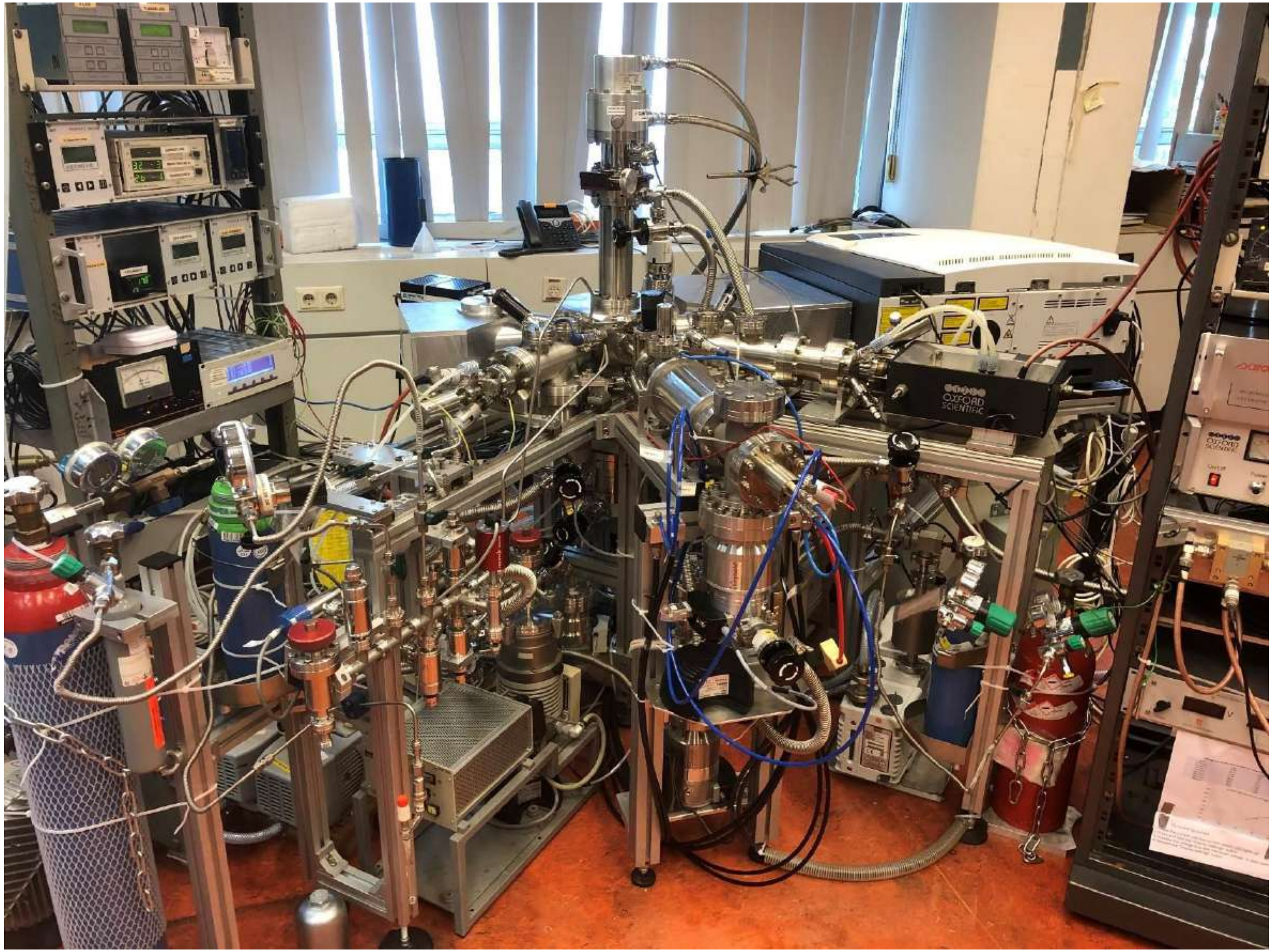


No Atom Source (QMS)

H/D Atom Source (FTIR + QMS)

O/N Atom Source

II. Bridging the gas-grain gap:
Interaction of ice and free atoms (SURFRESIDE)



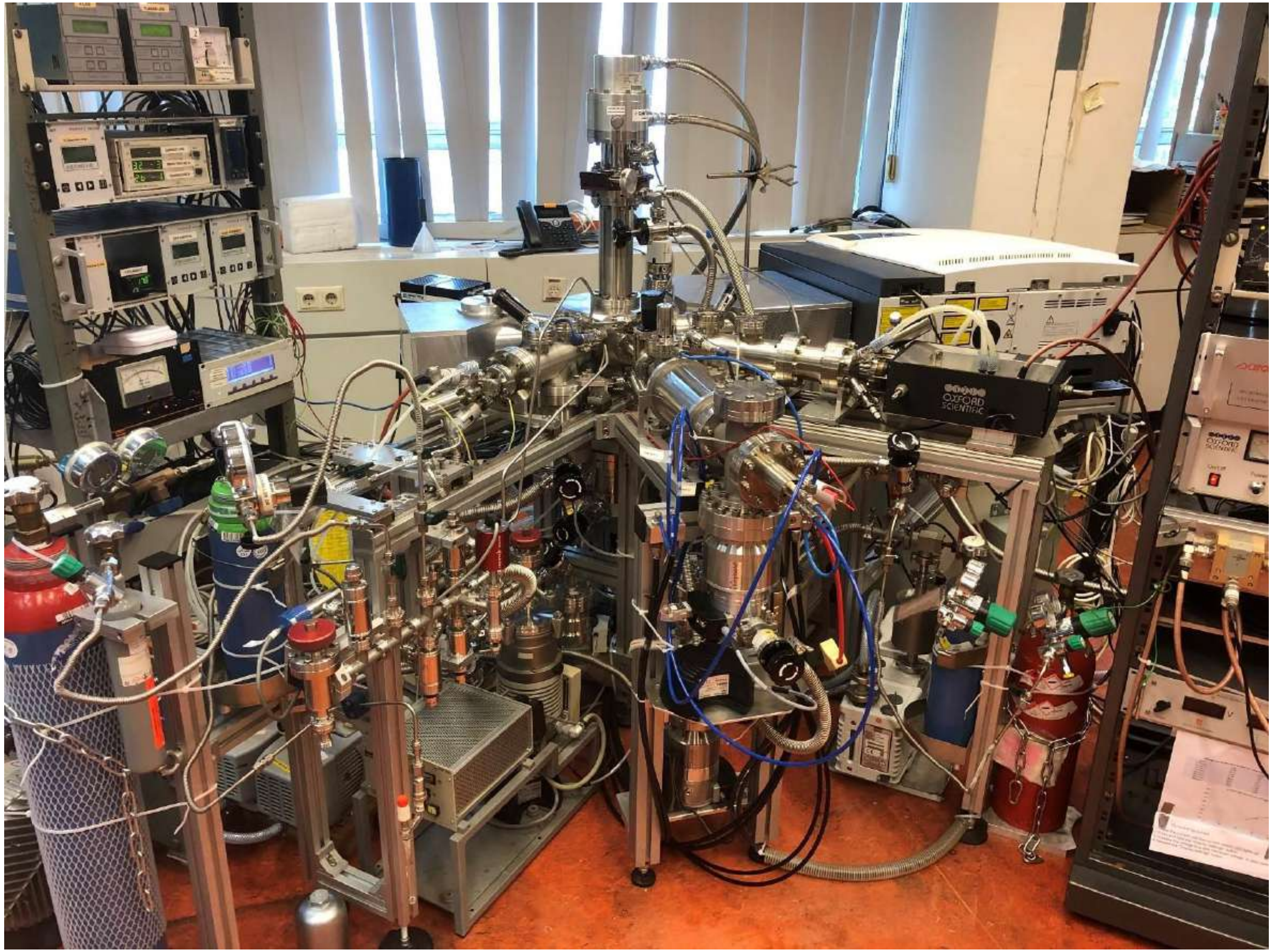
No Atom Source (QMS)

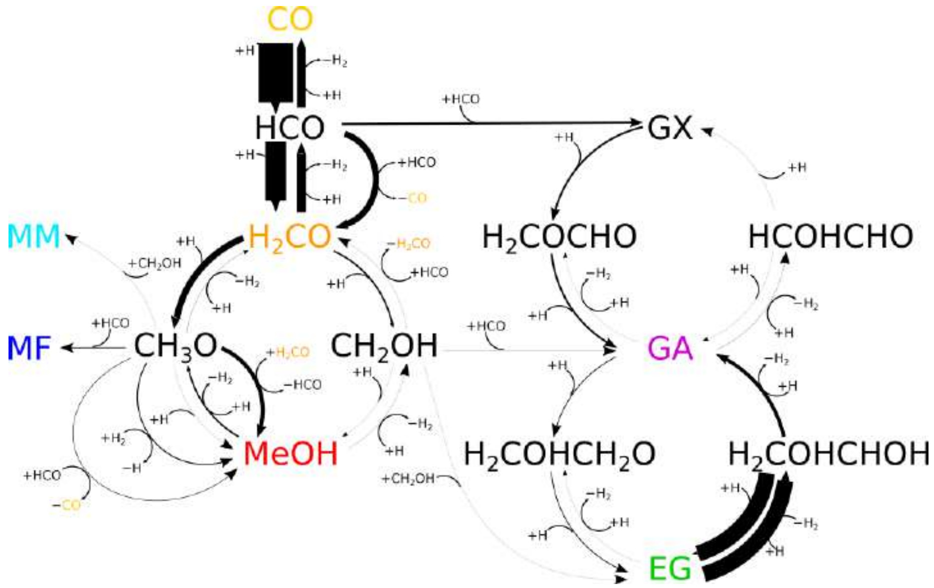
H/D Atom Source (FTIR + QMS)

O/N Atom Source

C Atom Source

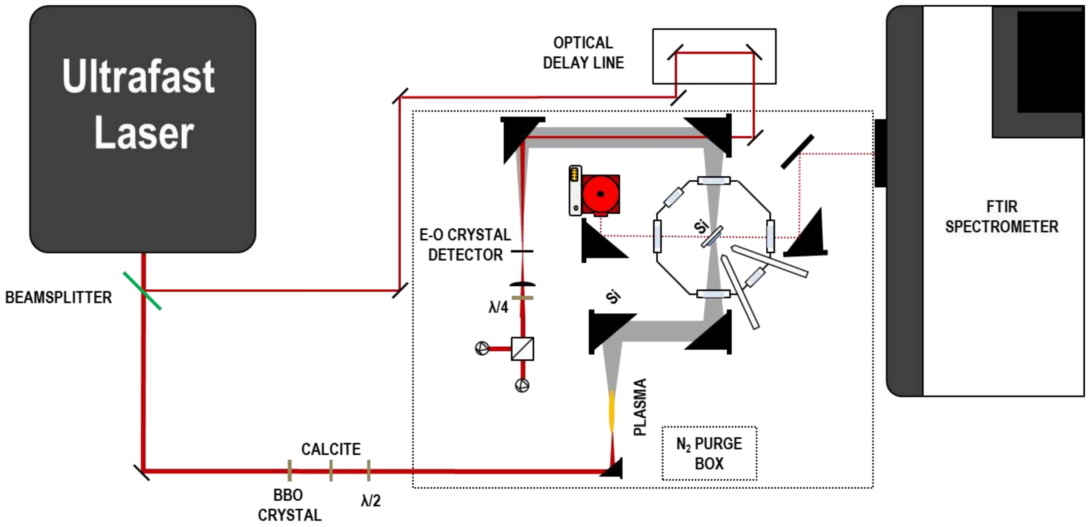
II. Bridging the gas-grain gap:
Interaction of ice and free atoms (SURFRESIDE)





Fuchs et al. *A&A* (2009)
Fedoseev et al. *ApJ* (2017)
Simons et al. *A&A* (2020)
He et al. *A&A* (2021)

II. Bridging the gas-grain gap:
Future time-resolved experiments



Single-shot coherent measurements:

10,000 spectra co-added in a second

Time-resolve dynamics within the ice

Surface reactions
Diffusion of molecules and radicals
Trapping
Segregation
Desorption

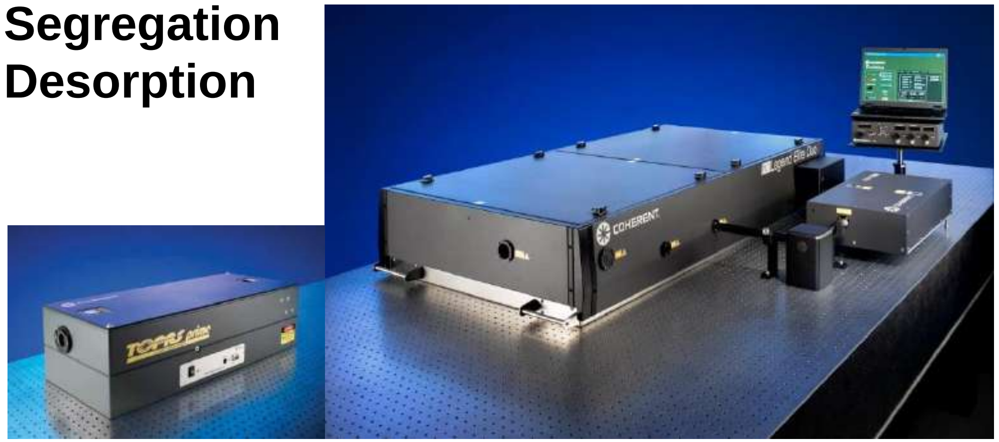


Table-top ultrafast lasers / (mass) spectrometers advances to time-resolved transient events in the IR/THz during ice processing.

