

Laboratory Ice Astrochemistry at Large Scale Facilities

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InterStellar Medium (ISM)

10% of Galaxy's mass

Gas 99% in mass

Dust 1% in mass

H (70%)

He (28%)

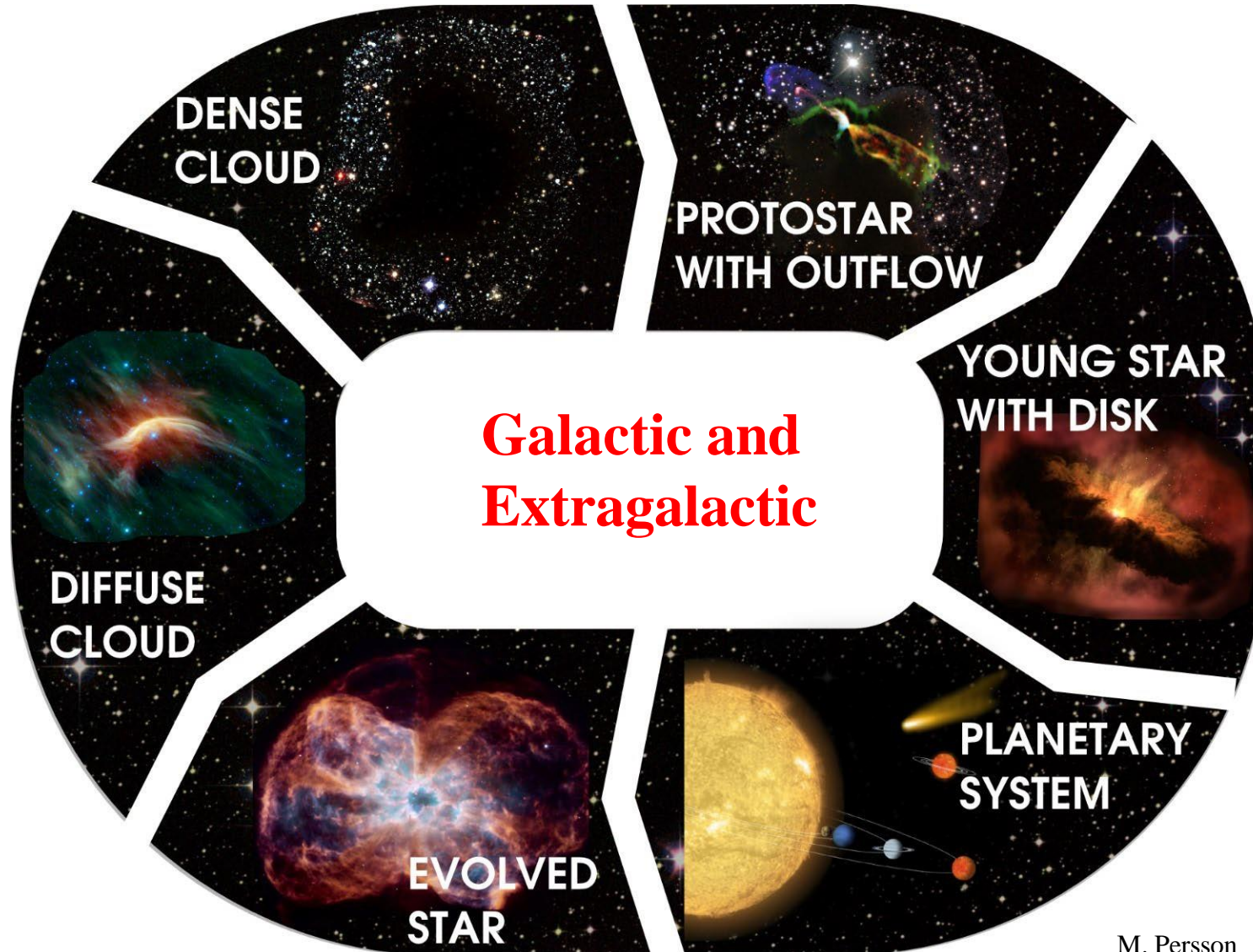
Heavier elements (2%)

Carbonaceous

Silicate Grains

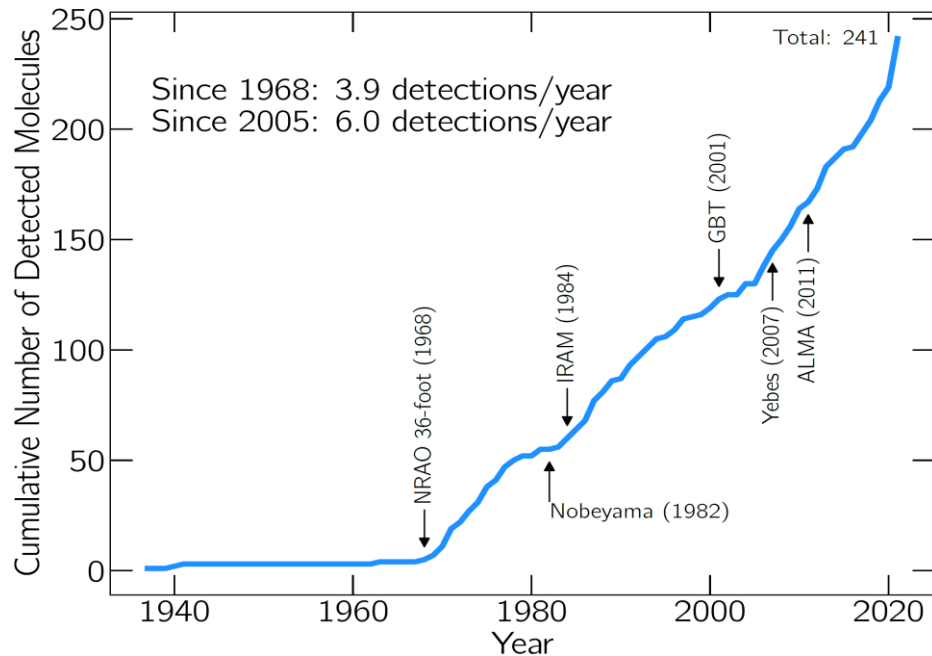


The Molecular Universe



Molecules in Space

More than 300 molecules detected in space in the gas phase



McGuire, *ApJS* (2021)

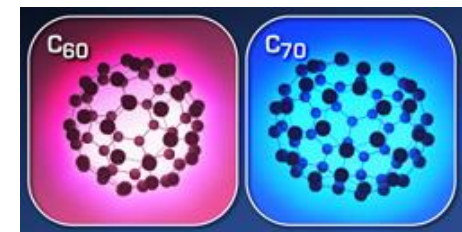
(The CDMS Catalog)

<https://cdms.astro.uni-koeln.de/classic/molecules>

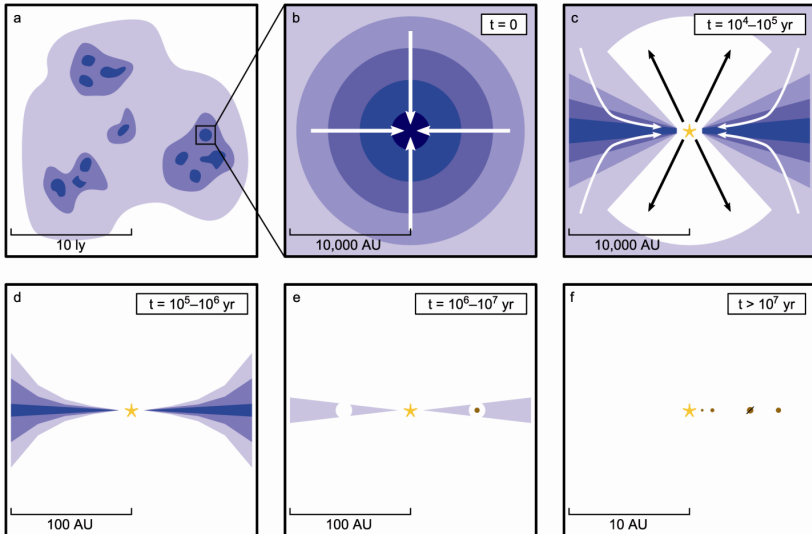
2 atoms	3 atoms	4 atoms	5 atoms	6 atoms	7 atoms	8 atoms	9 atoms	10 atoms	11 atoms	12 atoms				
H ₂	AlO	C ₃ [*]	H ₂ Cl [*]	c-C ₃ H	H ₂ NC	C ₆ [*]	HC(S)CN	C ₆ H	C ₆ H	CH ₃ C ₃ N	CH ₃ C ₄ H	CH ₃ C ₃ N	HC ₉ N	c-C ₆ H ₆ [*]
AlF	OH [*]	C ₂ H	KCN	I-C ₃ H	HCCS [*]	C ₄ H	HCCCO	I-H ₂ C ₄	CH ₂ CHCN	HC(O)OCH ₃	CH ₃ CH ₂ CN	(CH ₃) ₂ CO	CH ₃ C ₆ H	n-C ₃ H ₇ CN
AlCl	CN ⁻	C ₂ O	FeCN	C ₃ N		C ₄ Si		C ₂ H ₄ [*]	CH ₃ C ₂ H	CH ₃ COOH	(CH ₃) ₂ O	(CH ₂ OH) ₂	C ₂ H ₅ OCHO	i-C ₃ H ₇ CN
C ₂ ^{**}	SH [*]	C ₂ S	HO ₂	C ₃ O		I-C ₃ H ₂		CH ₃ CN	HC ₃ N	C ₇ H	CH ₃ CH ₂ OH	CH ₃ CH ₂ CHO	CH ₃ OC(O)CH ₃	C ₂ H ₅ OCH ₃
CH	SH	CH ₂	TiO ₂	C ₃ S		c-C ₃ H ₂		CH ₃ NC	CH ₃ CHO	C ₆ H ₂	HC ₇ N	CH ₃ CHCH ₂ O	CH ₃ C(O)CH ₂ OH	1-c-C ₃ H ₅ CN
CH [*]	HCl [*]	HCN	C ₂ N	C ₂ H ₂ [*]		H ₂ CCN		H ₂ CCN	CH ₃ OH	CH ₃ NH ₂	CH ₂ OHCHO	C ₆ H	CH ₃ OCH ₂ OH	2-c-C ₃ H ₅ CN
CN	TiO	HCO	Si ₂ C	NH ₃		CH ₄ [*]		CH ₃ SH	c-C ₂ H ₄ O	I-HC ₆ H [*]	CH ₃ C(O)NH ₂	c-C ₆ H ₄	HOCH ₂ CH ₂ NH ₂	CH ₃ C ₇ N (?)
CO	ArH [*]	HCO [*]	HS ₂	HCCN		HC ₃ N		HC ₃ NH [*]	H ₂ CCHOH	CH ₂ CHCHO	C ₆ H ⁻	H ₂ CCCHC ₃ N	H ₂ CCCHC ₄ H	n-C ₃ H ₇ OH
CO [*]	N ₂	HCS [*]	HCS	HCNH [*]		HC ₂ NC		HCCCHO	C ₆ H ⁻	CH ₂ CCHCN	C ₃ H ₆	C ₂ H ₅ NCO		i-C ₃ H ₇ OH
CP	NO ⁺ ?	HOC [*]	HSC	HNCO		HCCNC		NH ₂ CHO	CH ₃ NCO	H ₂ NCH ₂ CN	CH ₂ CH ₂ SH	C ₂ H ₆ NH ₂ (?)		
SiC	NS [*]	H ₂ O	NCO	HNCS		HCOOH		C ₃ N	HC ₃ O	HCOOH	CH ₃ CHNH	CH ₂ NHCHO	HC ₇ NH [*]	
HCl	HeH [*]	H ₂ S	CaNC	HOCO [*]		H ₂ CNH		I-HC ₄ H [*]	HOCH ₂ CN	CH ₃ SiH ₃	HC ₇ O	CH ₃ CHCHCN	CH ₃ CHCHCN	
KCl	PO [*]	HNC	NCS	H ₂ CO		H ₂ C ₂ O		I-HC ₄ N	HCCCHNH	H ₂ NC(O)NH ₂	HCCCHCHCN	CH ₃ C(CN)CH ₂	CH ₂ CHCH ₂ CN	
NH		HNO		H ₂ CN		H ₂ NCN		c-H ₂ C ₃ O	HC ₄ NC	HCCCH ₂ CN	H ₂ CCHC ₃ H	CH ₂ CHCH ₂ CN		
NO		MgCN		H ₂ CS		HNC ₃		H ₂ CCNH	c-C ₃ HCCH	HC ₃ NH [*]	H ₂ CCCHC ₃ H			
NS		MgNC		H ₃ O [*]		SiH ₄ [*]		C ₆ N ⁻	I-H ₂ C ₅	CH ₂ CHCCH	HOCHCHCHO (?)			
NaCl		N ₂ H [*]		c-SiC ₃		H ₂ COH [*]		HNCHCN	MgC ₆ N	MgC ₆ H				
OH		N ₂ O		CH ₃ [*]		C ₄ H ⁻		SiH ₃ CN	CH ₂ C ₃ N	C ₂ H ₃ NH ₂	(CHOH) ₂			
PN		NaCN		C ₃ N ⁻		HC(O)CN		C ₆ S			CH ₂ (H)C ₄			
SO		OCS		PH ₃		HNCNH		MgC ₄ H						
SO [*]		SO ₂		HCNO		CH ₃ O		CH ₃ CO ⁻						
SiN		c-SiC ₂		HOCN		NH ₄ [*]		C ₃ H ₃						
SiO		CO ₂ [*]		HSCN		H ₂ NCO [*]		H ₂ C ₂ S						
SiS		NH ₂		H ₂ O ₂		NCCNH [*]		HCCCHS						
CS		H ₃ ^(*)		C ₃ H [*]		CH ₃ Cl		C ₆ O						
HF		SiCN		HMgNC		MgC ₃ N		C ₅ H [*]						
HD		AlNC		HCCO		NH ₂ OH		HCCNCH [*]						
FeO ?		SiNC		CNCN		HC ₃ O [*]		c-C ₃ C ₂ H						
O ₂		HCP		HONO		HC ₃ S [*]		HC ₄ S						
CF [*]		CCP		MgC ₂ H		H ₂ C ₂ S								
SiH ?		AlOH		HCCS		C ₄ S								
PO		H ₂ O [*]		HNCN		HC(O)SH								

>12 atoms

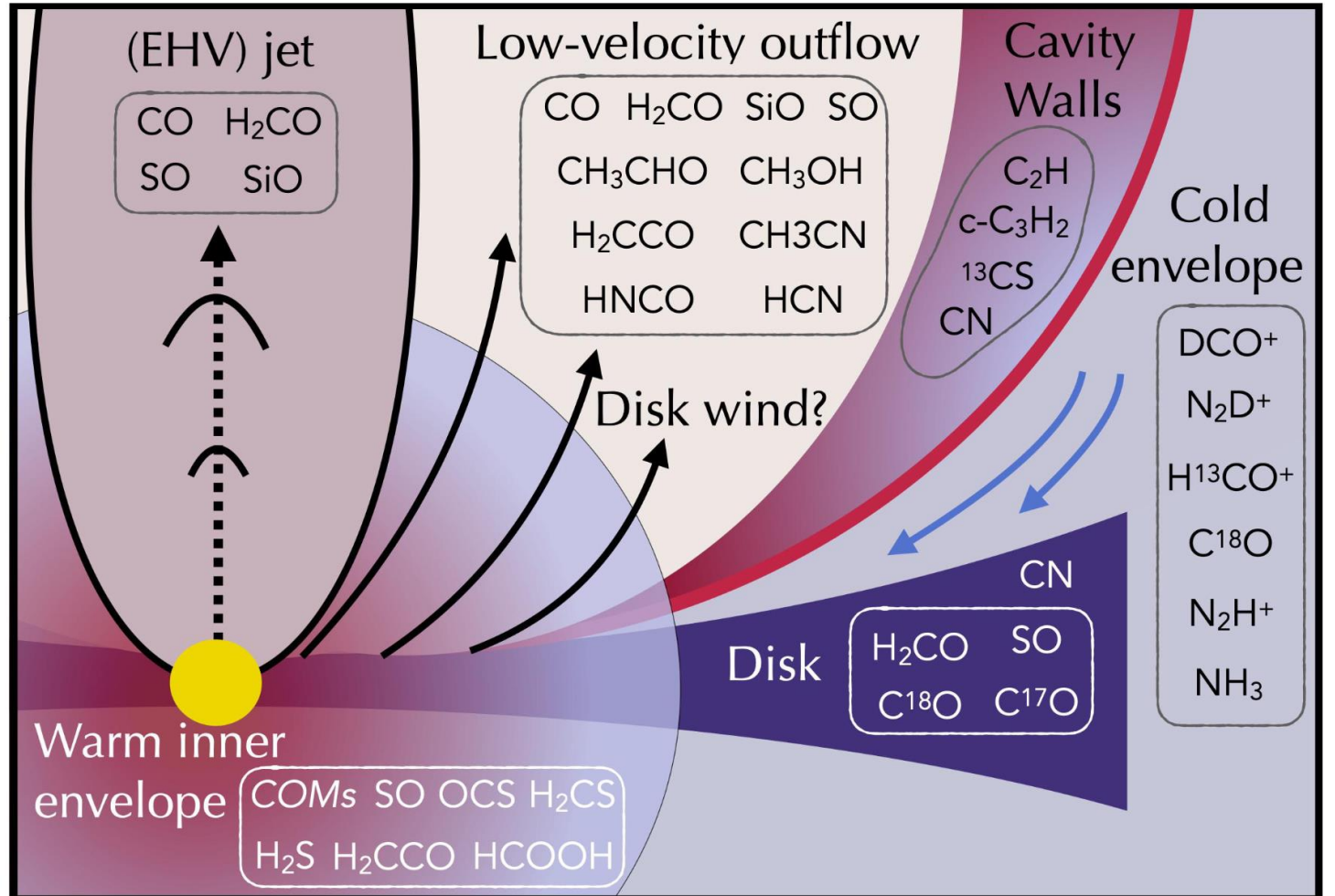
- C₆₀^{*}
- C₇₀^{*}
- C₆₀^{**}
- c-C₆H₆CN
- HC₁₁N
- 1-C₁₀H₇CN
- 2-C₁₀H₇CN
- c-C₆H₆
- 1-c-C₆H₅CCH
- 2-c-C₆H₅CCH
- c-C₃H₂CCH₂
- 2-C₆H₇CN



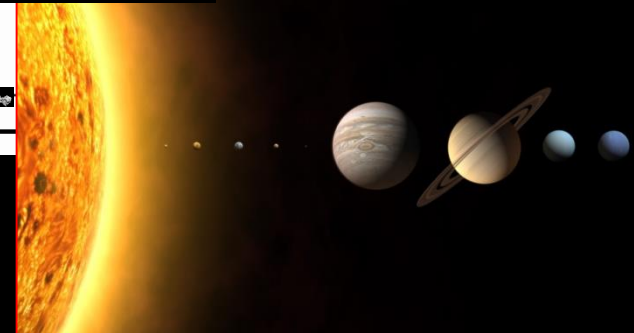
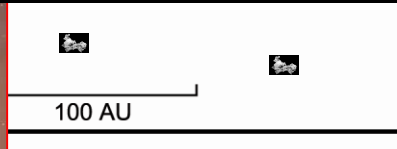
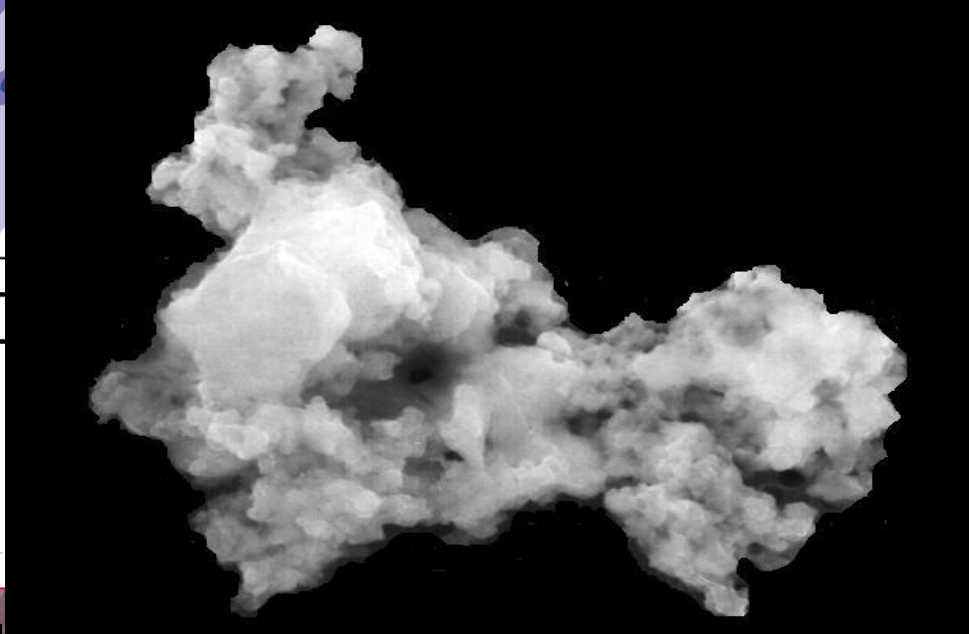
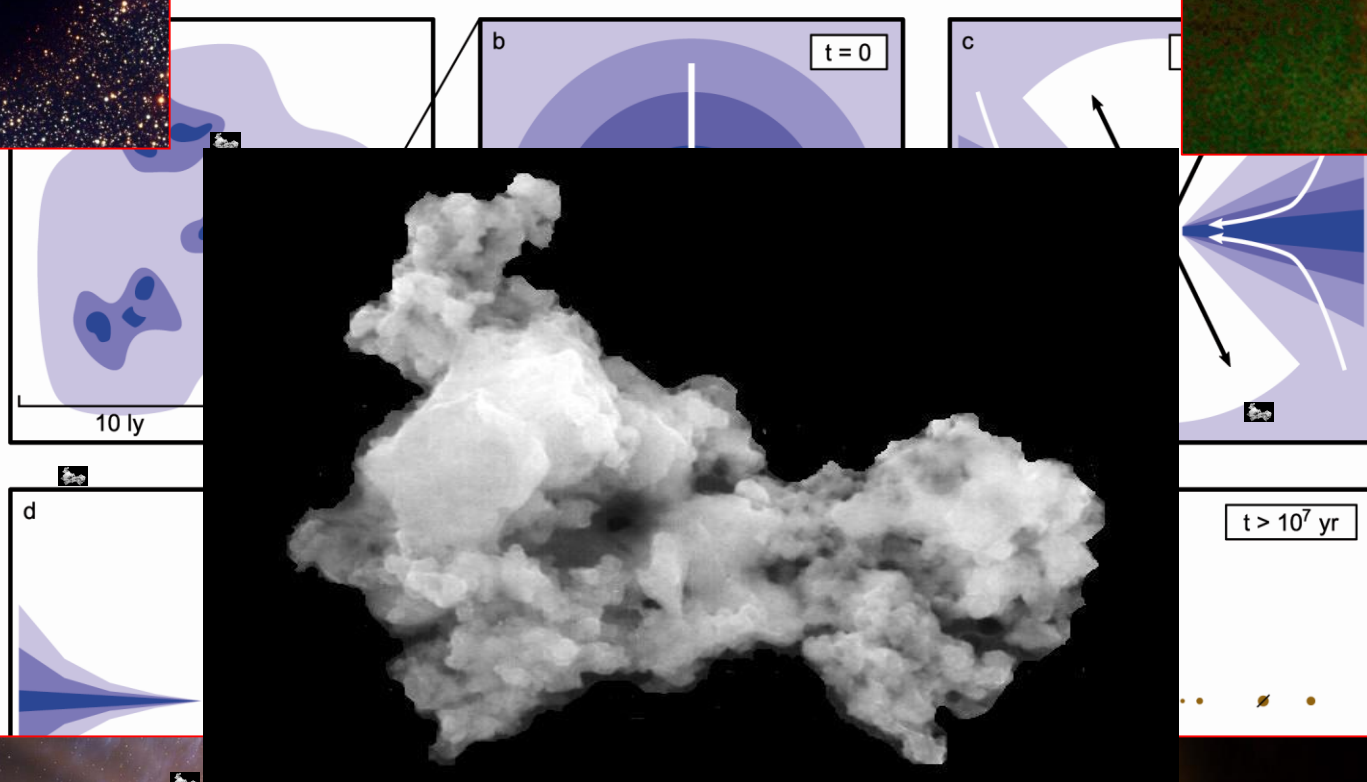
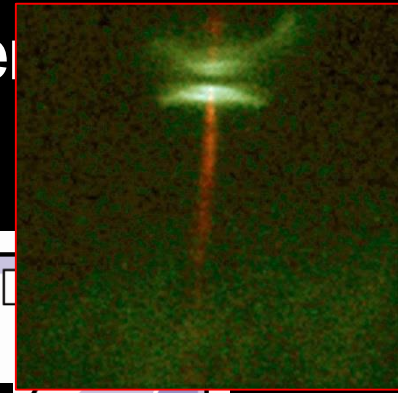
Star- and Planet Formation