II. Bridging the gas-grain gap:
Transmission electron microscopy (TEM)

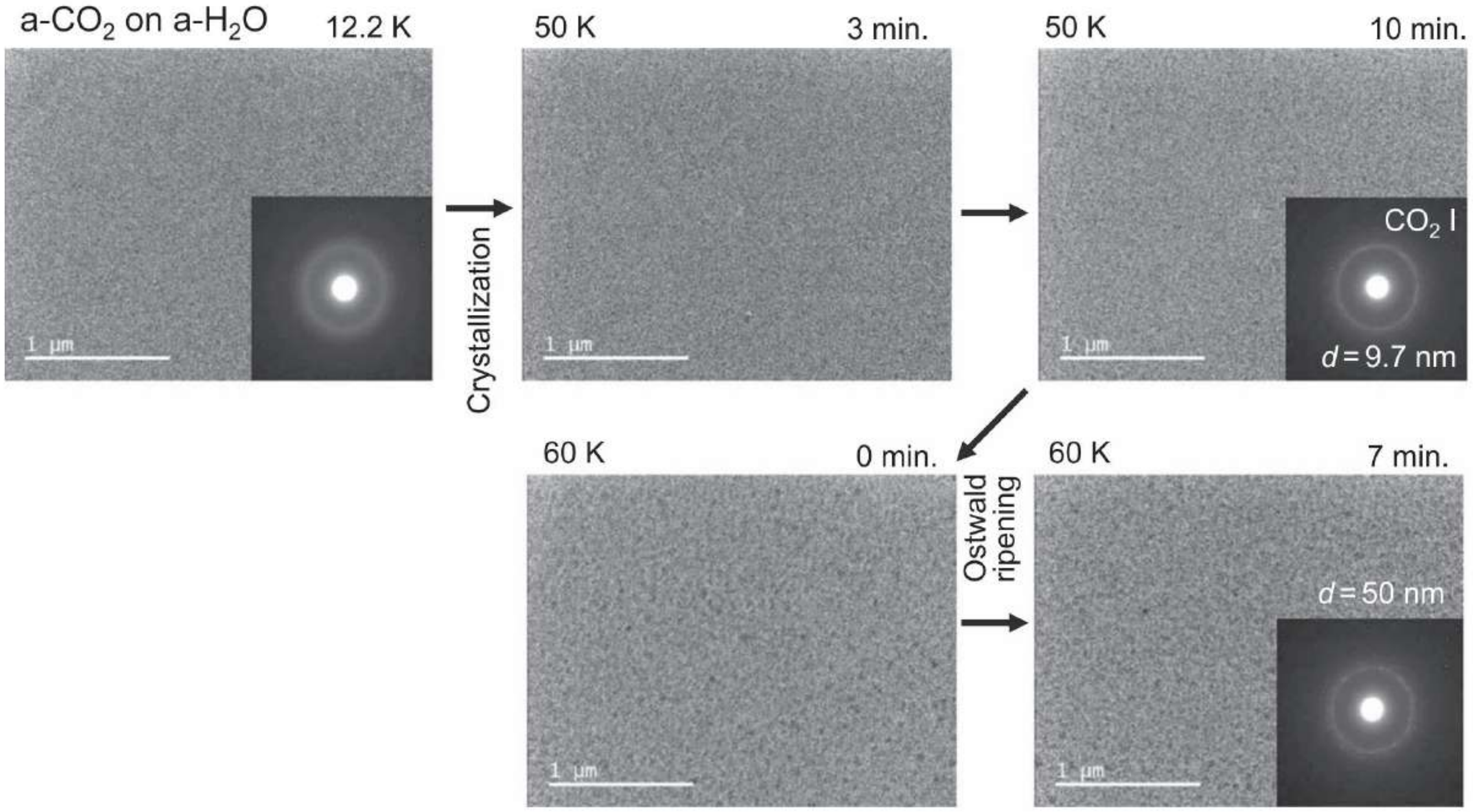
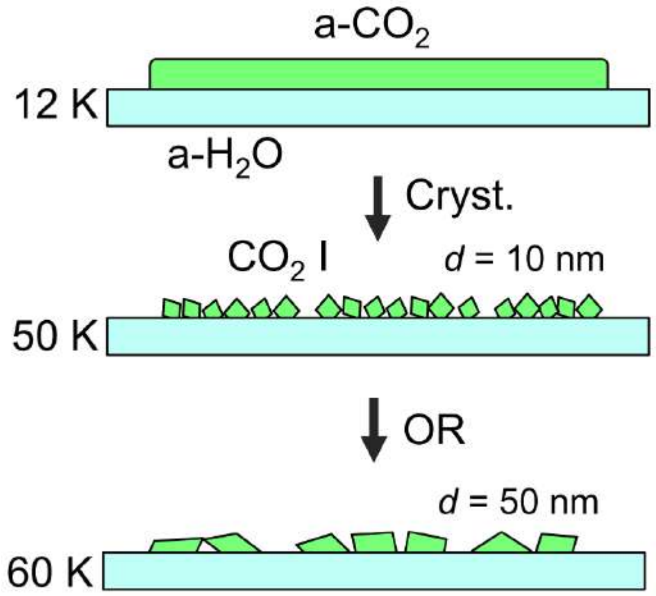


Figure 5. TEM observation of the crystallization of a-CO_2 on a-H_2O substrate at 50 and 60 K.

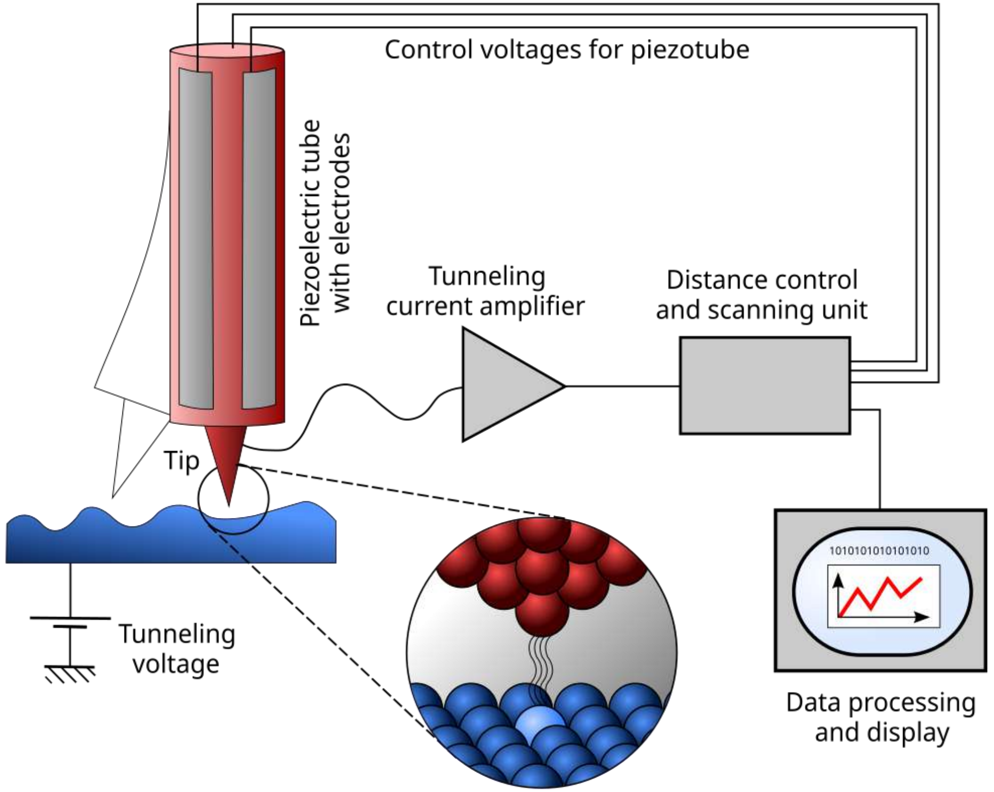


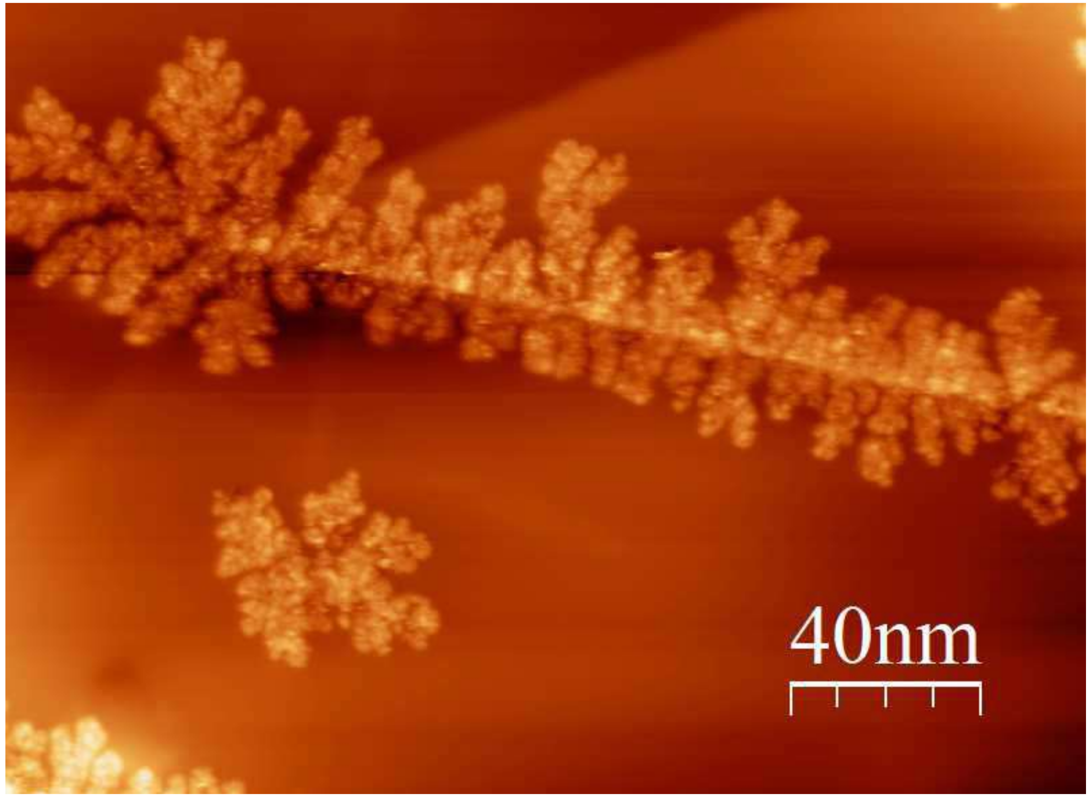
Kouchi *et al.*, ApJ (2021)

II. Bridging the gas-grain gap:
Scanning tunneling microscopy (STM)

INTERCAT
Center for Interstellar Catalysis

Low temperature – STM of D_2O ice growth on HOPG at 40 K

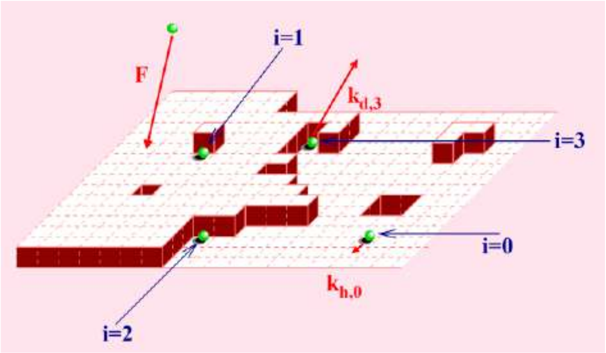


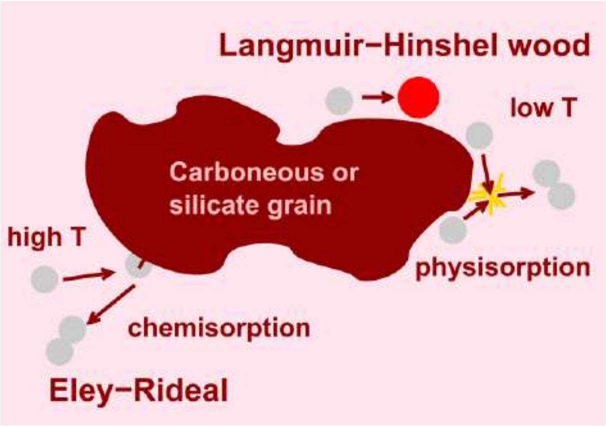


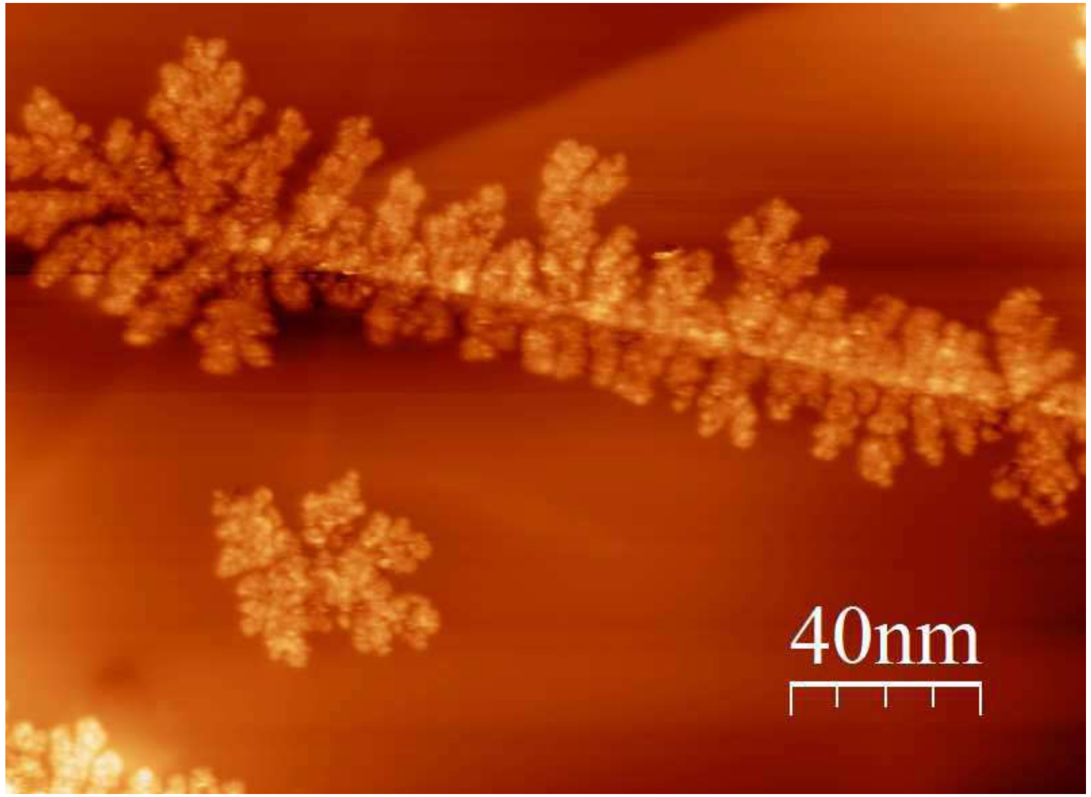
Credit: Liv Hornekær's Group

II. Bridging the gas-grain gap:
Scanning tunneling microscopy (STM)

Low temperature – STM of D_2O ice growth on HOPG at 40 K





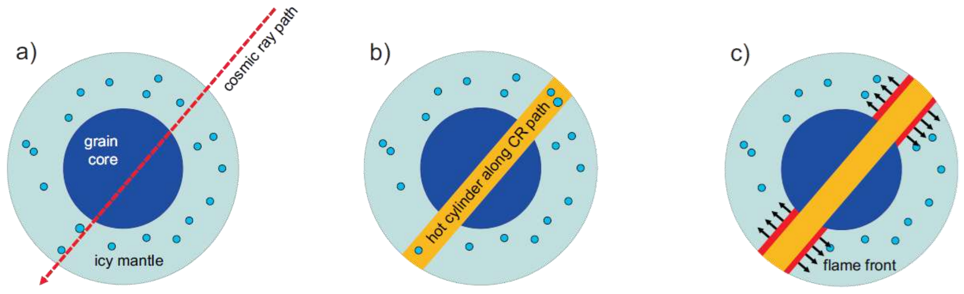


Credit: Liv Hornekær's Group

II. Bridging the gas-grain gap:
(Non)Thermal Desorption

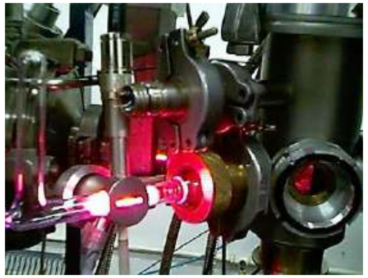
- Thermal sublimation

- Cosmic-ray spot heating
- Cosmic-ray sputtering

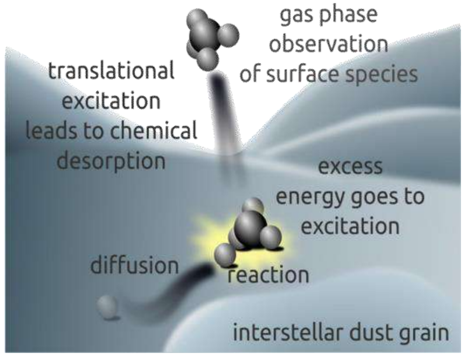


Ivlev et al. (2015)