Credit: Ruud Visser

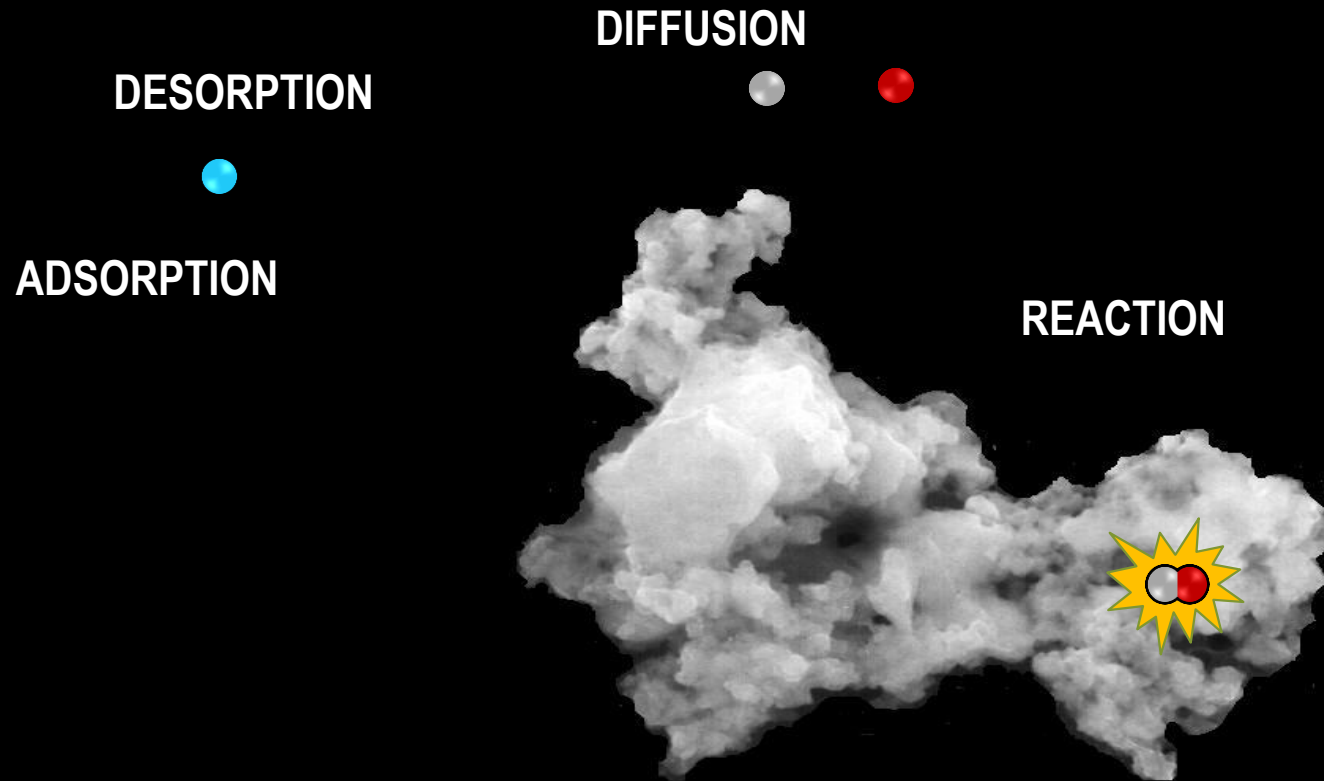


Formation and origin of a Solar-like System



Interstellar ice chemistry

Carbonaceous/Silicate Grains

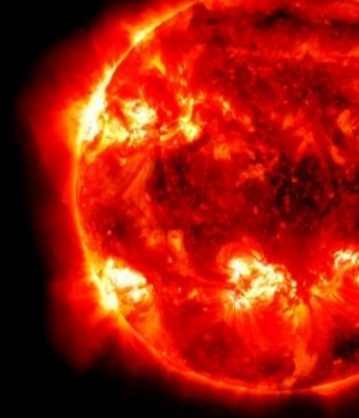


$T = 10-20 \text{ K}$
 $n > 10^2 \text{ cm}^{-3}$

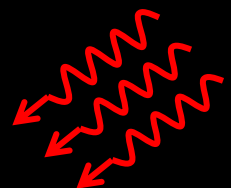
$< 1 \mu\text{m}$

Interstellar ice chemistry

Carbonaceous/Silicate Grains

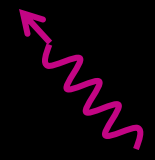
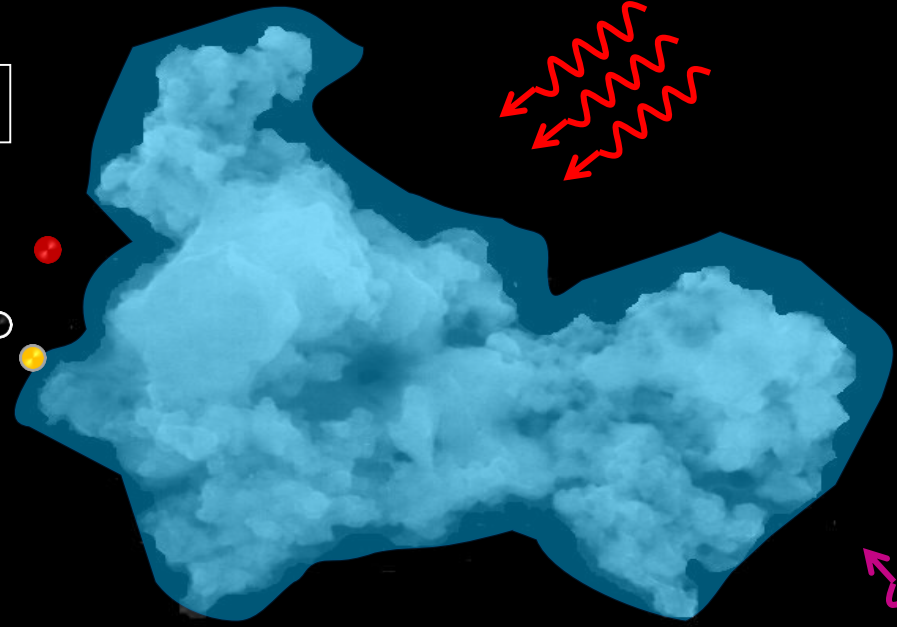
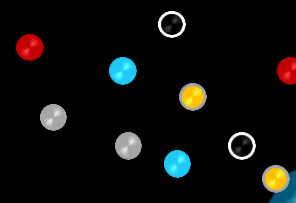


UV PHOTOLYSIS & COSMIC RAY IRRADIATION



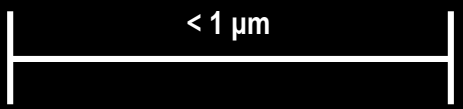
ATOM BOMBARDMENT

H, N, O,
C, S, D

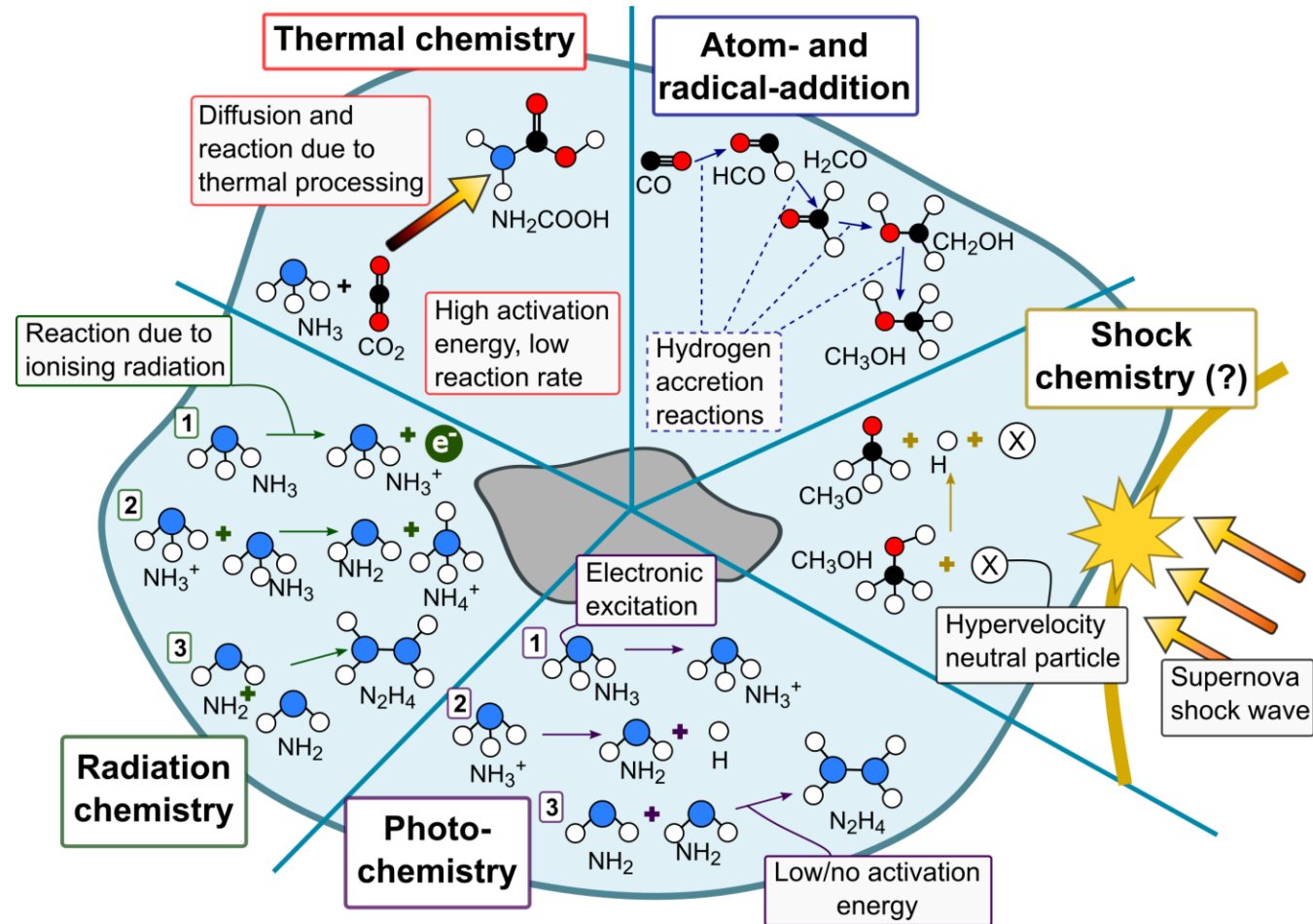


THERMAL PROCESSING

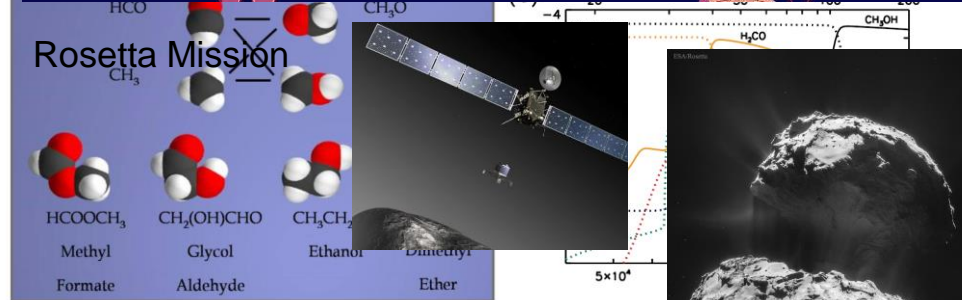
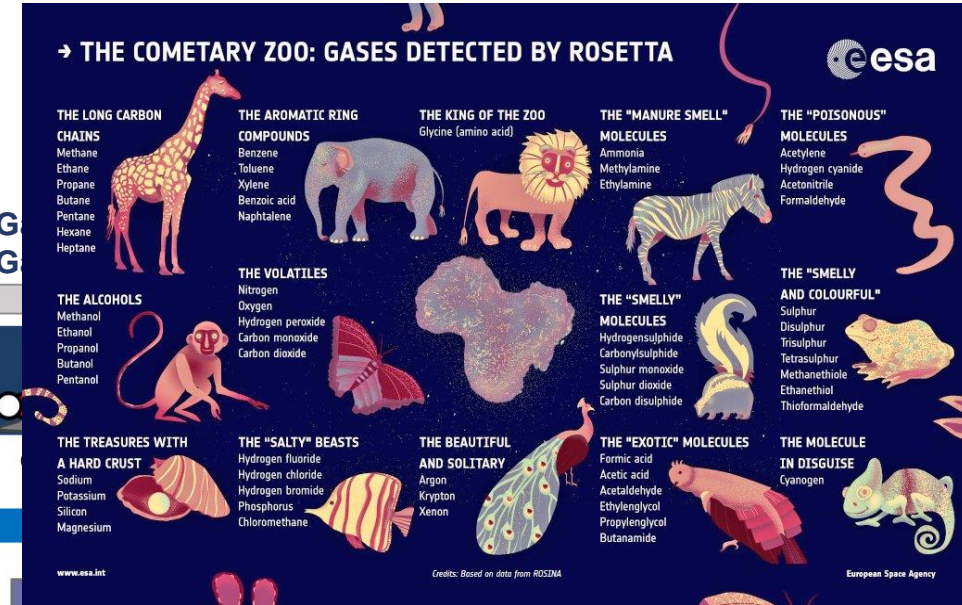
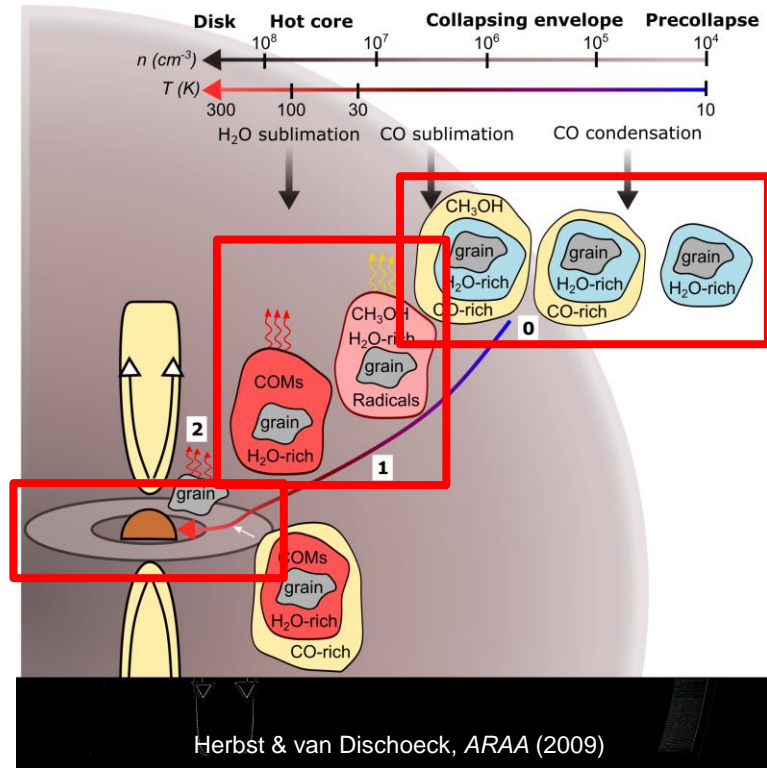
$T = 10-20 \text{ K}$
 $n > 10^2 \text{ cm}^{-3}$