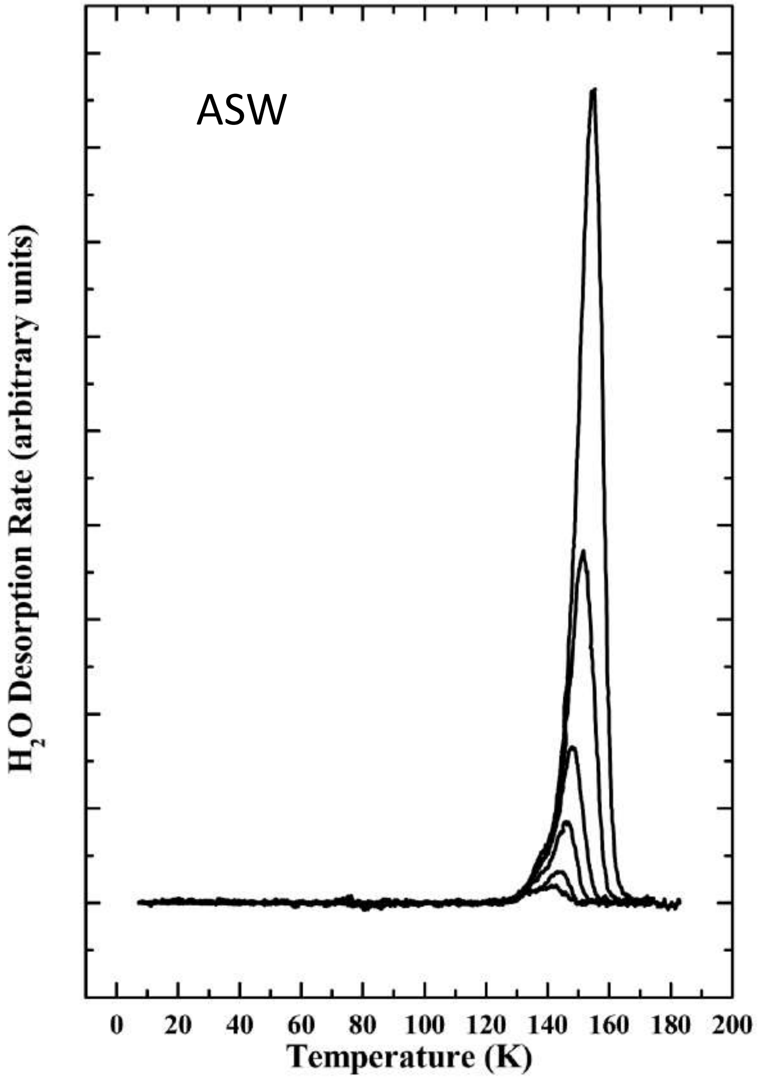
- UV photodesorption
- IR photodesorption



- Chemical desorption

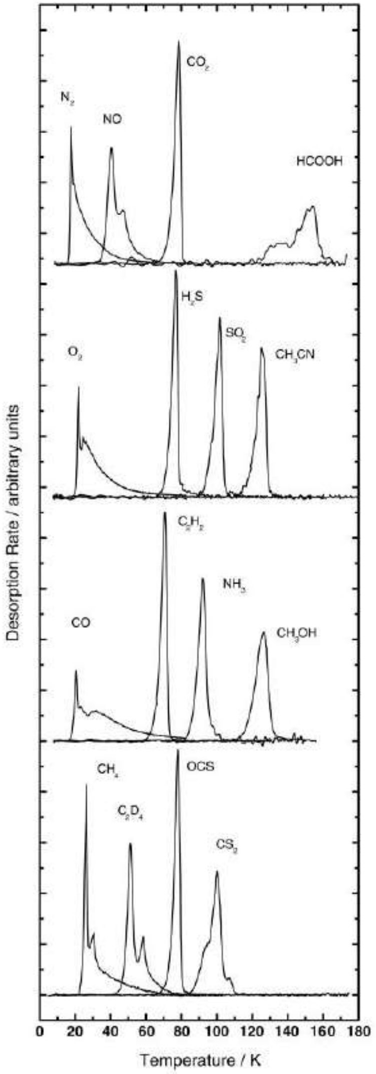


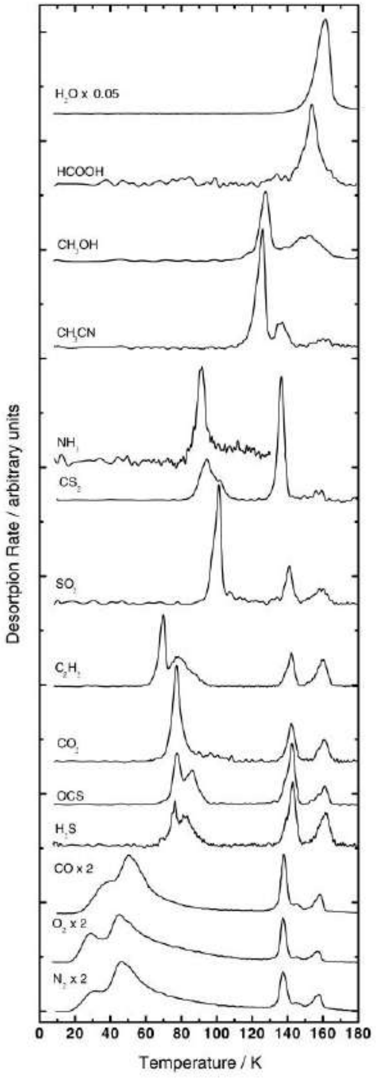
II. Bridging the gas-grain gap:
Thermal Desorption – Temperature Programmed Desorption



On Au

Fraser et al. (2001)



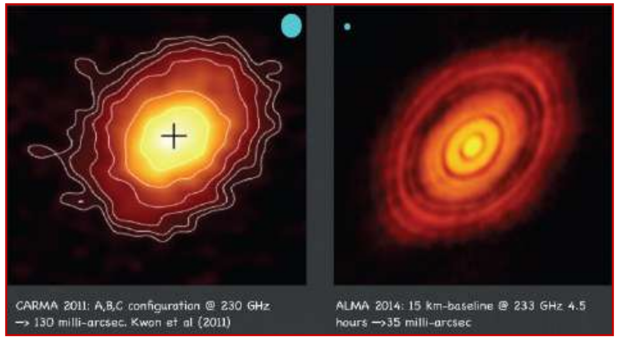


On ASW

Collings et al. (2004)

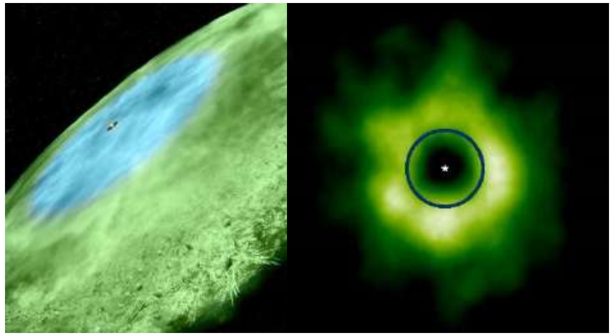
II. Bridging the gas-grain gap:
Thermal Desorption – Observations

HL TAU - ALMA High Resolution Results



CREDIT: P. Salomé, Paris Obs.

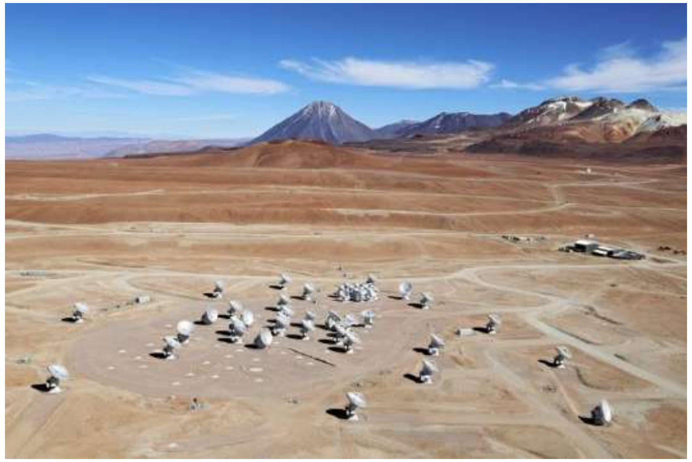
CO Snow Line - ALMA High Resolution Results

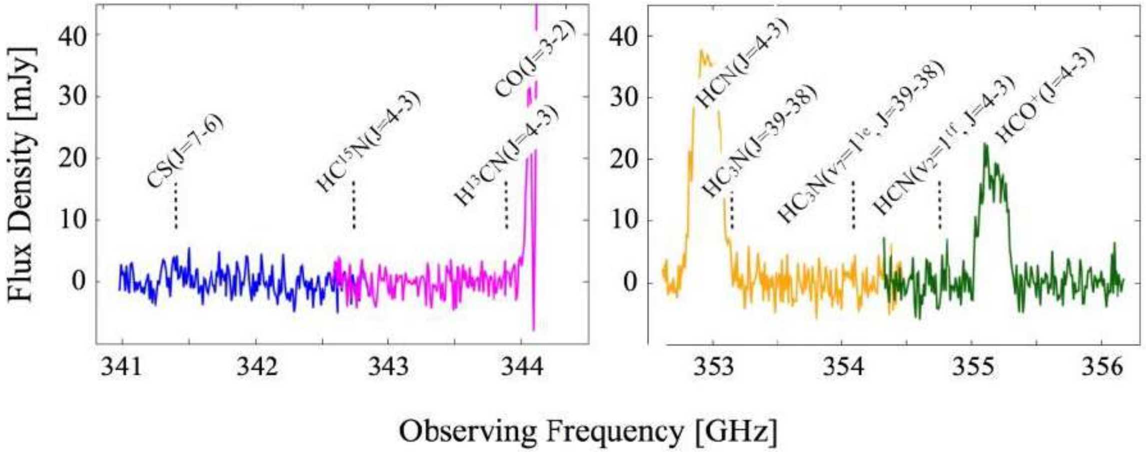


CREDIT: B. Saxton, NRAO/NSF
CREDIT: K. Öberg, Harvard

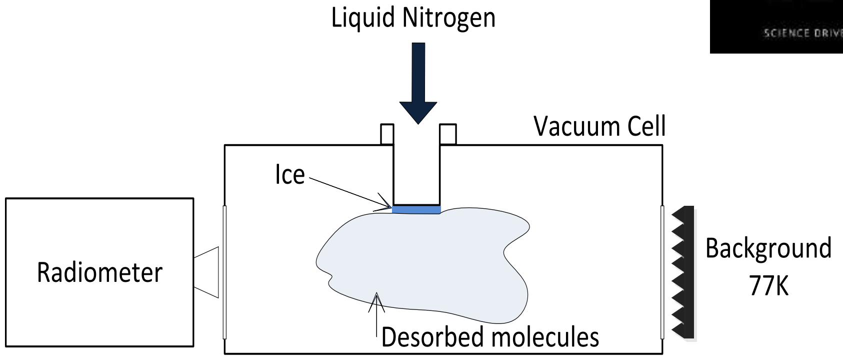
II. Bridging the gas-grain gap:
Thermal Desorption – Observations vs Experiments

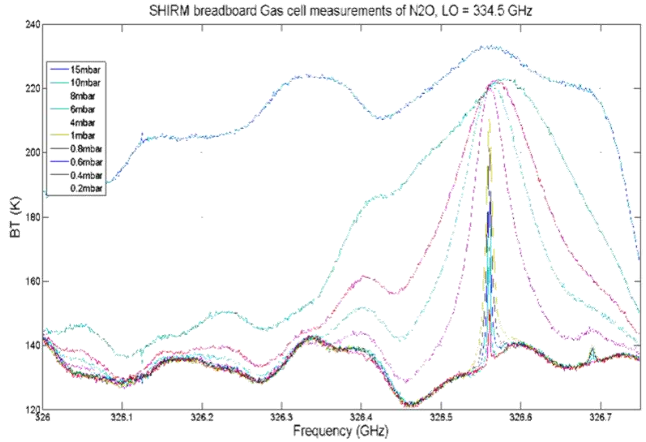
(sub)mm Observations





Laboratory Measurements



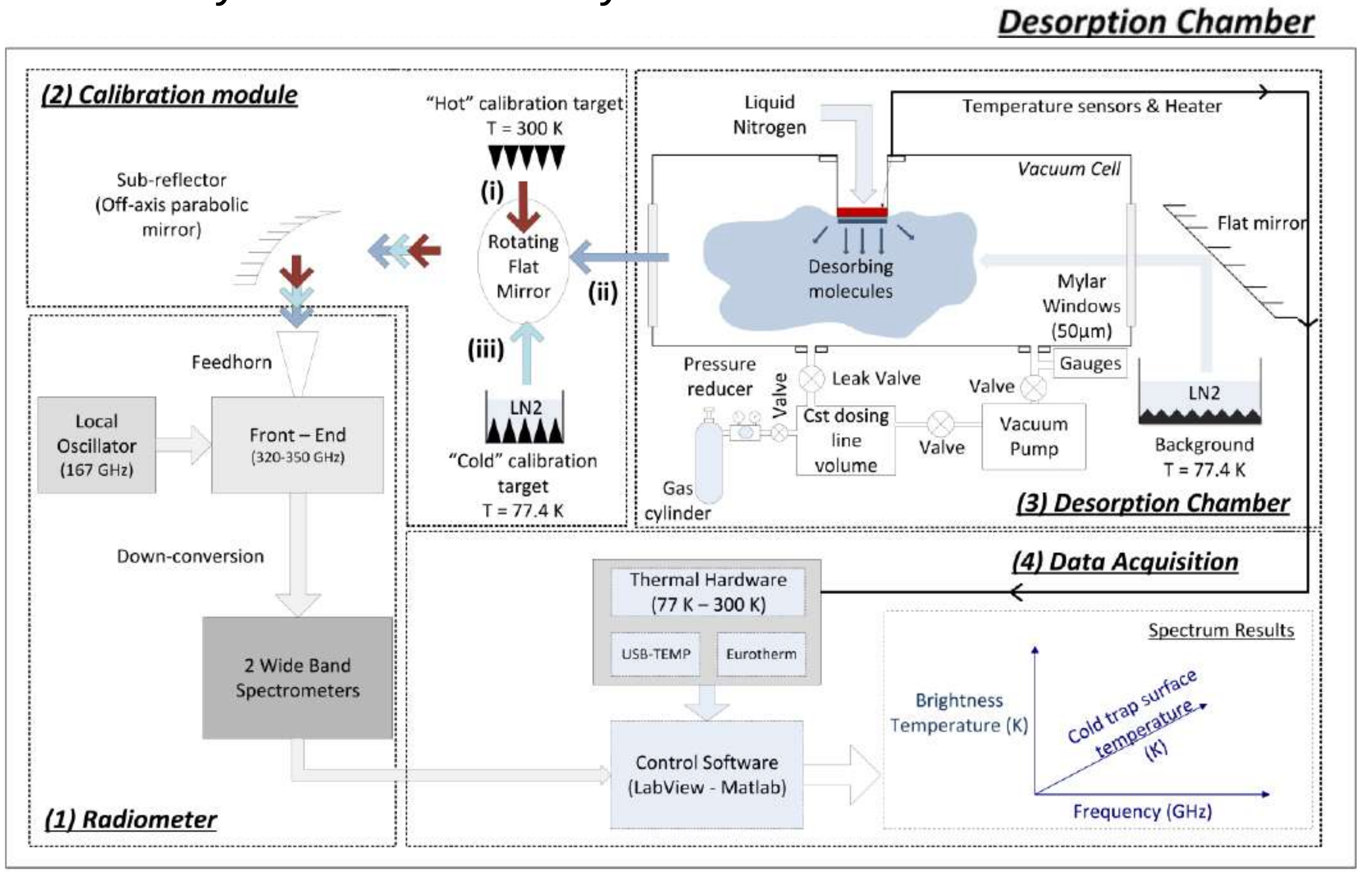


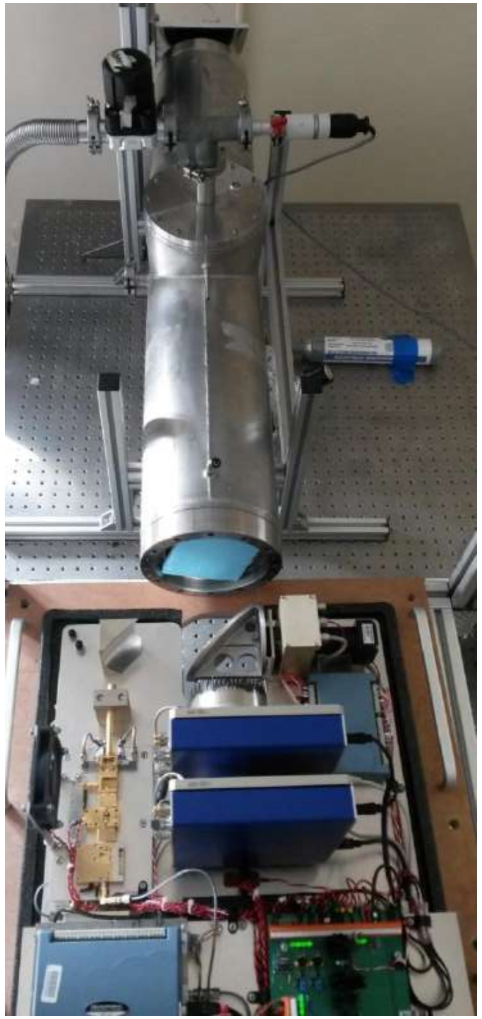
Auriacombe et al. *MNRAS* (2022)

II. Bridging the gas-grain gap:
TeraHertz Desorption Emission Spectroscopy (THz DES)

(sub)mm Heterodyne Radiometer System

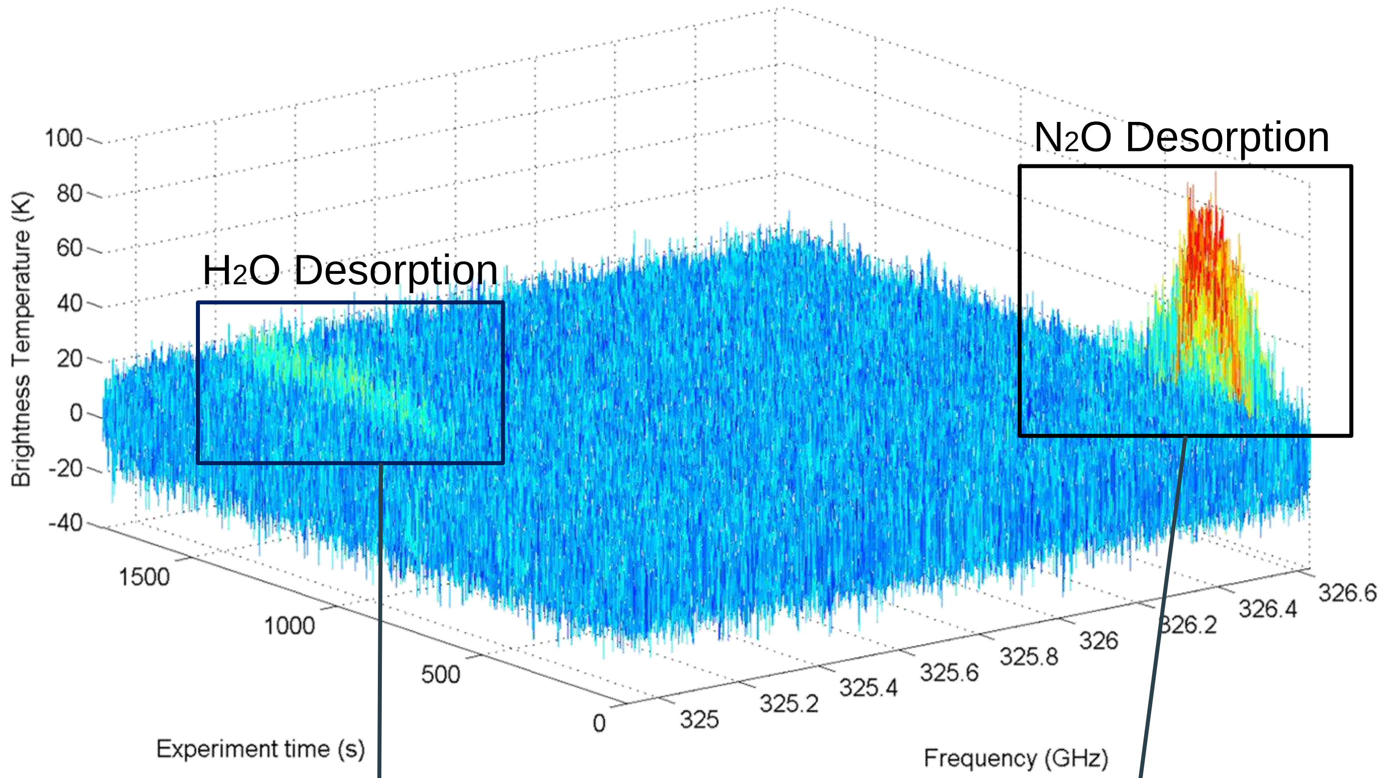
Top-View





Auriacombe et al. *MNRAS* (2022)

II. Bridging the gas-grain gap:
TeraHertz Desorption Emission Spectroscopy (THz DES)

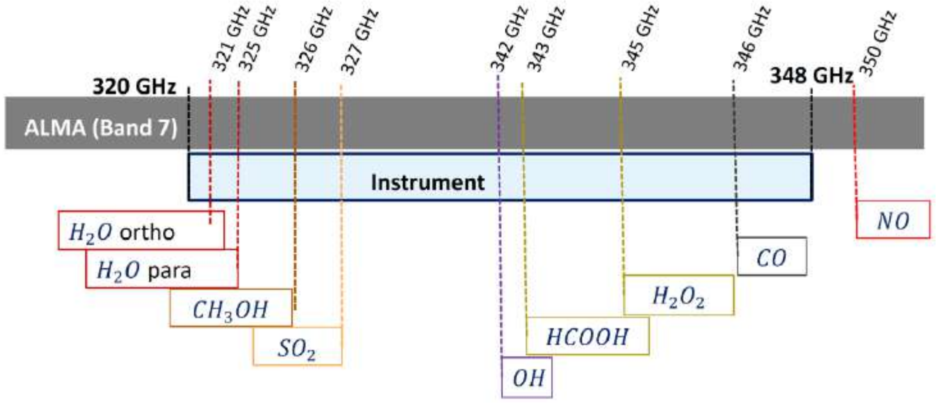


H_2O Desorption

- Start:~ 230 K
- Peak: ~ 250 K

N_2O Desorption

- Start: ~ 90 K
- Peak: ~ 130 K

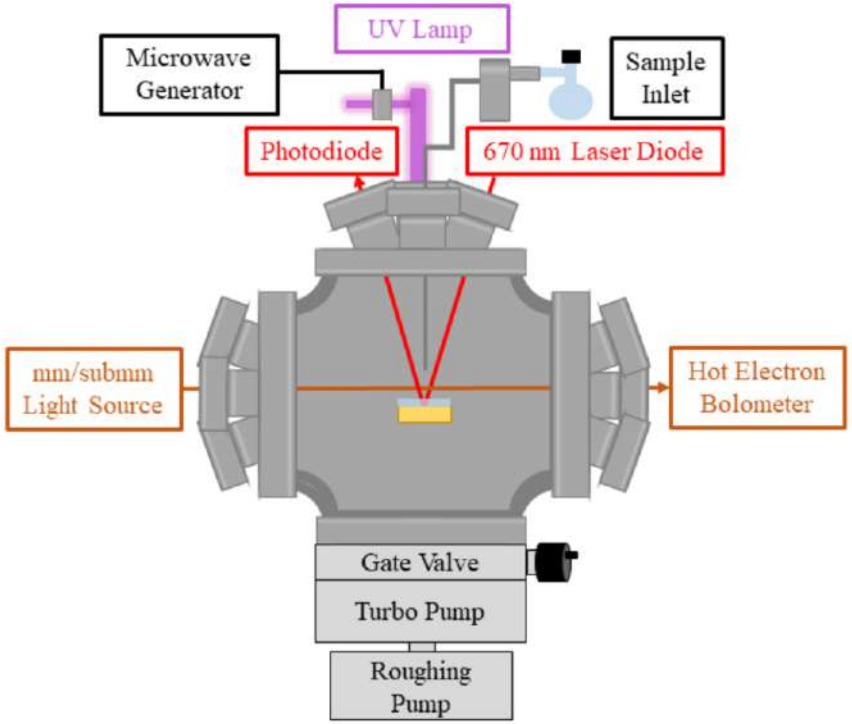


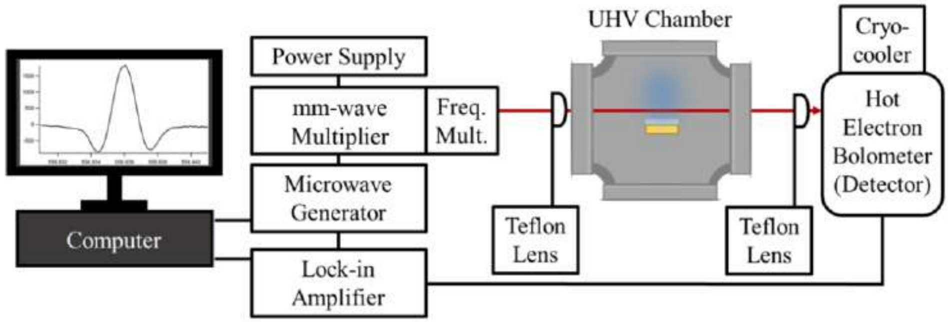
Target Molecules

Molecules	Frequency Line
Water	325,15 GHz
Methanol	326 GHz,…
Nitrous Oxide (N_2O)	326,55 GHz

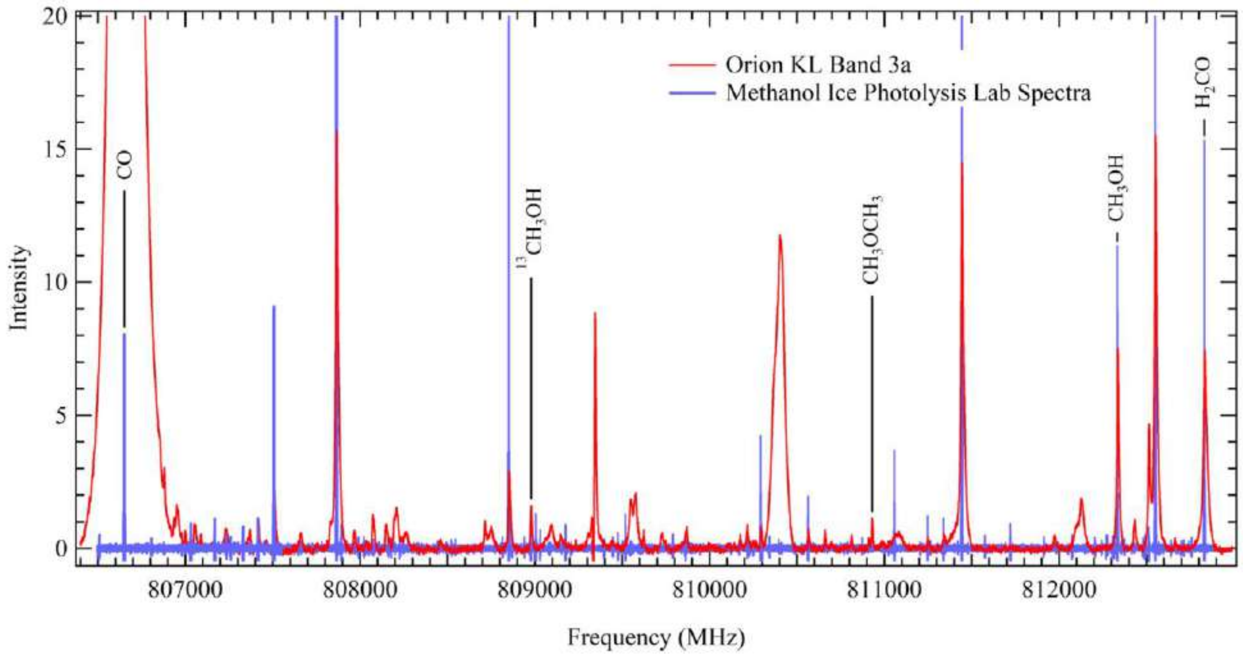
Auriacombe et al. *MNRAS* (2022)

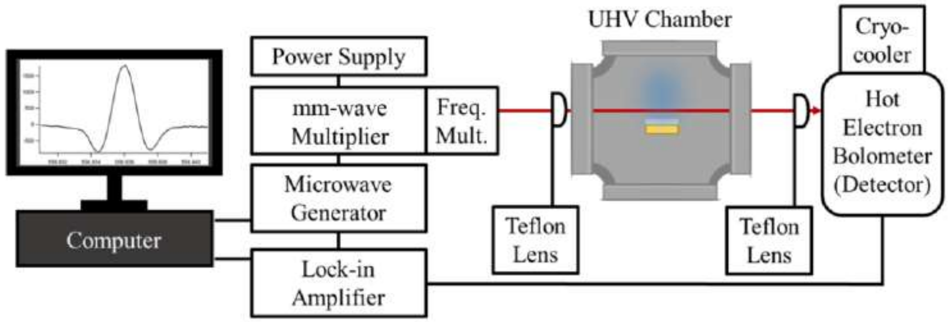
II. Bridging the gas-grain gap:
Sublimation Lab Ice (sub)Millimeter Experiment (SubLIME)





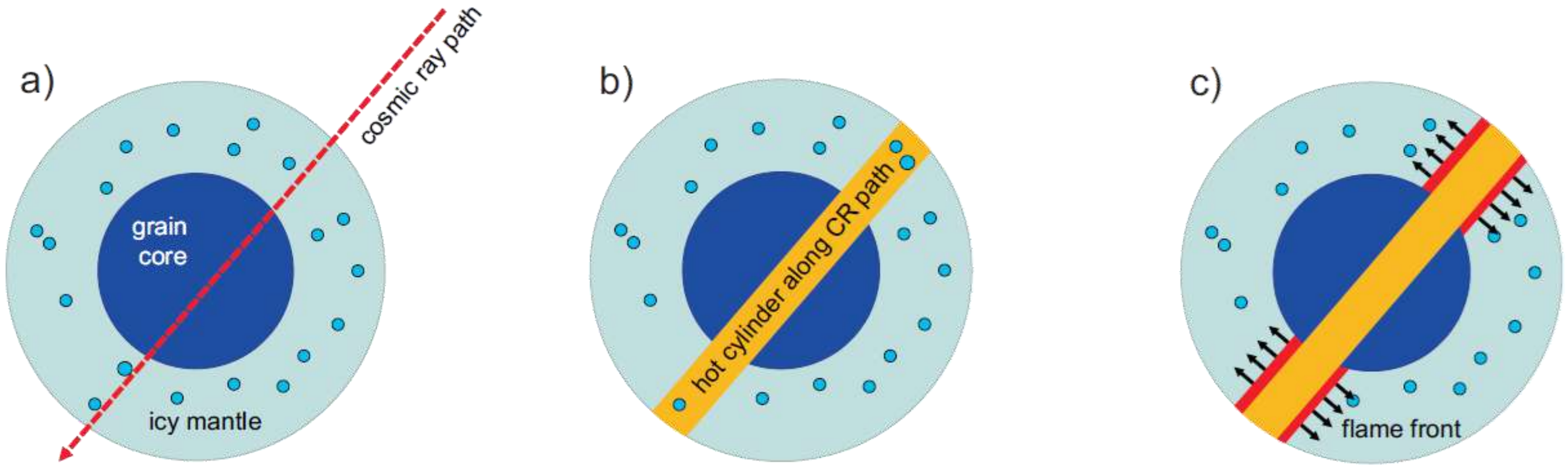
II. Bridging the gas-grain gap:
Sublimation Lab Ice (sub)Millimeter Experiment (SubLIME)