Ice Grain Chemistry



Standard Picture



Comet 67P/CG

Challenges in Astrochemistry



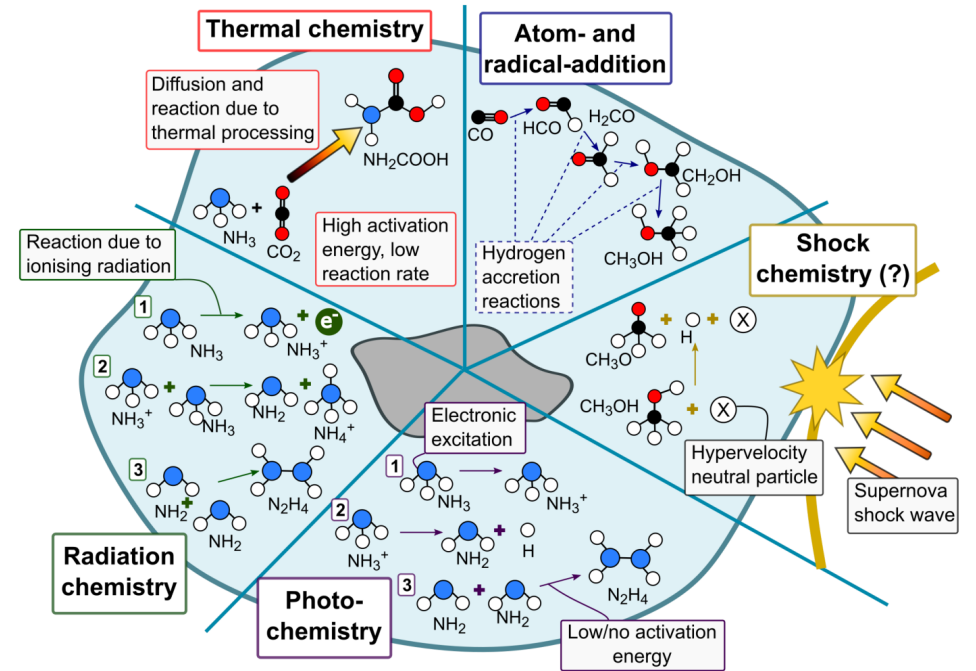
Can COMs form in ices?



Can COMs be detected in ices?

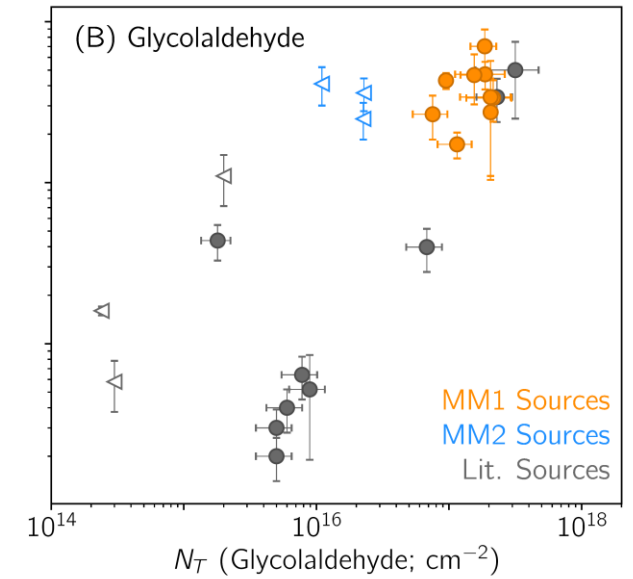
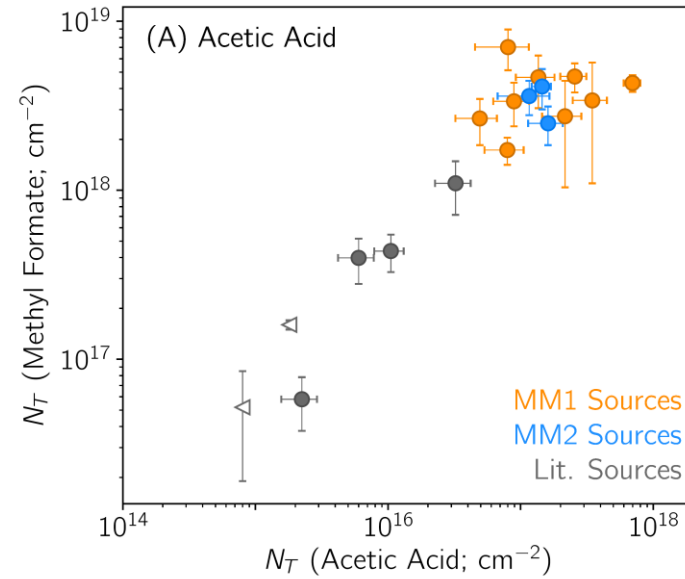
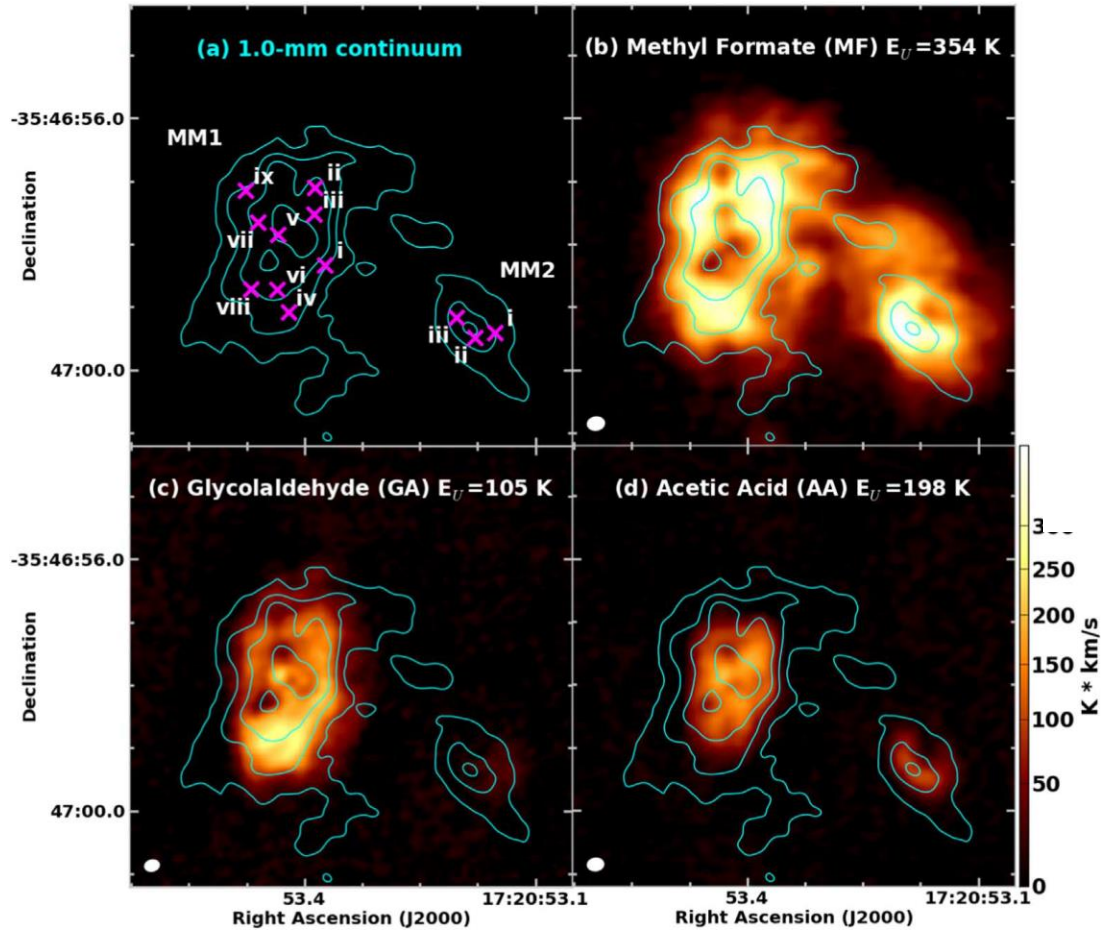
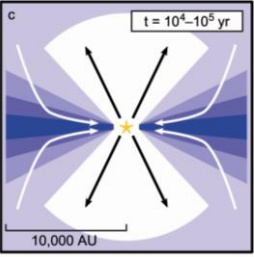


What is the physicochemical evolution of COMs in the ISM?

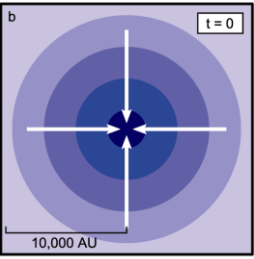


Credit: Chris R. Arumainayagam

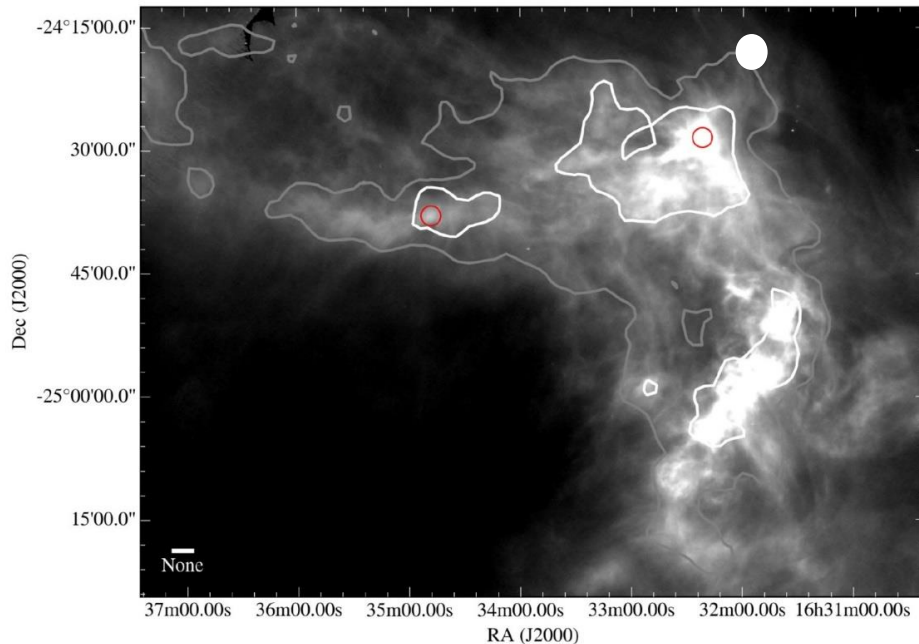
COMs in Hot Cores



COMs in Prestellar Cores



Bacmann *et al.*, A&A (2012) (L1689B)



Complex Organic Molecules in L1544 O-bearing COMS

Firm detections ($> 5 \sigma$)

methanol: CH_3OH (7) $^{13}\text{CH}_3\text{OH}$ (2) CH_2DOH

acetaldehyde: CH_3CHO (8)

formic acid: HCOOH (1)

ketene: H_2CCO (4)

propyne: CH_3CCH (6)

+ C_3O (3), HCO (4)