II. Bridging the gas-grain gap:
(Non)Thermal Desorption

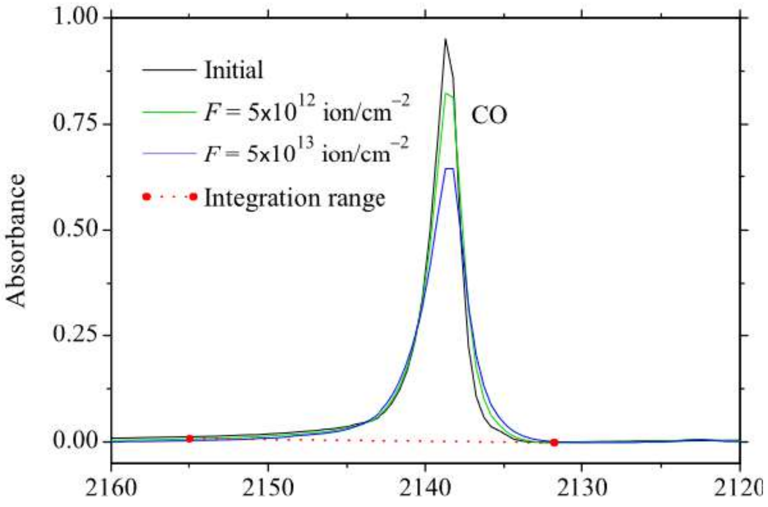
- Cosmic-ray spot heating
  - $t_{CR} \approx 4 \times 10^6 - 10^7$ yr

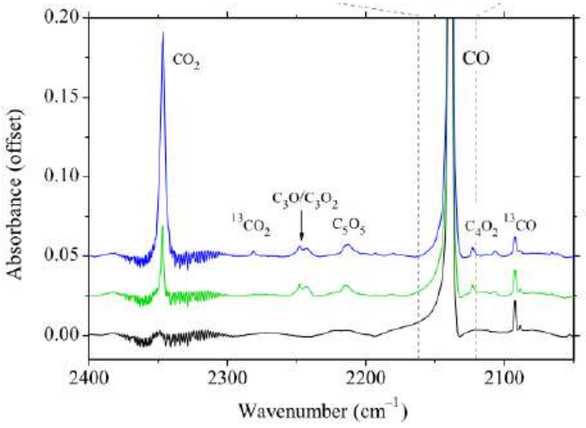


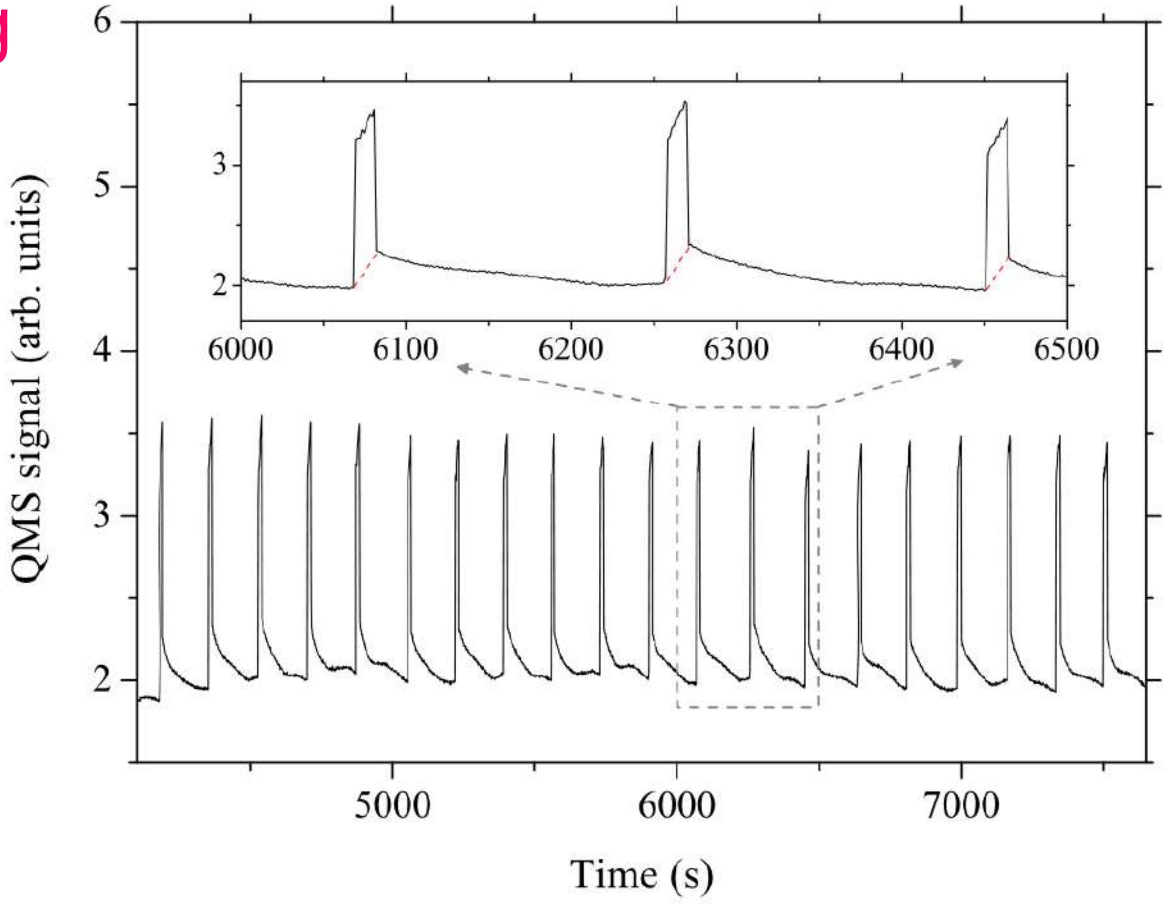
Ivlev et al. (2015)

II. Bridging the gas-grain gap:
(Non)Thermal Desorption

- Cosmic-ray sputtering





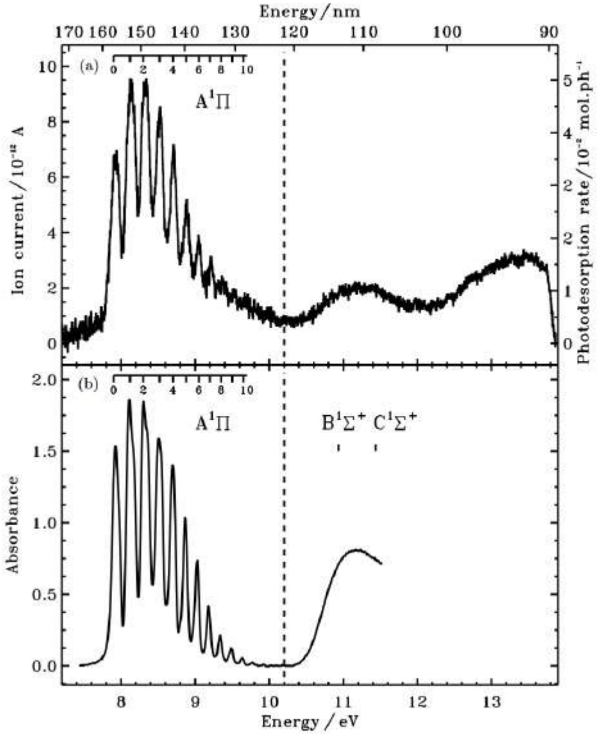


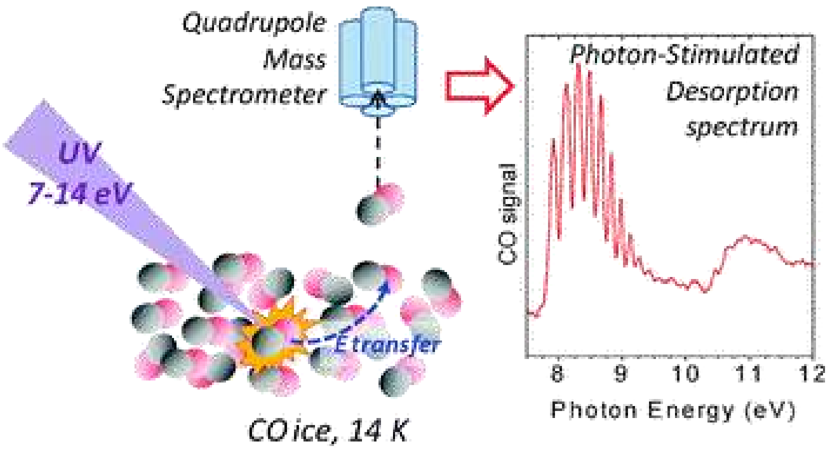
0.3 MeV He^+ ions on CO ice

Ivlev et al. (2023)

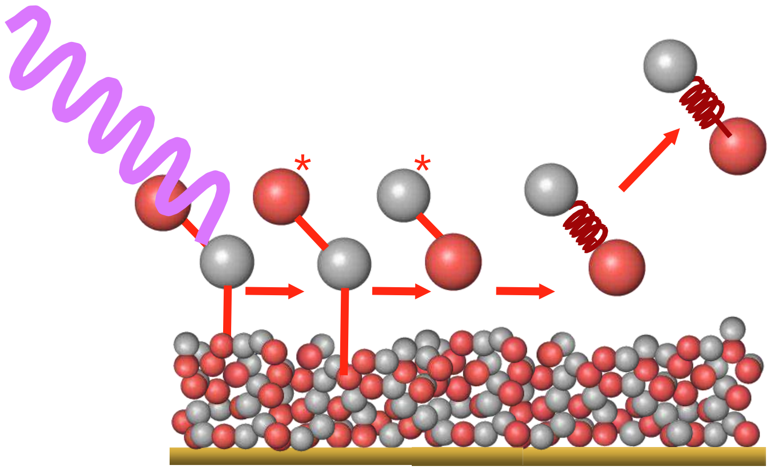
II. Bridging the gas-grain gap:
(Non)Thermal Desorption

- UV Photodesorption
  - Shown by lab experiments and calculations to have efficiencies of 10^{-3} - 10^{-4} per incident photon



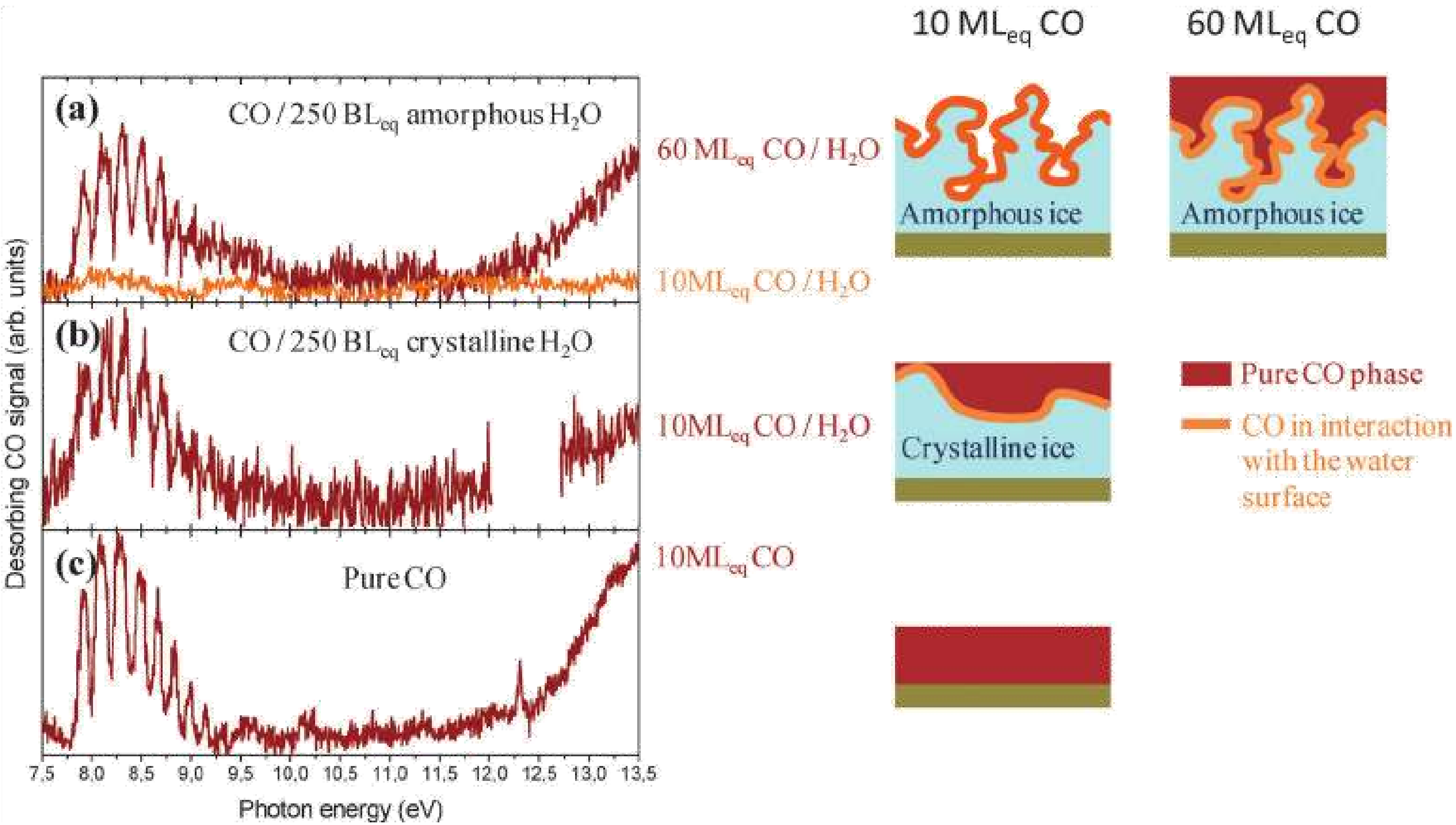


Fayolle et al. (2011)



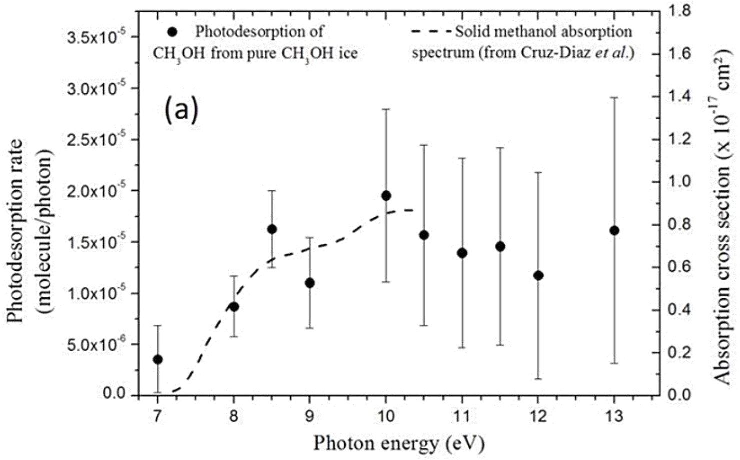
Öberg et al. (2007, 2009)

II. Bridging the gas-grain gap:
(Non)Thermal Desorption



Bertin et al. (2012)

II. Bridging the gas-grain gap:
(Non)Thermal Desorption



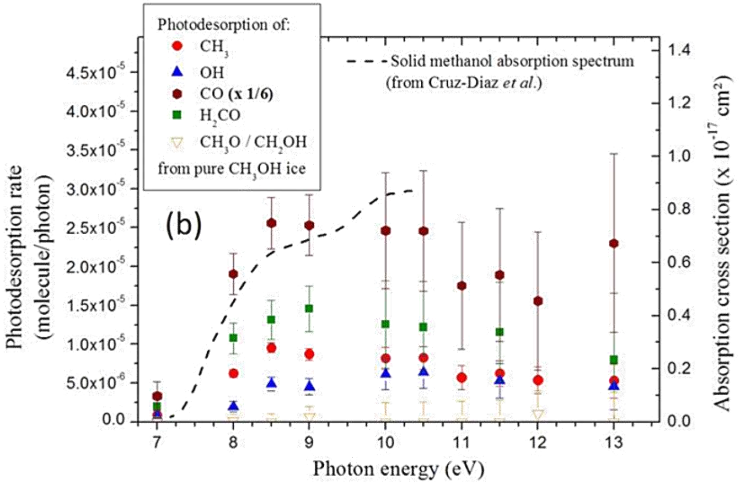


Table 1
Integrated Photodesorption Rates of CH_3OH and Photofragments of CH_3OH from Pure CH_3OH Ice and CH_3OH:CO Mixtures at 10 K for Different Astronomical Environments

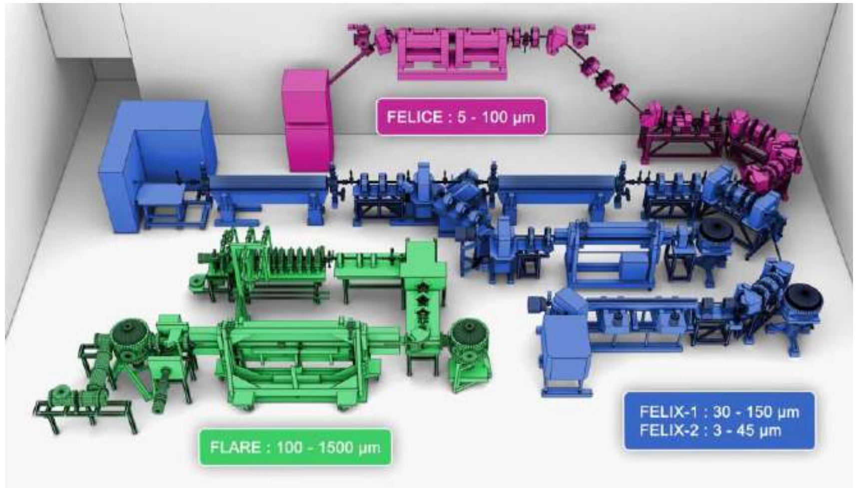
Photodesorbed Species	CH_3OH Ice	Integrated Photodesorption Rate ($\times 10^{-5}$ Molecule/Photon)	
		ISRF[a]	Prestellar Cores[b] and Protoplanetary Disks[c]
CH_3OH	Pure	1.2 ± 0.6	1.5 ± 0.6
	Mixed with CO	<0.3	<0.3
CH_3O/CH_2OH	Pure	<0.3	<0.3
	Mixed with CO	0.7 ± 0.3	0.8 ± 0.5
CO	Pure	19 ± 3	21 ± 3
H_2CO	Pure and Mixed with CO	0.7 ± 0.3	1.2 ± 0.4
OH	Pure and Mixed with CO	0.3 ± 0.1	0.7 ± 0.3
CH_3	Pure and Mixed with CO	0.3 ± 0.1	0.8 ± 0.4

Notes. Rates have been derived considering our energy-resolved photodesorption rates shown in Figures 1 and 2 and several interstellar-relevant UV fields, between 7 and 14 eV. Using UV field from.
[a] Mathis et al. (1983).
[b] Gredel et al. (1987).
[c] Johns-Krull & Herczeg (2007).

Bertin et al. (2016)

II. Bridging the gas-grain gap:
(Non)Thermal Desorption

- IR Photodesorption
  - First investigations by lab experiments and calculations



II. Bridging the gas-grain gap:
(Non)Thermal Desorption

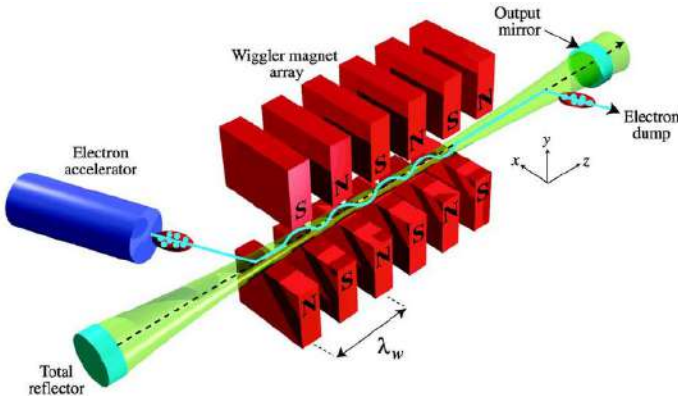
End Station at FEL-1 & FEL-2 (2.7 – 150 µm):

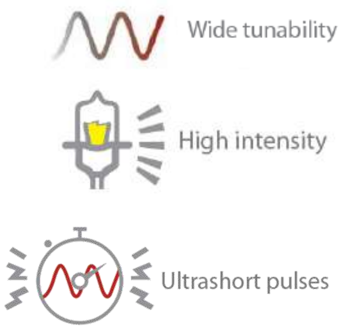
UHV Chamber (P = 1x10^{-10} mbar)

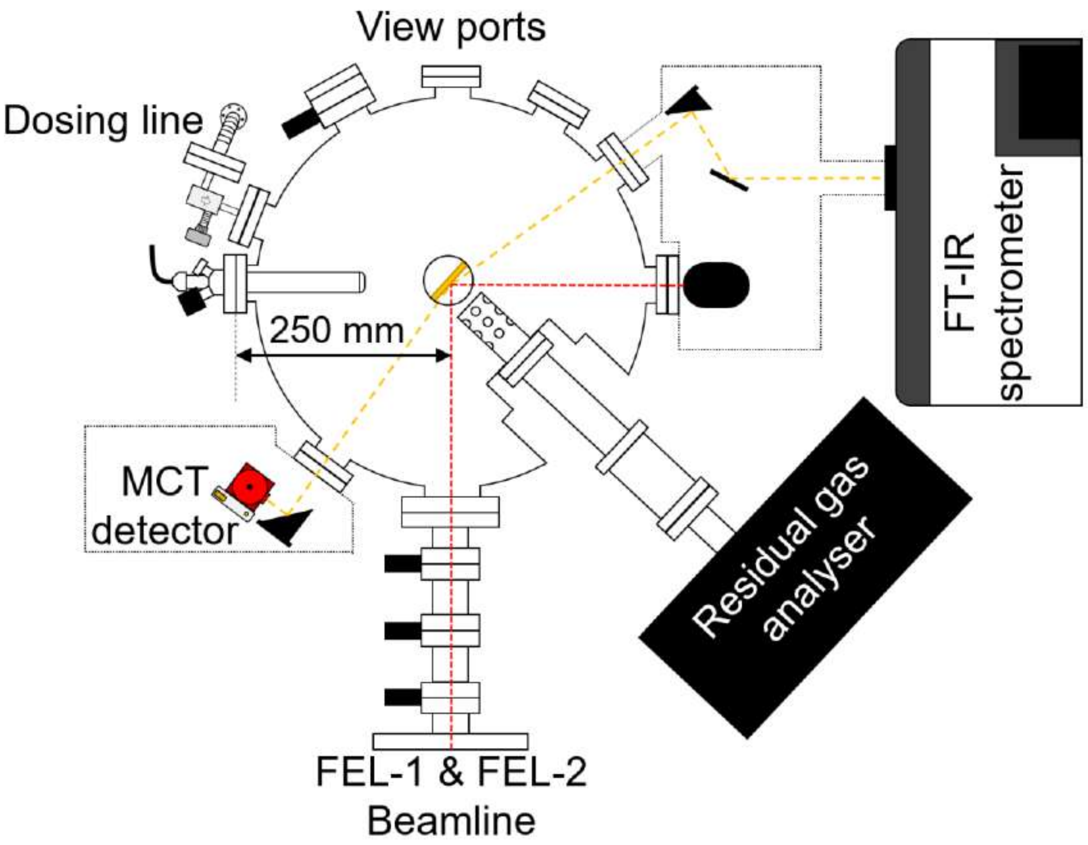
Analytical Tools (FTIR & QMS)

Sample Manipulation (Rotation + XYZ)

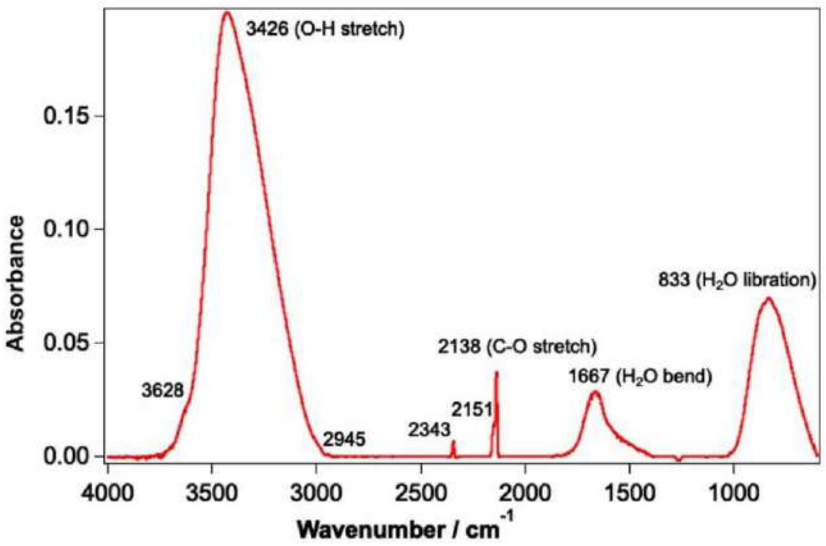
Source (5 keV electron gun)

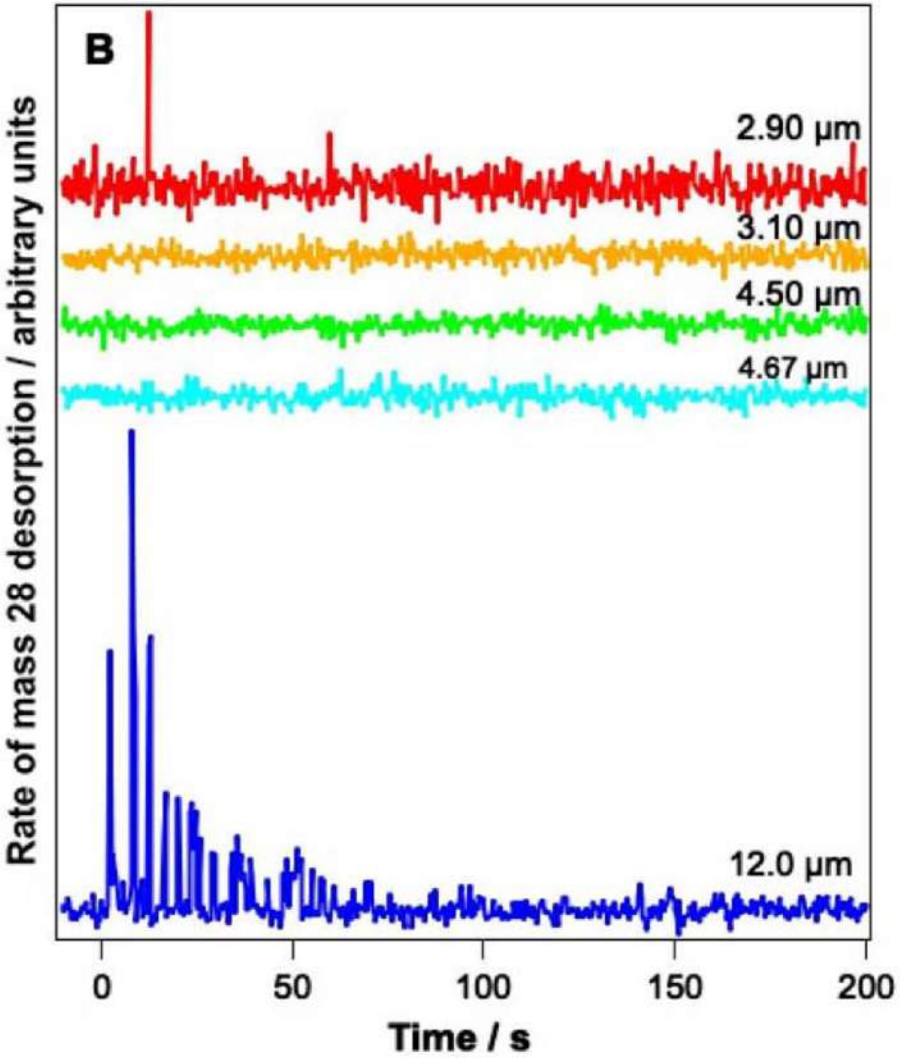






II. Bridging the gas-grain gap:
(Non)Thermal Desorption

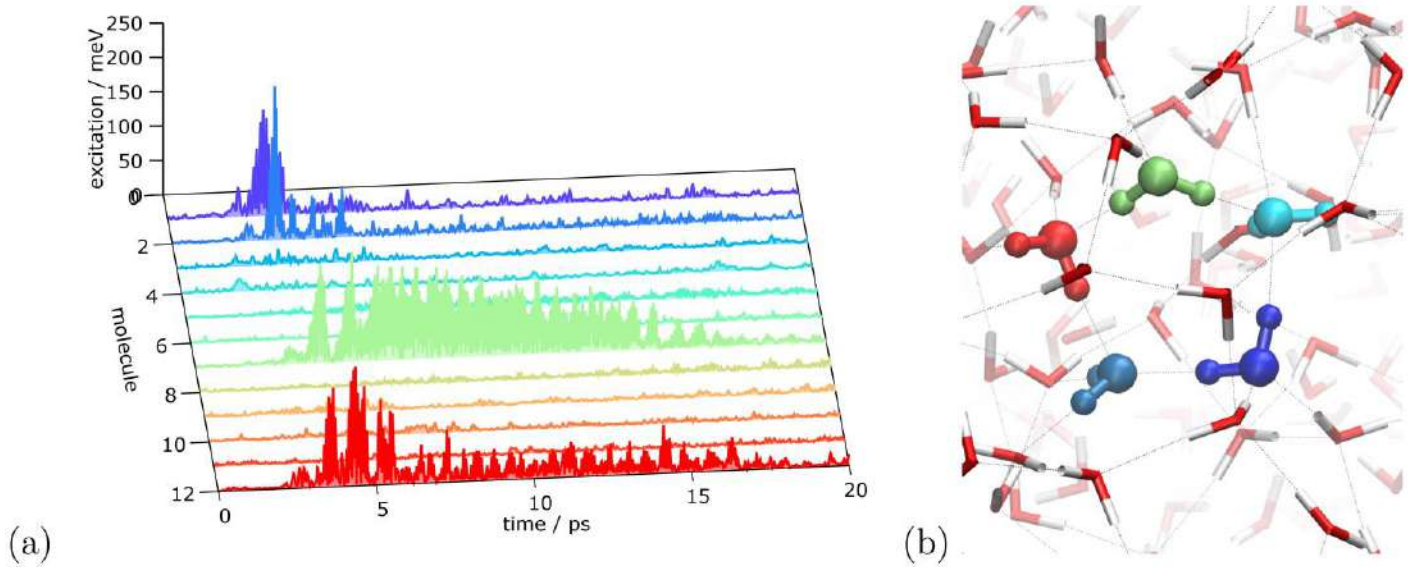




Ingman et al. *FD* (2023)

II. Bridging the gas-grain gap:
(Non)Thermal Desorption

Modelling energy relaxation in ASW:



Vibrational excitation heats ice locally causing crystallization-like effect (increased number of H-bonds) and desorption