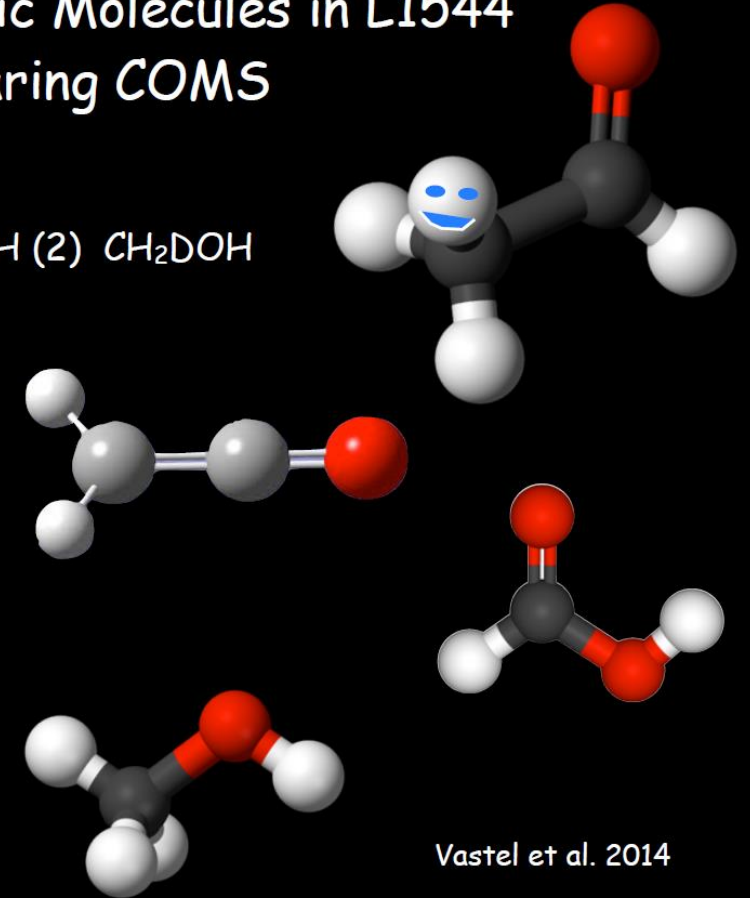
Upper Limits

Dimethyl ether: CH_3OCH_3

Methyl formate: HCOOCH_3

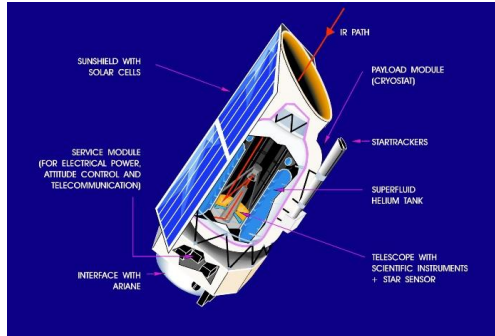
Methoxy: CH_3O

propynal: $\text{C}_3\text{H}_2\text{O}$

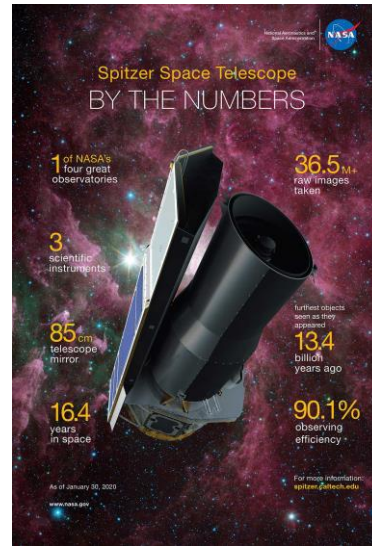


Vastel *et al.* 2014

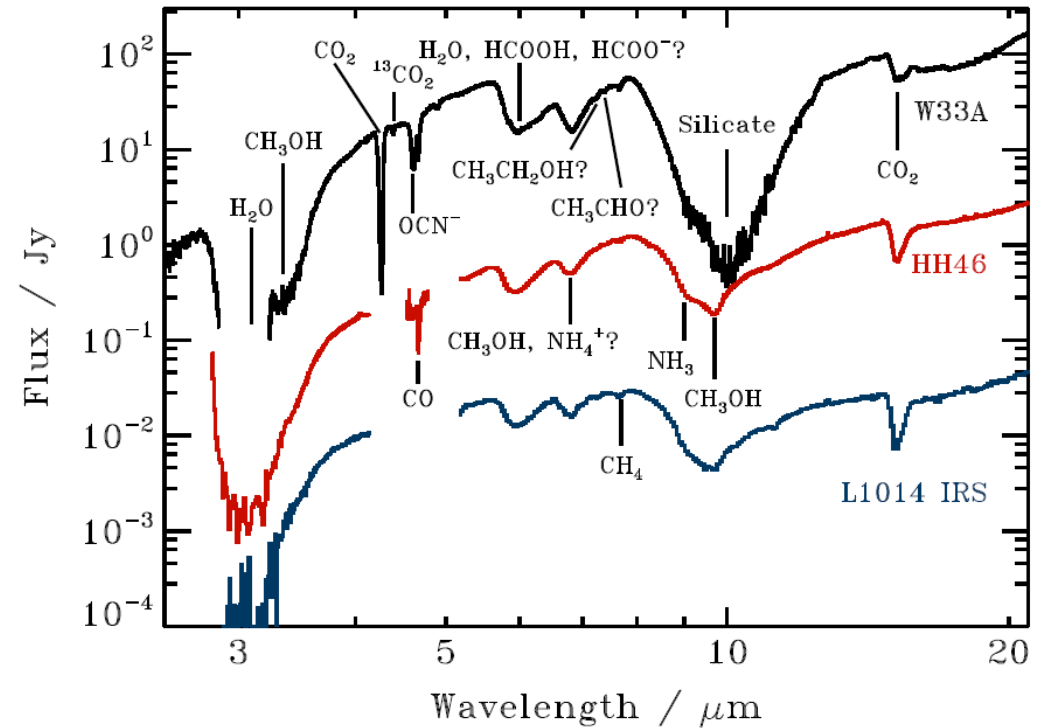
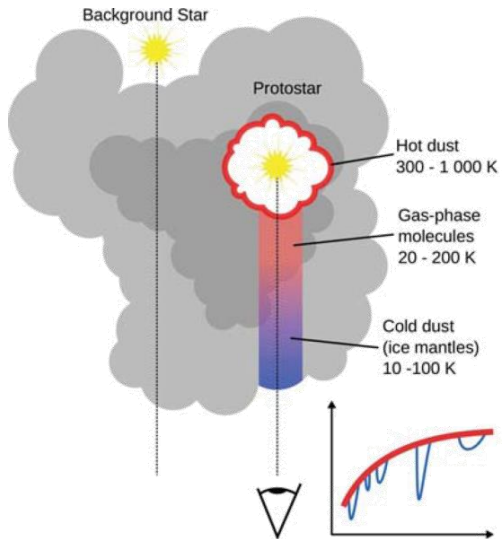
Infrared Space Observatory & Spitzer Ice Legacy



SST

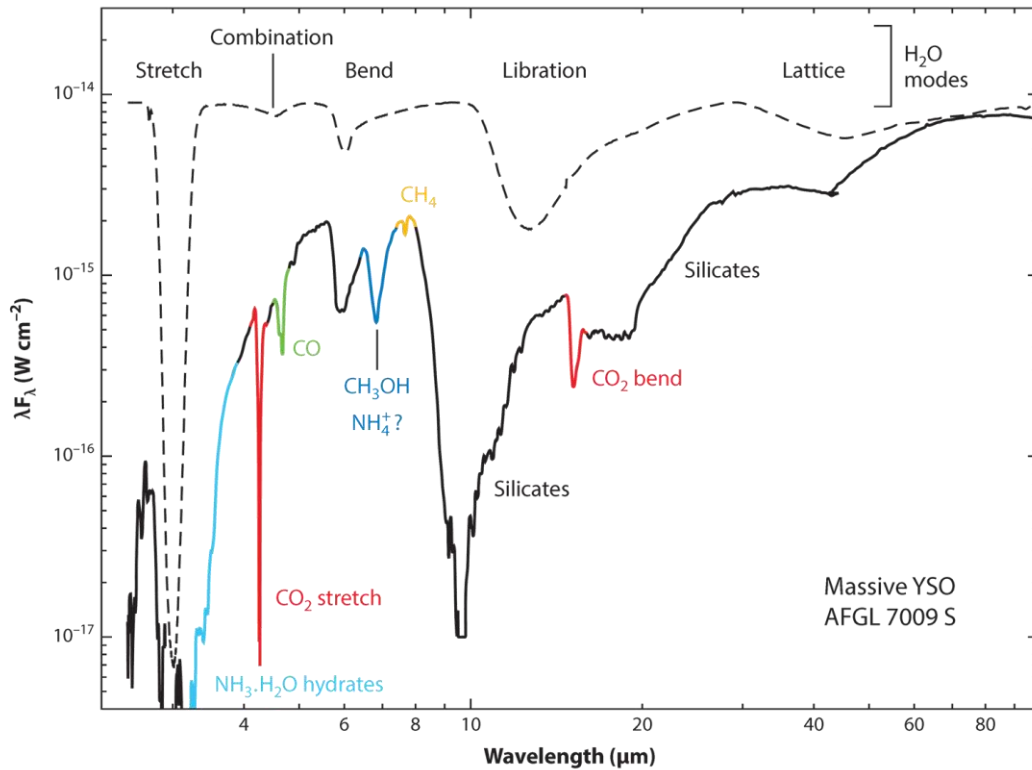


ISO

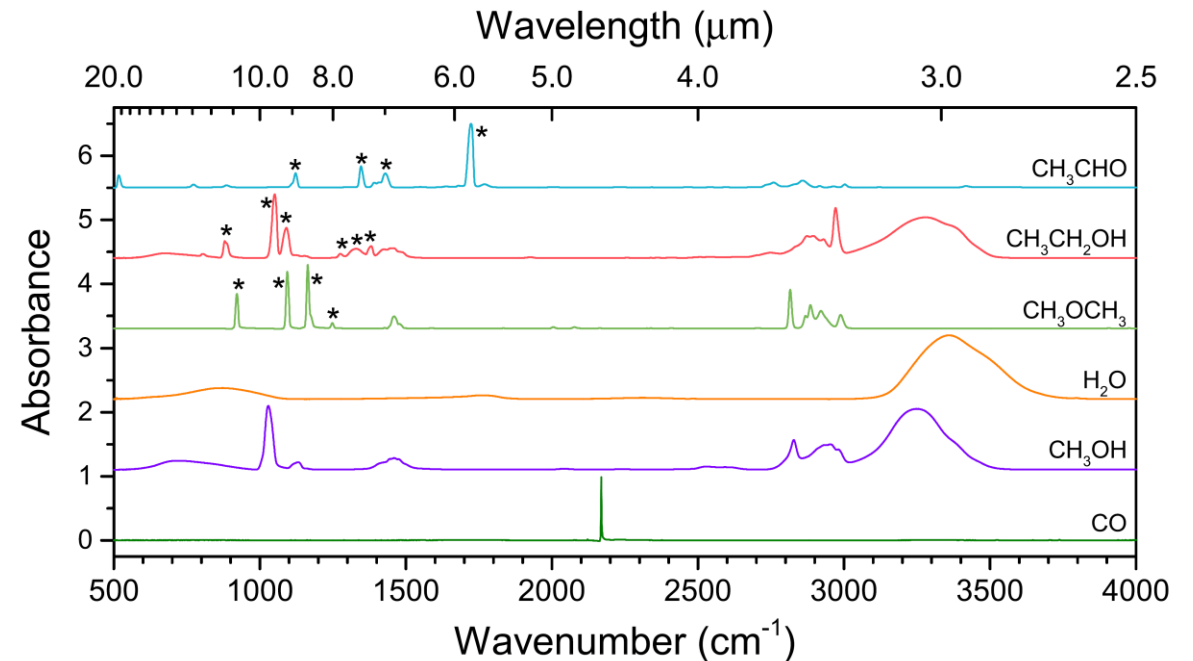
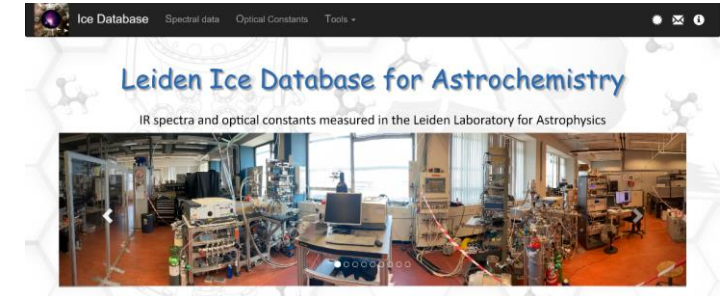


Öberg *et al.*, *ApJ* (2011)

Observations vs Laboratory

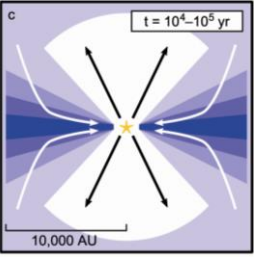


Boogert, Gerakines and Whittet, *ARAA* (2015)



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

First Ice Data from JWST



DRAFT VERSION AUGUST 24, 2022
Typeset using L^AT_EX twocolumn style in AASTeX62

CORINOS I: JWST/MIRI Spectroscopy and Imaging of a Class 0 protostar IRAS 15398–3359

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NEAL J. EVANS II,⁵ ROBIN T. GARROD,⁶ MIHWA JIN,^{7,8} CHUL HWAN KIM,⁹ JAEYEONG KIM,¹⁰ JEONG-EUN LEE,⁵
NAMI SAKAI,¹ CHRISTOPHER N. SHINGLEDECKER,¹¹ BRIELLE SHOPE,¹² JOHN J. TOBIN,¹³ AND EWINE F. VAN DISHOECK^{14,15}

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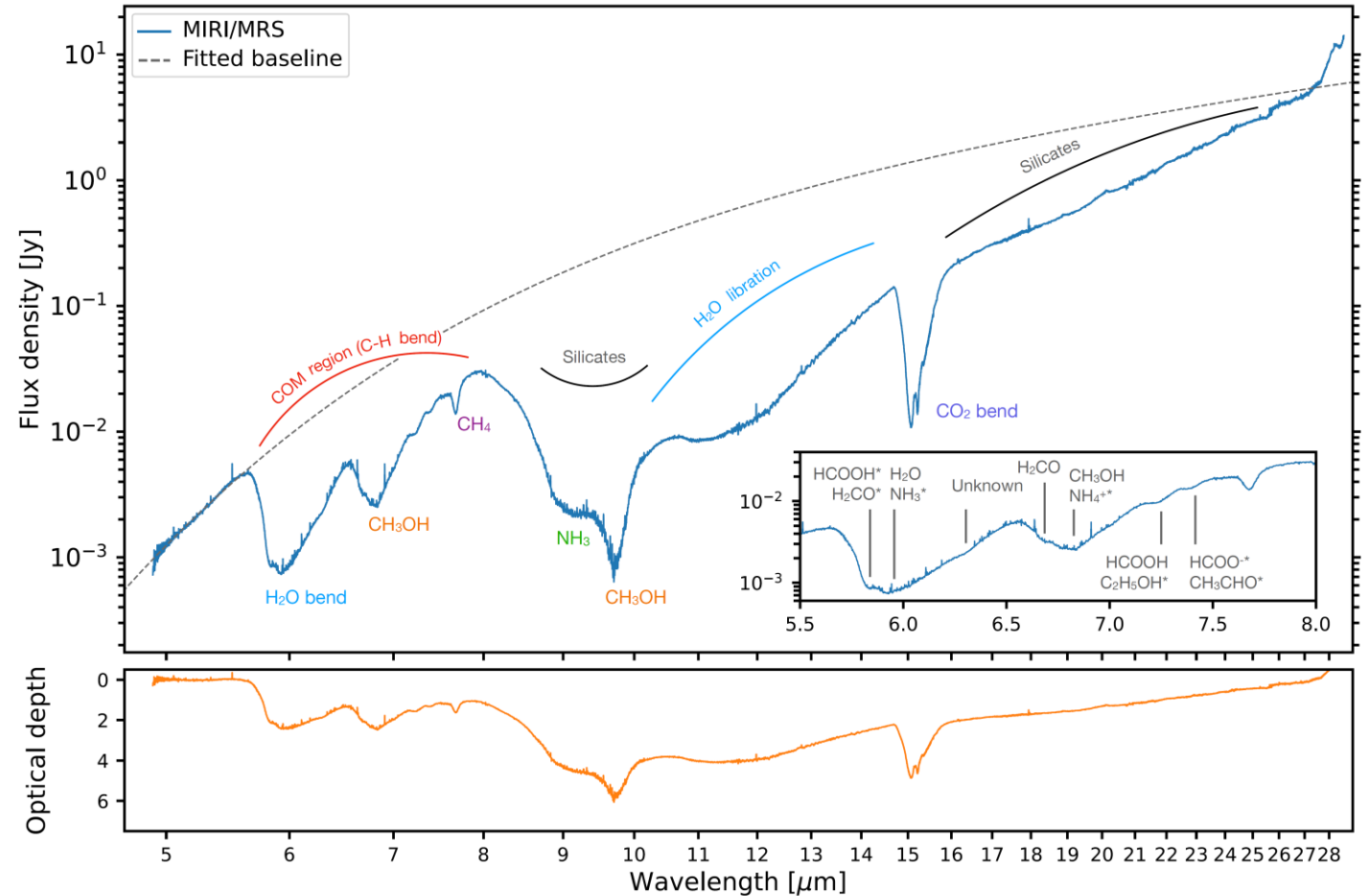
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¹⁴Leiden Observatory, Leiden University, Netherlands

¹⁵Max Planck Institute for Extraterrestrial Physics, Garching, Germany

ABSTRACT

The origin of complex organic molecules (COMs) in young Class 0 protostars has been one of the major questions in astrochemistry and star formation. While COMs are thought to form on icy dust grains via gas-grain chemistry, observational constraints on their formation pathways have been



Extracted MIRI MRS spectrum of the IRAS 1539-3359 point source.
Yang et al. ApJL (2023)

Early Release Science program on JWST



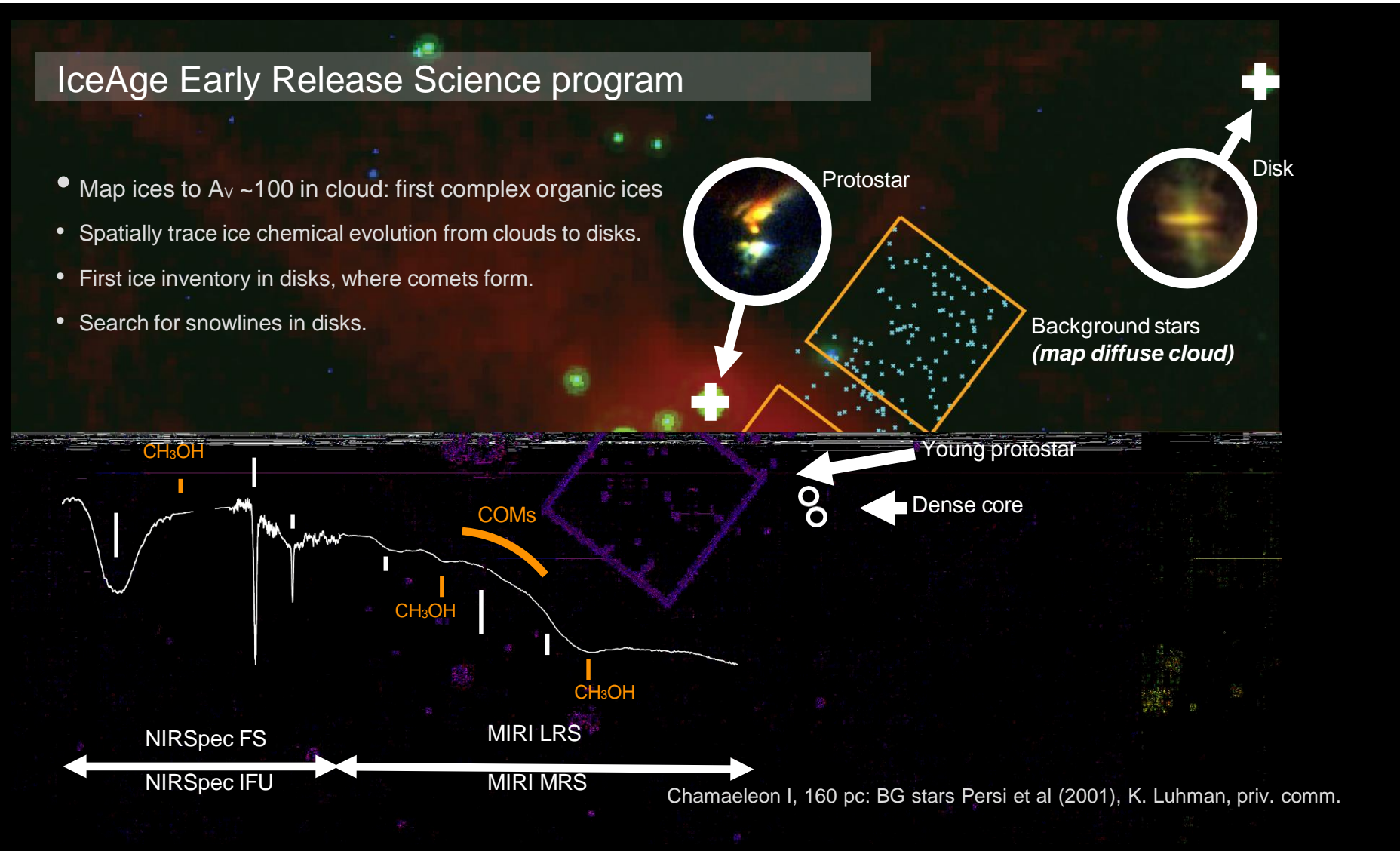
ERS: PI McClure, co-PI Boogert, co-PI Linnartz,
co-I Ioppolo + 46 co-Is

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

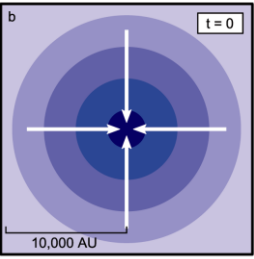
400 hours of observational time in first
year to study cosmic ices

IceAge Early Release Science program

- Map ices to $A_V \sim 100$ in cloud: first complex organic ices
- Spatially trace ice chemical evolution from clouds to disks.
- First ice inventory in disks, where comets form.
- Search for snowlines in disks.



IceAge - Dense Cores



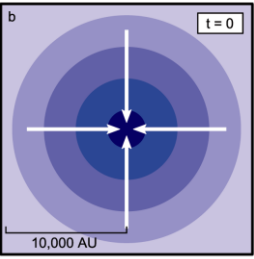
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400 hours of observational time in first
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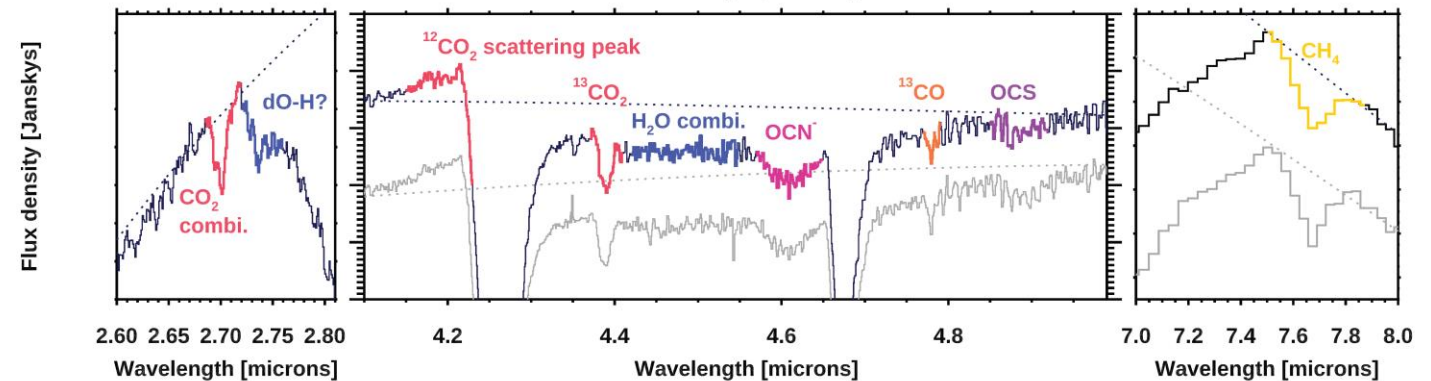
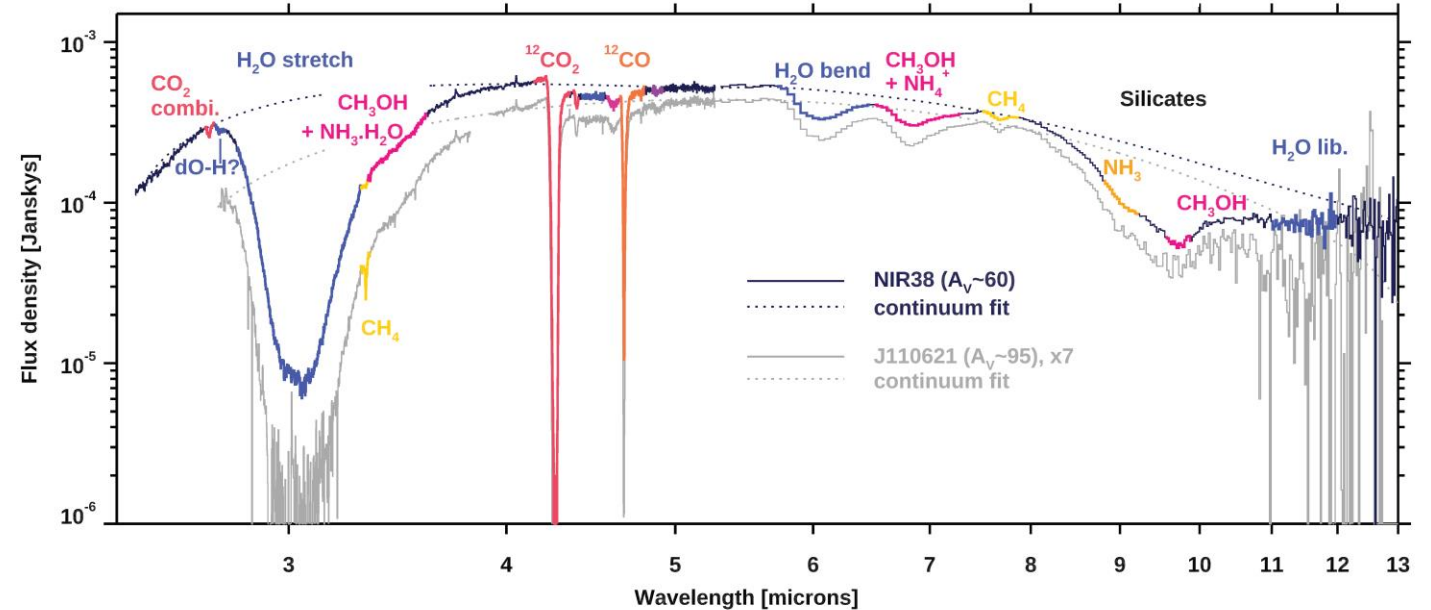
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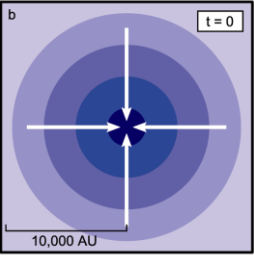
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400 hours of observational time in first
year to study cosmic ices