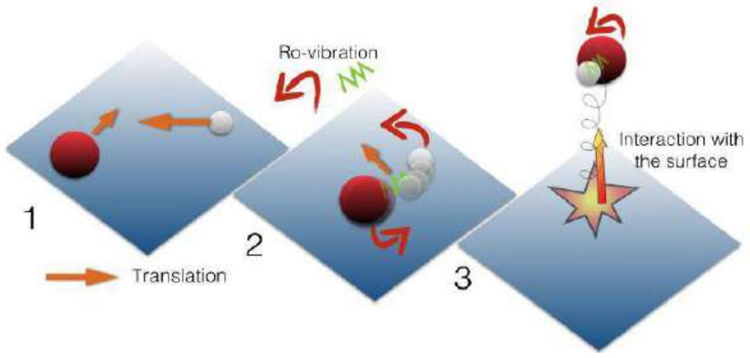
Noble et al., *JPCC* (2020), Cuppen et al. JPCA (2022)

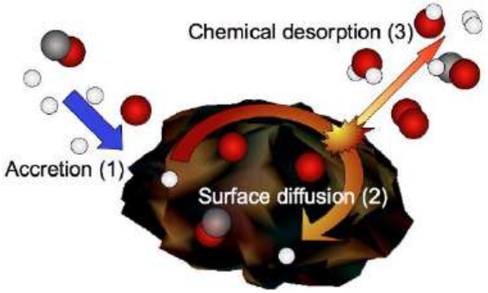
II. Bridging the gas-grain gap:
(Non)Thermal Desorption

- Explosive desorption
  - Exothermic reactions between stored radicals at $T \approx 30$ K
  - Cosmic-ray induced: $t_{exp\text{-}CR} \approx 10^5$ yr
  - Grain-grain collisions at v≥0.1 km s^{-1}: $t_{exp\text{-}gg} \approx 2\times10^9/n_H$ yr

- Grain-grain collisions in turbulent boundary layers
  - E.g., ice mantle sputtering by shocks

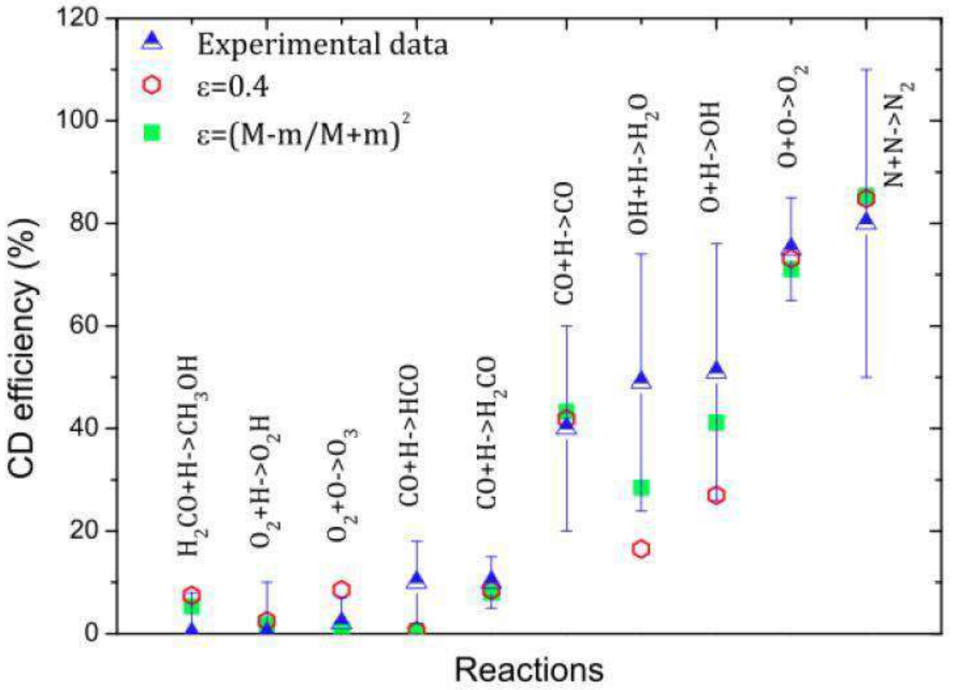
II. Bridging the gas-grain gap:
(Non)Thermal Desorption





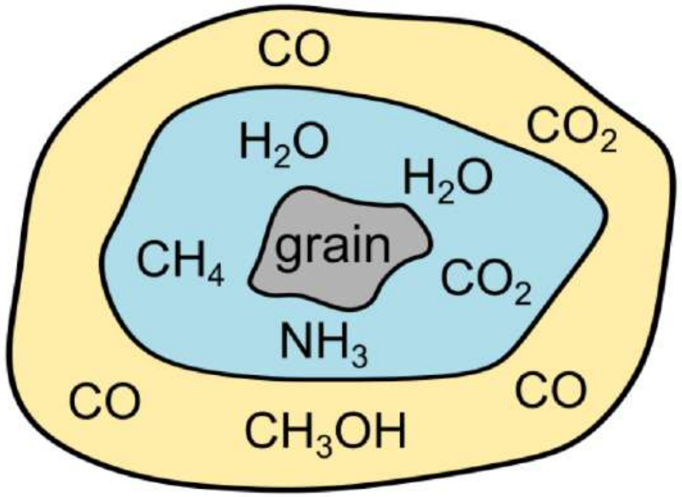
Desorption efficiencies range from <1% to >50%, with large uncertainties

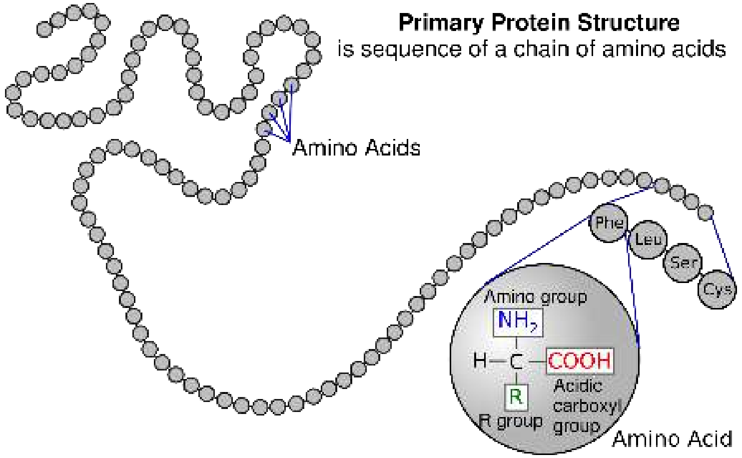
Depend sensitively on surface (e.g., silicate vs ice)

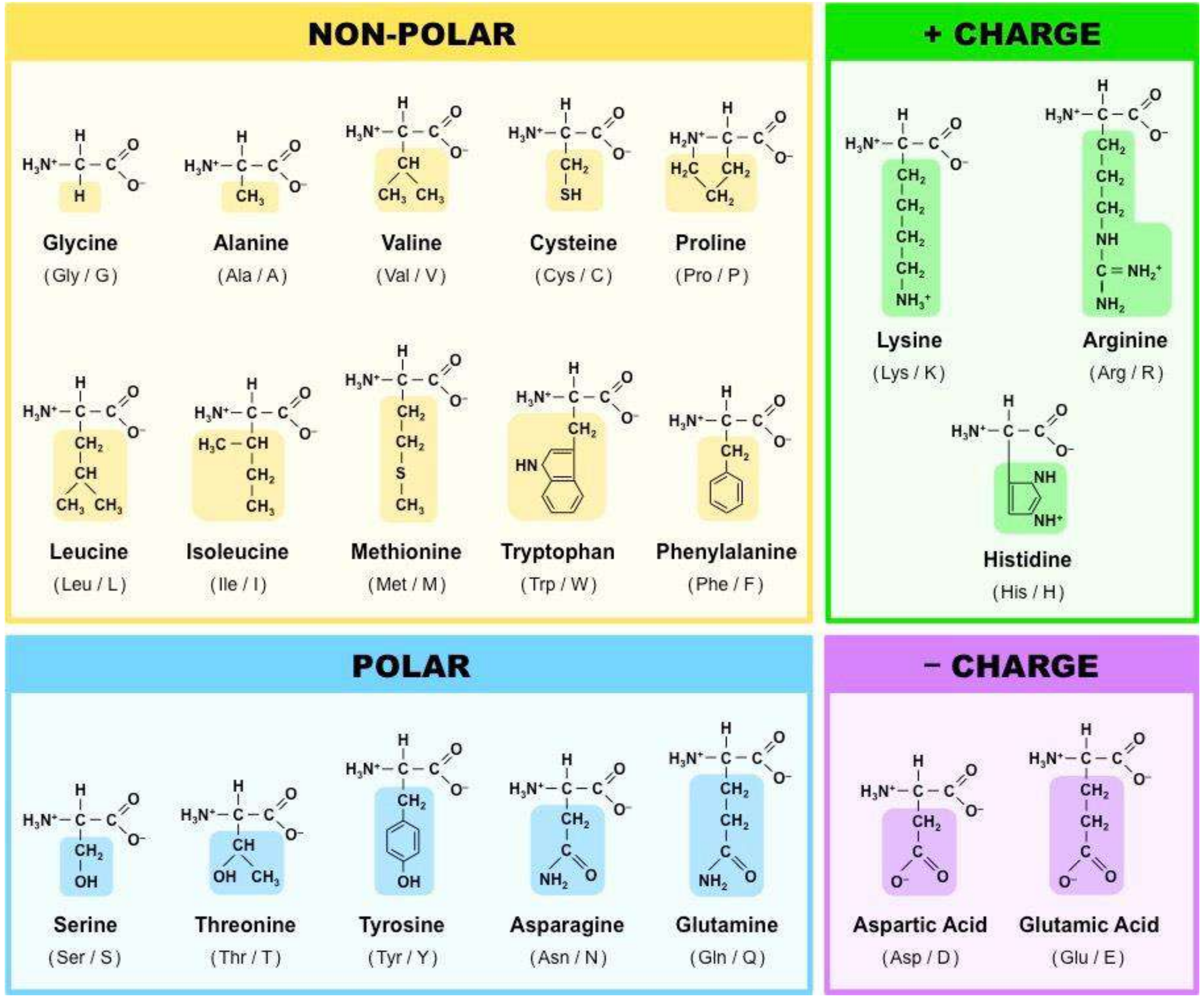


Minissale et al. 2016

III. From Astrochemistry to Astrobiology:
Surface Formation of the Building Blocks of Life in Space

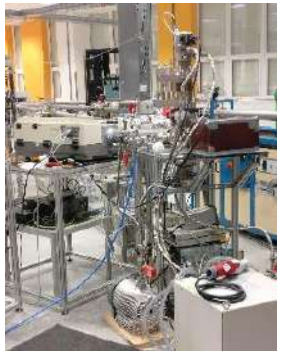




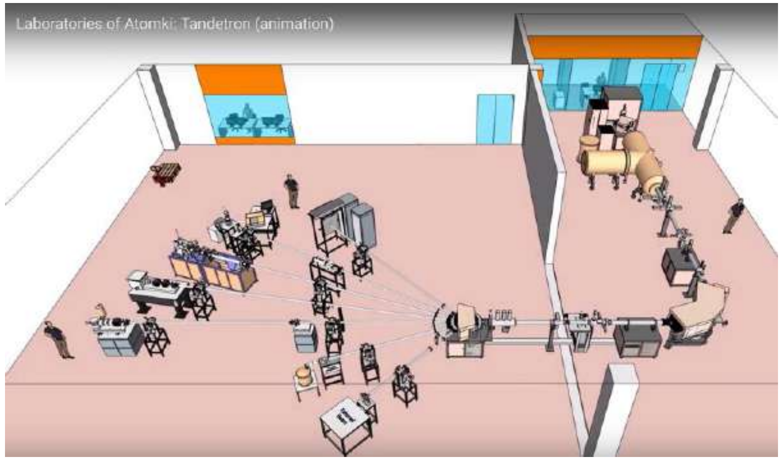


III. From Astrochemistry to Astrobiology:
Interaction of ice and particles (HUN-REN ATOMKI)

CRs and electron irradiation of ice material relevant to ISM & Solar System



ICA
P < 1x10^{-9} mbar
T_{surf} = 20 - 300 K
E_{ions} = 200 keV – 4 MeV H^+
H^+, He^+, He^{++}, C^+, C^{++}, O^+, O^{++}, S^+, S^{++}
Current = nA - µA
- **2 keV electron gun**
- **Effusive Cell**



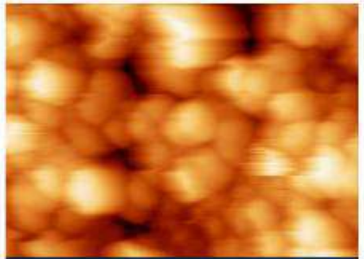
AQUILA
P < 1x10^{-9} mbar
T_{surf} = 20 - 300 K
E_{ions} = 100s eV – 10s keV
Solar Wind: H, He, C, O, Si, Fe, Ni ions
High charge state of ions
Positive/negative ions or molecular ions

ECR Ion Source (ECRIS)

III. From Astrochemistry to Astrobiology:
Interaction of ice and dust (InterCat)

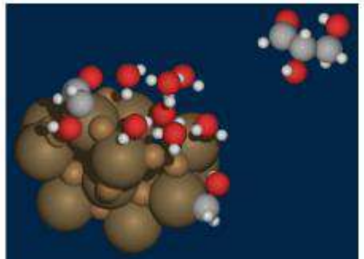
INTERCAT
Center for Interstellar Catalysis

INTERCAT
Center for Interstellar Catalysis



Theme 1

Synthesis of carbonaceous and silicate interstellar dust grain analogue nanoparticles and nanostructures



Theme 2

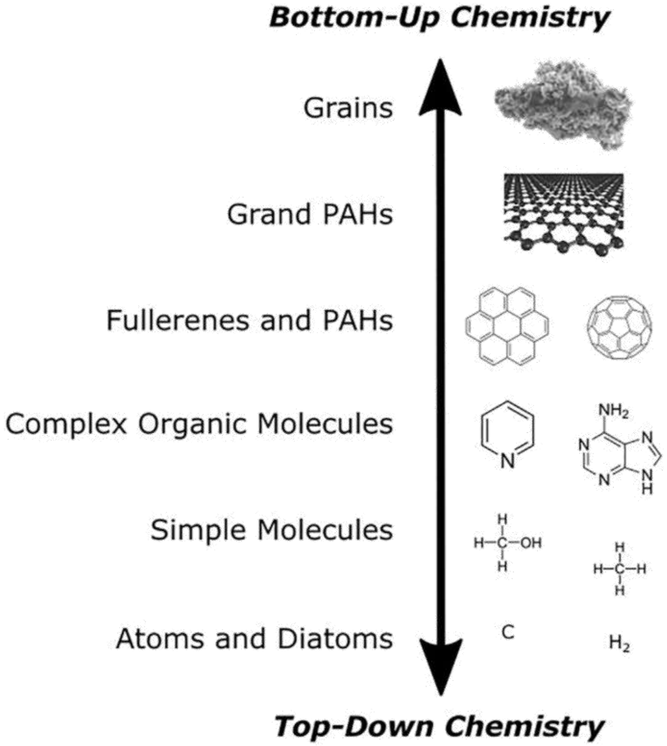
Catalytic activity of carbonaceous and silicate interstellar dust grain analogue nanoparticles and nanostructures

Theme 3

Gauging the effect on catalytic activity of ice growth on silicate and carbonaceous grain surfaces

Theme 4

Solid ice photo-processing pathways to complex organic molecule formation



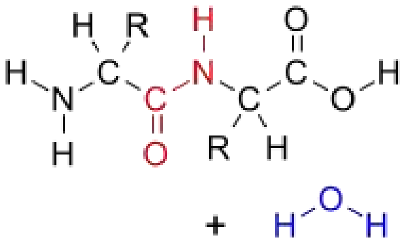
III. From Astrochemistry to Astrobiology:
Interaction of ice and dust (InterCat)