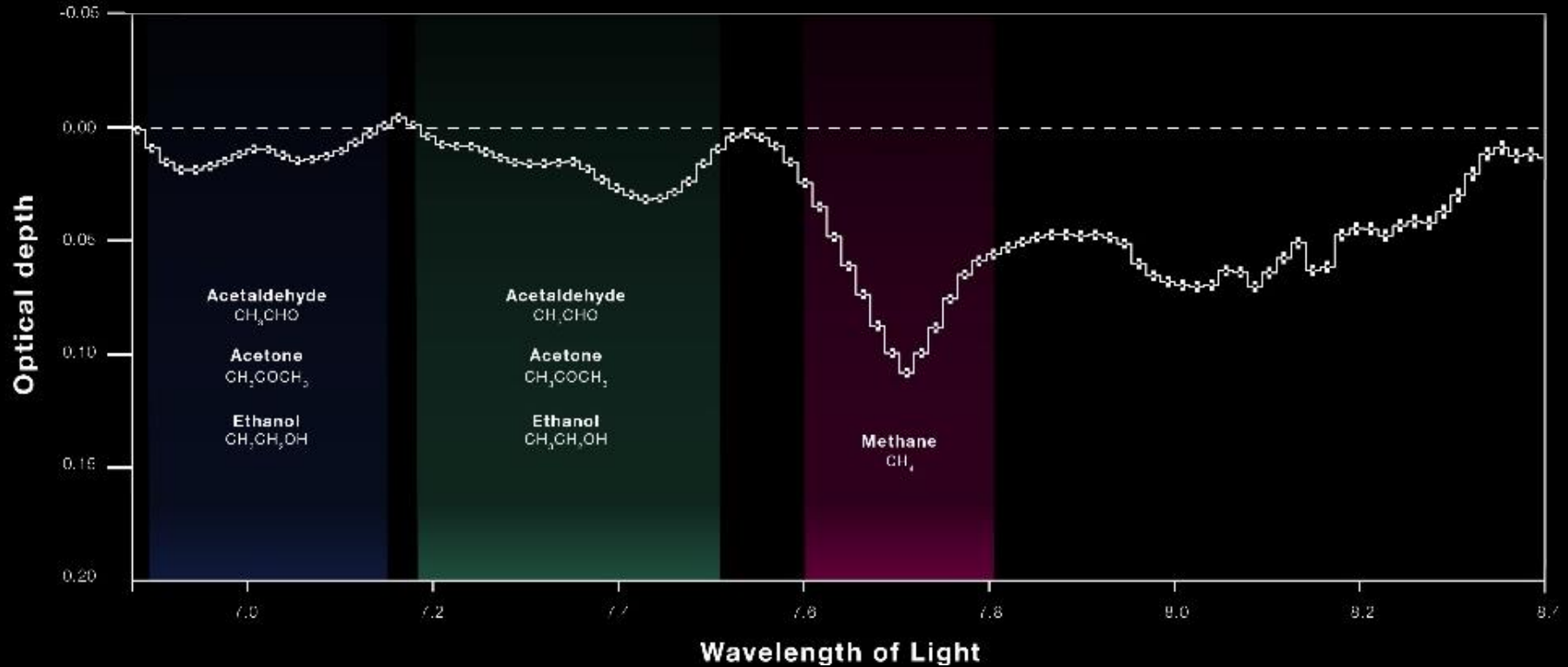


McClure et al. *Nat. Astron.* (2023)

IceAge - Dense Cores



CHAMAELEON I DARK CLOUD BACKGROUND STAR NIR38 ICE CHEMICAL COMPOSITION



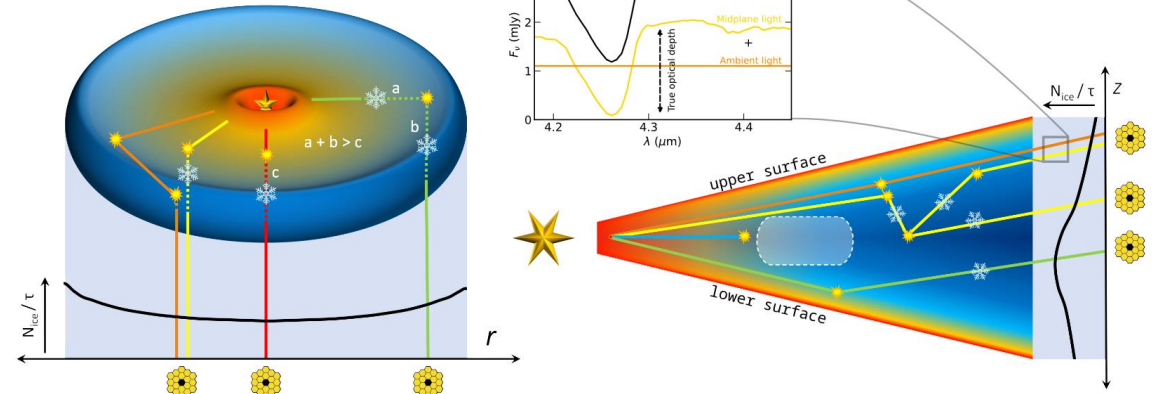
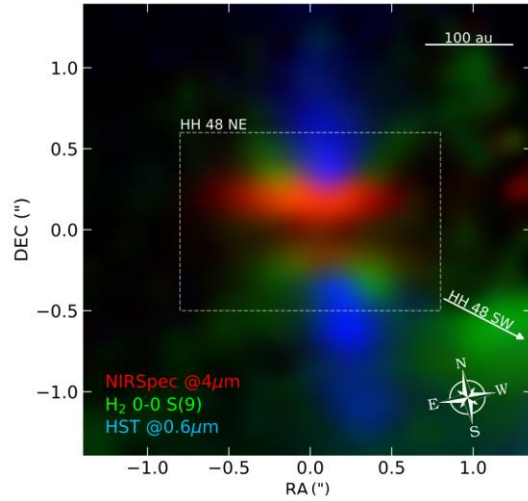
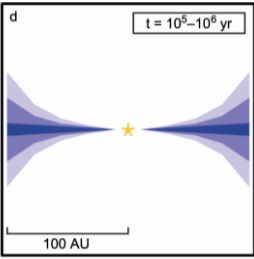
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Cycle 1: PI McClure, co-I Ioppolo + 25 co-Is

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

McClure *et al.* (2023)

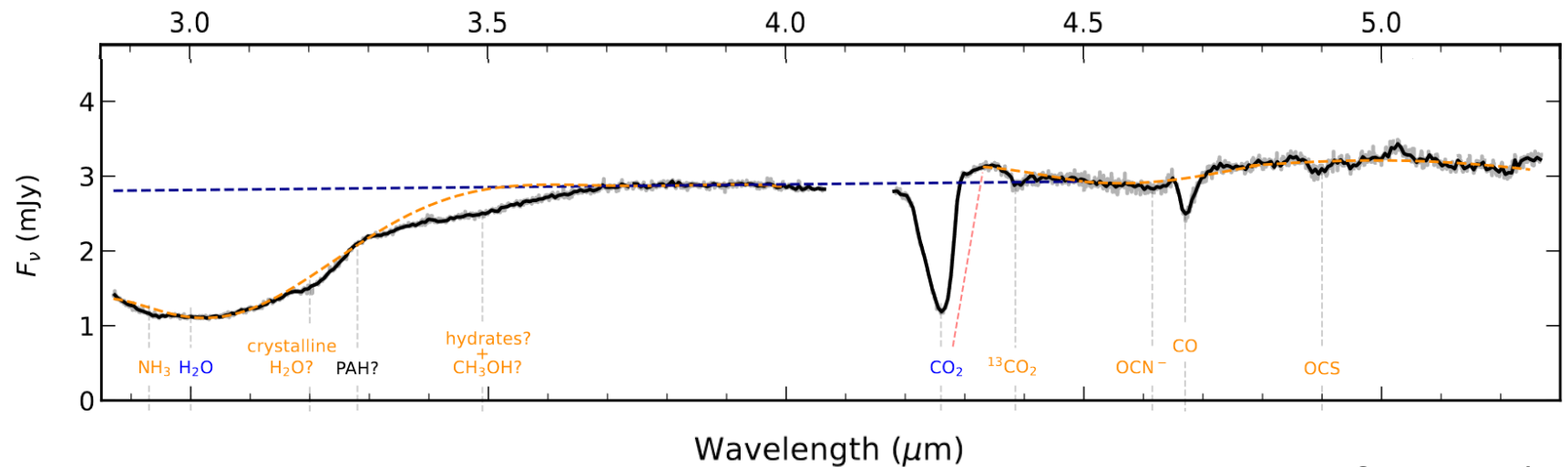
IceAge - Disk



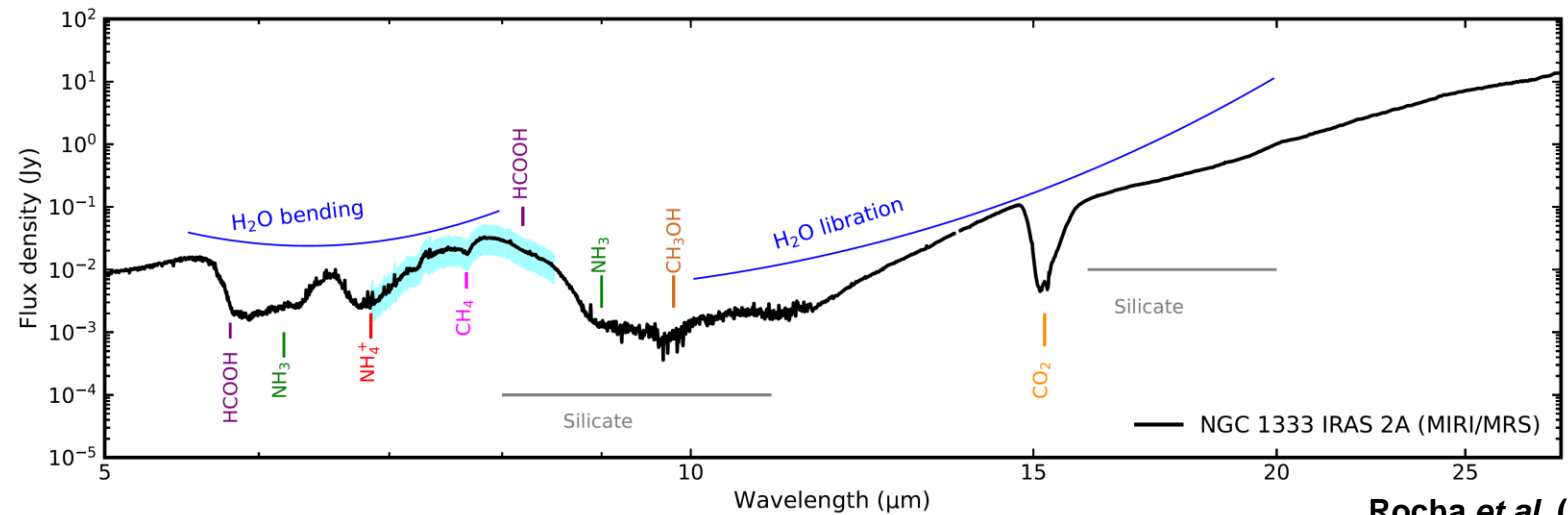
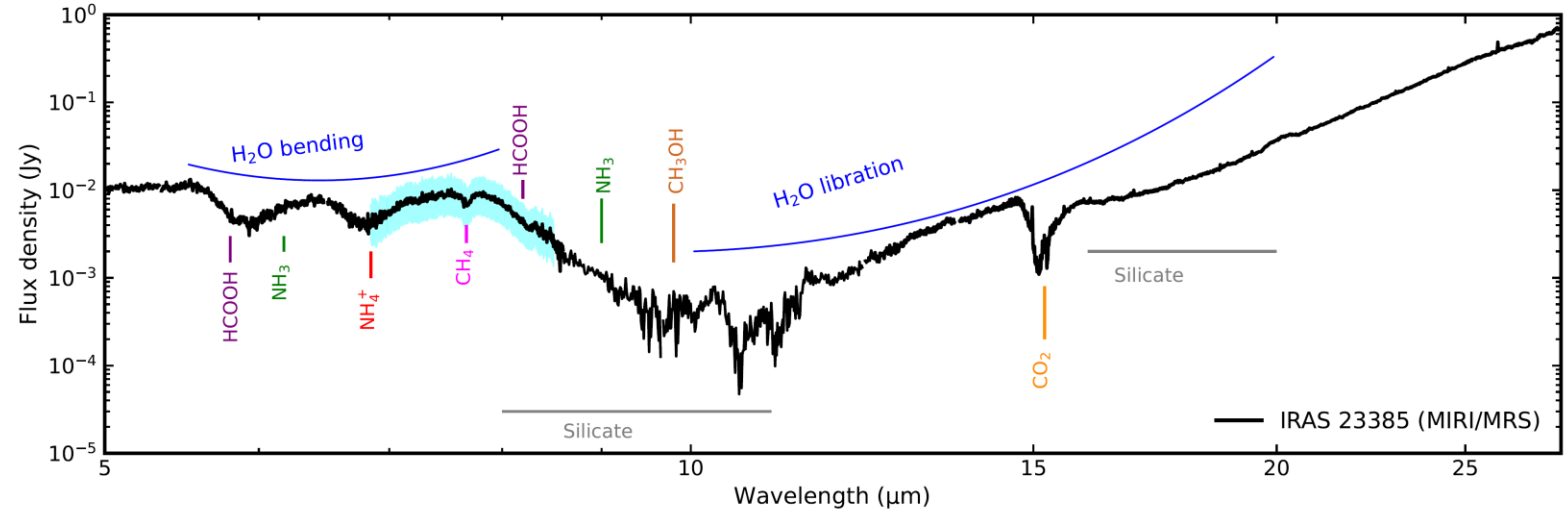
ERS: PI McClure, co-PI Boogert, co-PI Linnartz,
co-I Ioppolo + 46 co-Is