INTERCAT
Center for Interstellar Catalysis

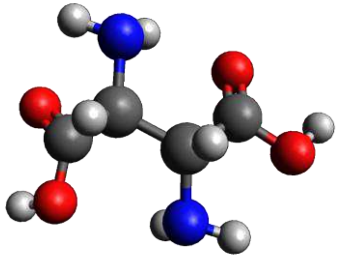
Investigation of peptide bond formation

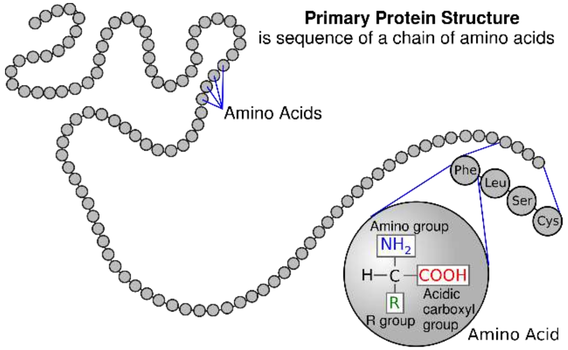
Alfred Hopkinson

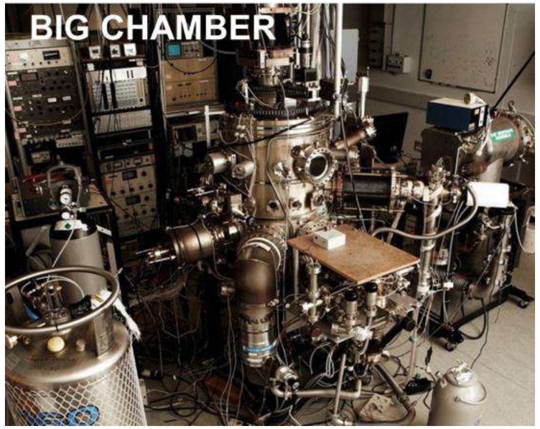
1) **Hydrogenation/Deuteration of Gly on cold grain analogs**
   Deuterium exchange observed
   Formation of **larger species**
2) **1 keV e⁻ irradiation of Gly**
3) **20 keV H^+ irradiation of Gly**
4) **1 MeV H^+ irradiation of Gly**
   Peptide-like bonds

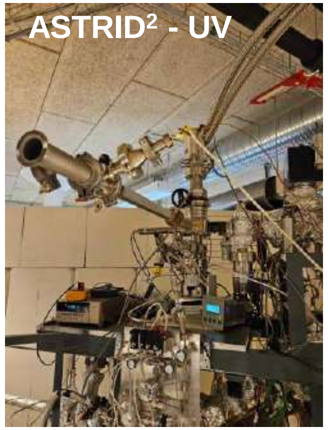


3-Aminoaspartic Acid



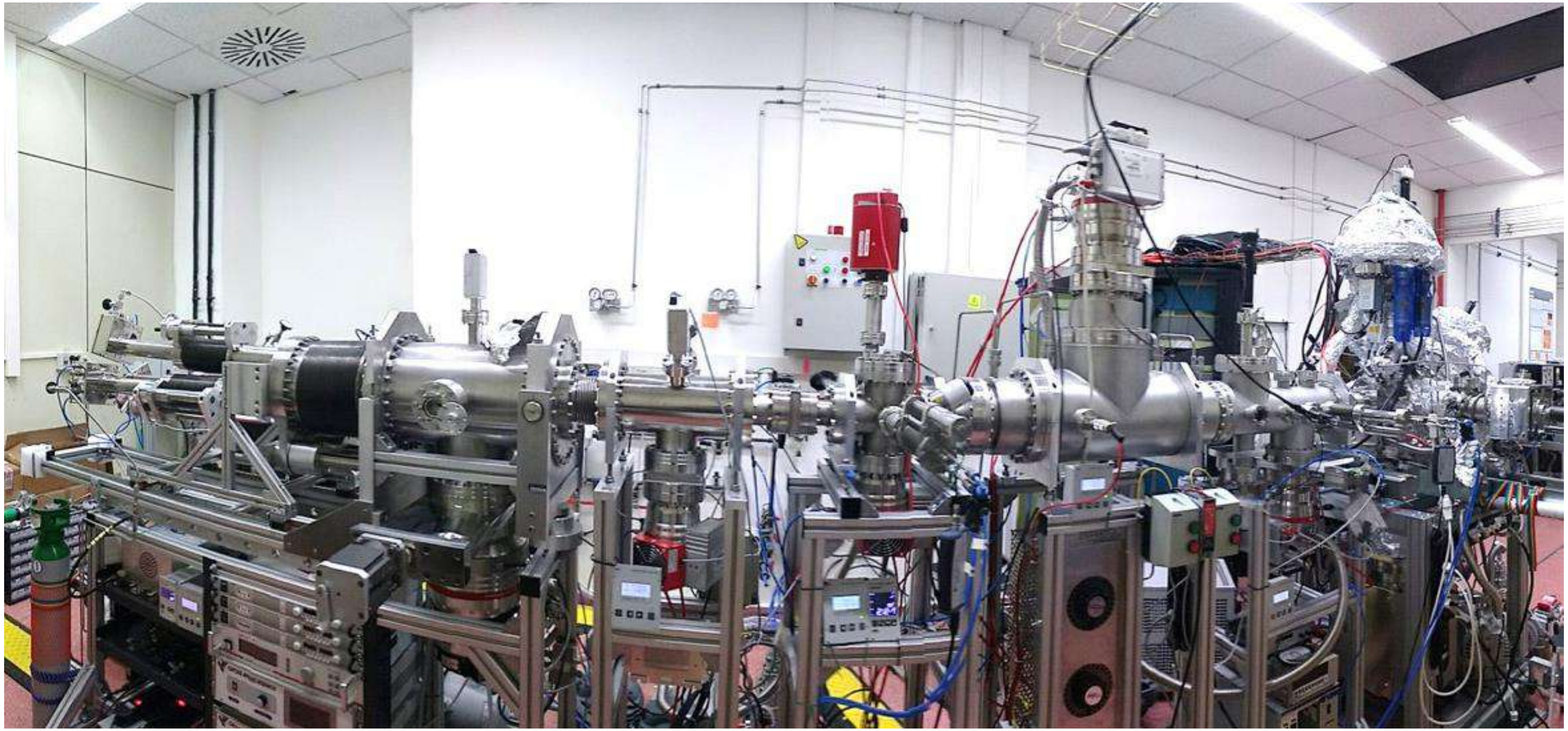






III. From Astrochemistry to Astrobiology:
Interaction of ice and dust (Stardust)

STARDUST MACHINE



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III. From Astrochemistry to Astrobiology:
Interaction of ice and dust (Impact Chemistry)

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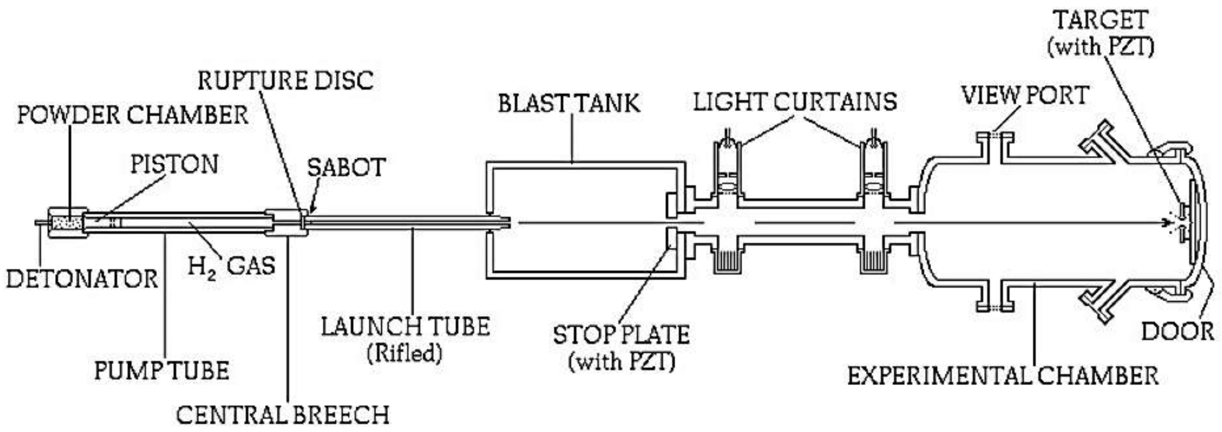

Schematic diagram of the Light Gas Gun

Speed regime: 0.3 to 7.5 km/s

Projectile Type: Can fire single projectiles between 0.1 mm and 3.0 mm in diameter, or 1 micron to 400 microns diameter bodies in buck-shot style firings.

Firing Rate: Upper rate of two shots a day (dependent on projectile and target).

Target Specifications: Objects of up to 1m x 1m x 1m can be used as targets. In addition (depending on the size of the target) and there is also an option to have the target cooled by liquid nitrogen, or heated to up to 1000 K in our customised target holder.

III. From Astrochemistry to Astrobiology:

Interaction of ice and dust (Impact Chemistry)

University of Kent

nature geoscience ARTICLES
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Shock synthesis of amino acids from impacting cometary and icy planet surface analogues

Zita Martins[1†], Mark C. Price[2*†], Nir Goldman[3], Mark A. Sephton[1] and Mark J. Burchell[2]

Comets are known to harbour simple ices and the organic precursors of the building blocks of proteins—amino acids—that are essential to life. Indeed, glycine, the simplest amino acid, was recently confirmed to be present on comet 81P/Wild-2 from samples returned by NASA's Stardust spacecraft. Impacts of icy bodies (such as comets) onto rocky surfaces, and, equally, impacts of rocky bodies onto icy surfaces (such as the jovian and saturnian satellites), could have been responsible for the manufacture of these complex organic molecules through a process of shock synthesis. Here we present laboratory experiments in which we shocked ice mixtures analogous to those found in a comet with a steel projectile fired at high velocities in a light gas gun to test whether amino acids could be produced. We found that the hypervelocity impact shock of a typical comet ice mixture produced several amino acids after hydrolysis. These include equal amounts of D- and L-alanine, and the non-protein amino acids α-aminoisobutyric acid and isovaline as well as their precursors. Our findings suggest a pathway for the synthetic production of the components of proteins within our Solar System, and thus a potential pathway towards life through icy impacts.

Table 1 | Summary of the average total amino acid abundances (in nanograms) in the target ice samples no. 1 and no. 2 measured by GC-MS*.

Amino acid	Target ice sample no. 1 (ng)	Target ice sample no. 2 (ng)
α-AIB	5.6±0.4	51.4±0.8
D,L-isovaline†	4.1±0.2	152.8±3.5
D-alanine	54.3±2.1	61.0±0.7
L-alanine	54.7±1.8	61.8±0.6
D,L-α-ABA‡	60.0	90.0
Glycine	3,722.1±196.4	1,161.0±39.8
D-norvaline	10.3±0.3	11.8±0.1
L-norvaline	10.6±0.3	12.2±0.2

*The associated errors are based on the standard deviation of the average value between six separate measurements (*N*) with a standard error, $\delta x = \sigma x \cdot N^{-1/2}$. †Enantiomers could not be separated under the chromatographic conditions. ‡Optically pure standard, not available for enantiomeric identification.

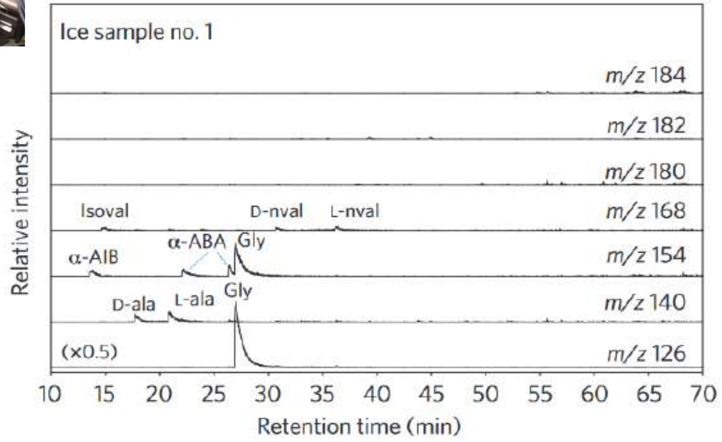

Figure 1 | Chromatogram of extracts from shocked ice sample no. 1. The 10–70 min region of the single-ion GC-MS traces (*m/z* 126, 140, 154, 168, 180, 182 and 184) of the derivatized (*N*-TFA, *O*-isopropyl) HCl-hydrolysed extracts of ice sample no. 1 (impact-shocked). Gly, glycine; D-ala, D-alanine; L-ala, L-alanine; α-AIB, α-aminoisobutyric acid; α-ABA, α-aminobutyric acid; Isoval, isovaline; D-nval, D-norvaline; L-nval, L-norvaline. No other amino acid was detected above the detection limit of the GC-MS (10 pg). The single-ion trace for *m/z* 126 is scaled by ×0.5 to aid comparison.

III. From Astrochemistry to Astrobiology:
Interaction of ice and dust (Impact Chemistry)

University of Kent

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Research Article **Open Access**

Tardigrade Survival Limits in High-Speed Impacts —Implications for Panspermia and Collection of Samples from Plumes Emitted by Ice Worlds

Alejandra Traspas and Mark J. Burchell

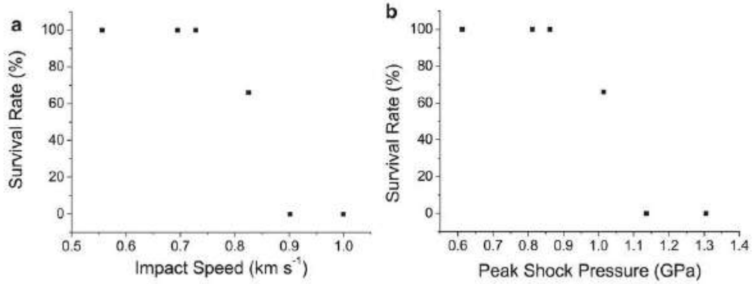

FIG. 2. Results of impact experiments onto sand. **(a)** Tardigrade survival rate vs. impact speed. **(b)** Tardigrade survival rate vs. peak shock pressure.

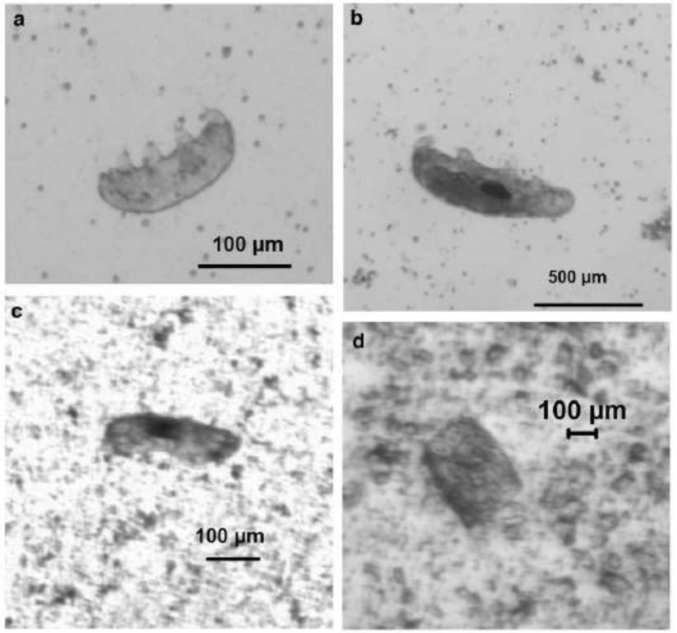

FIG. 1. **(a, b)** Example tardigrades before impact testing. Tardigrades ranged in size from 150 to 850 μm. **(c)** Tardigrade recovered after an impact at 0.728 km s^{-1}. **(d)** Tardigrade fragment from shot at 0.901 km s^{-1}.

Outlook

ALMA and JWST are revolutionizing our understanding of star formation

New dedicated set of lab data are needed!

Complementary VUV/IR/THz and novel techniques at large scale facilities can help understand the evolution of ices in space.

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