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

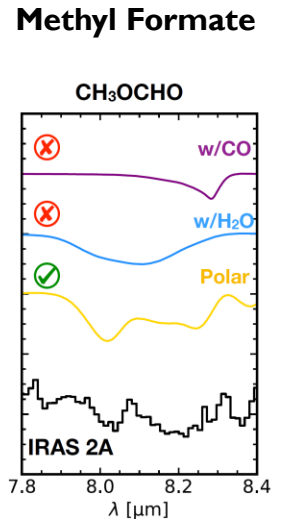
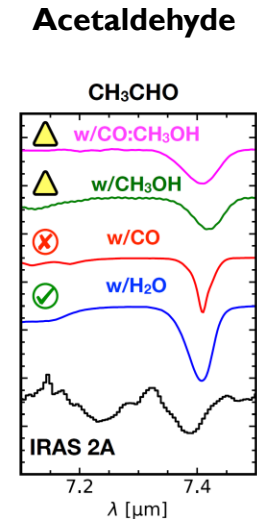
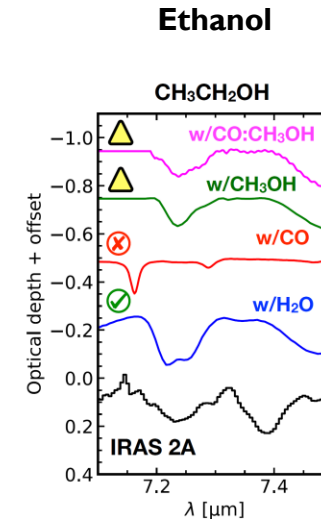
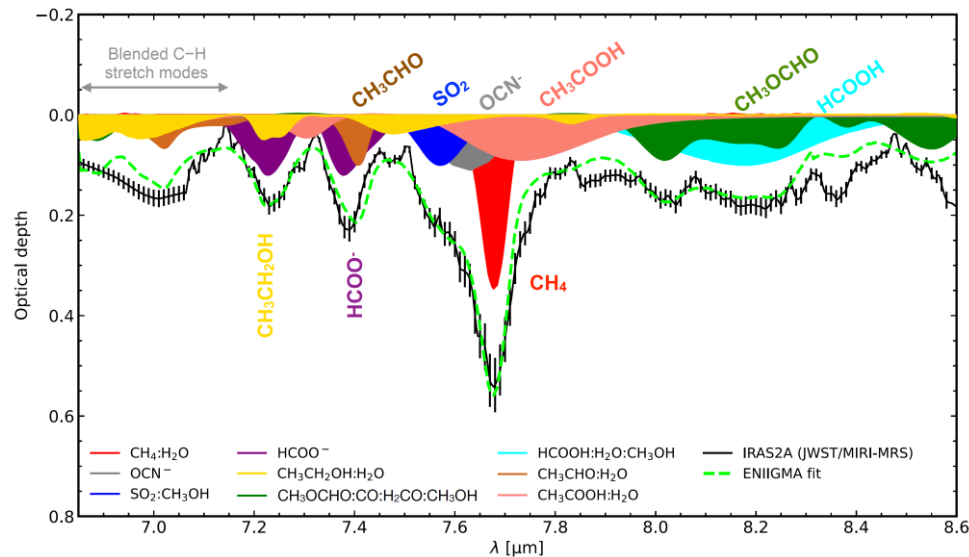
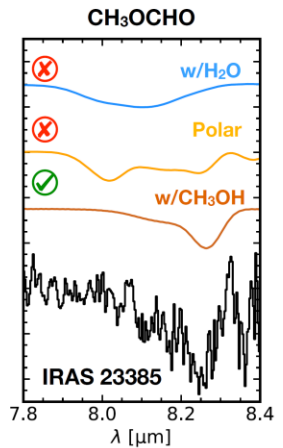
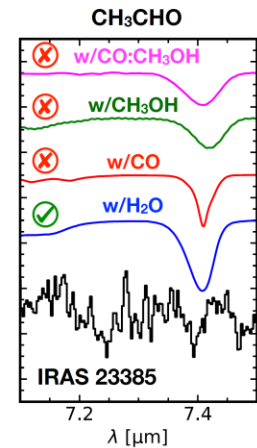
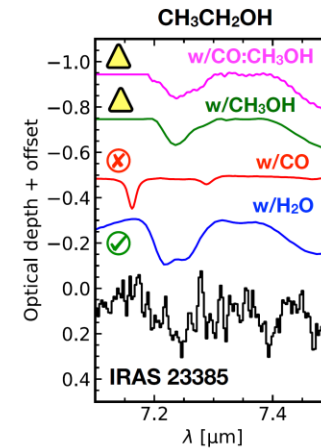
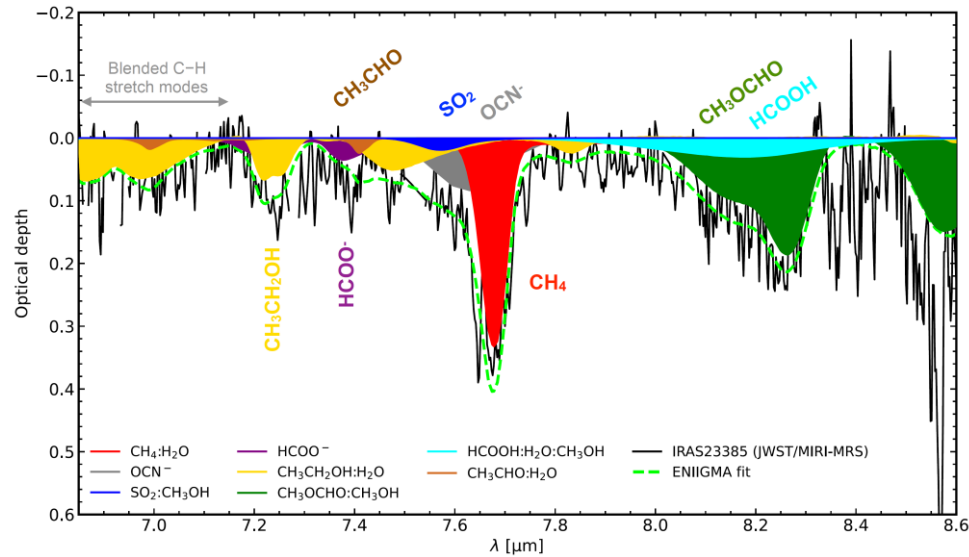
400 hours of observational time in first
year to study cosmic ices



Jwst Observations of Young protoStars (JOYS)



Jwst Observations of Young protoStars (JOYS)



Challenges in Astrochemistry



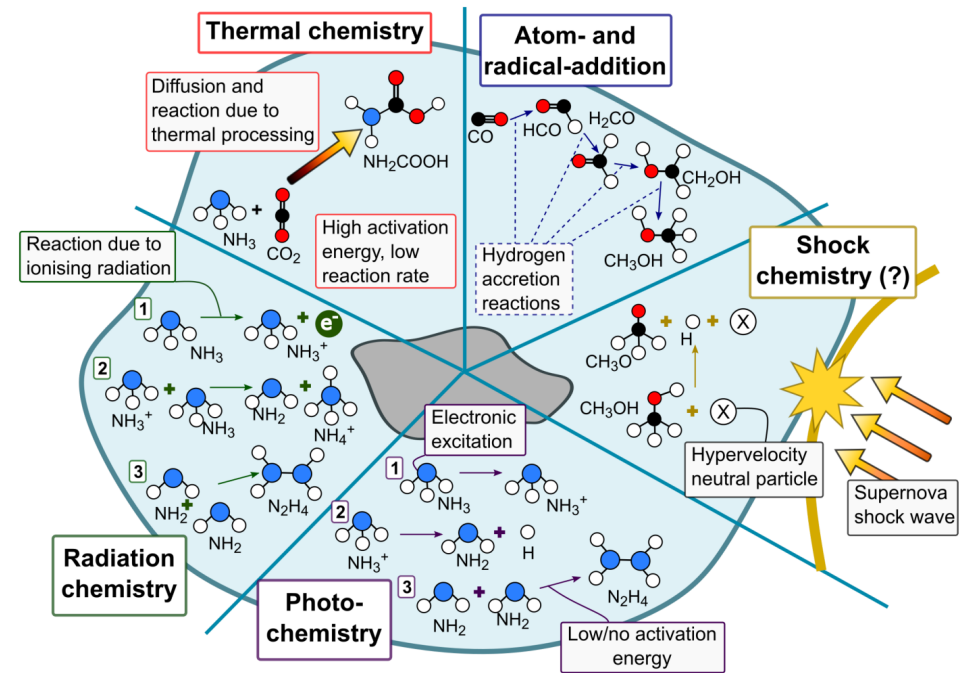
COMs form in ices



COMs are detected in ices



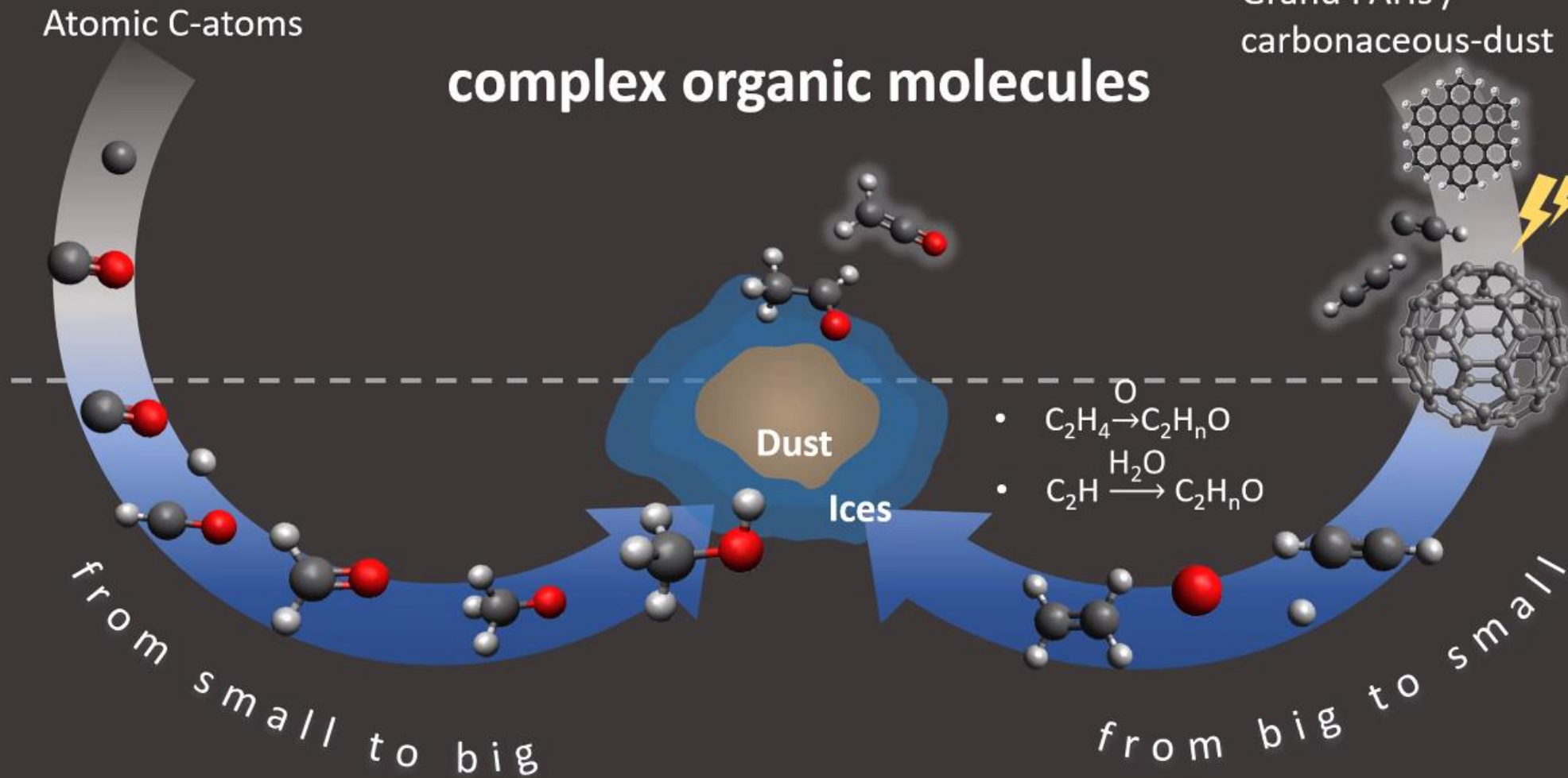
What is the physicochemical evolution of COMs in the ISM?



Credit: Chris R. Arumainayagam

Bottom-up route

Top-down route



Jäger et al. 2011; Alata et al. 2014; Zhen et al. 2014;
Maté et al. 2016; Dartois et al. 2017; West et al. 2018

Tielens 1992; Bennett et al. 2005; Ward &
Price 2011; Bergner et al. 2019
Perrero, Enrique Romero et al. 2022

SURFRESIDE TEAM

Leiden University



Prof. Harold Linnartz
(1965 - 2023)



Dr. Ioppolo



Dr. Fedoseev



Dr. Lamberts



Dr. Chuang



Dr. Qasim



Ms. Santos

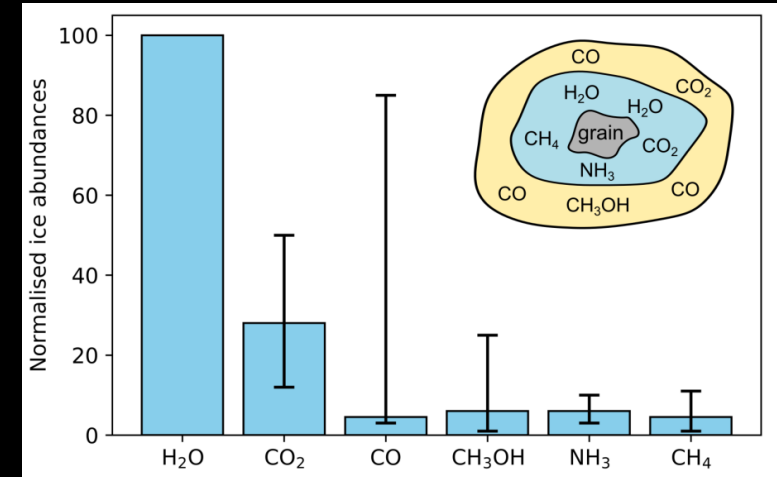
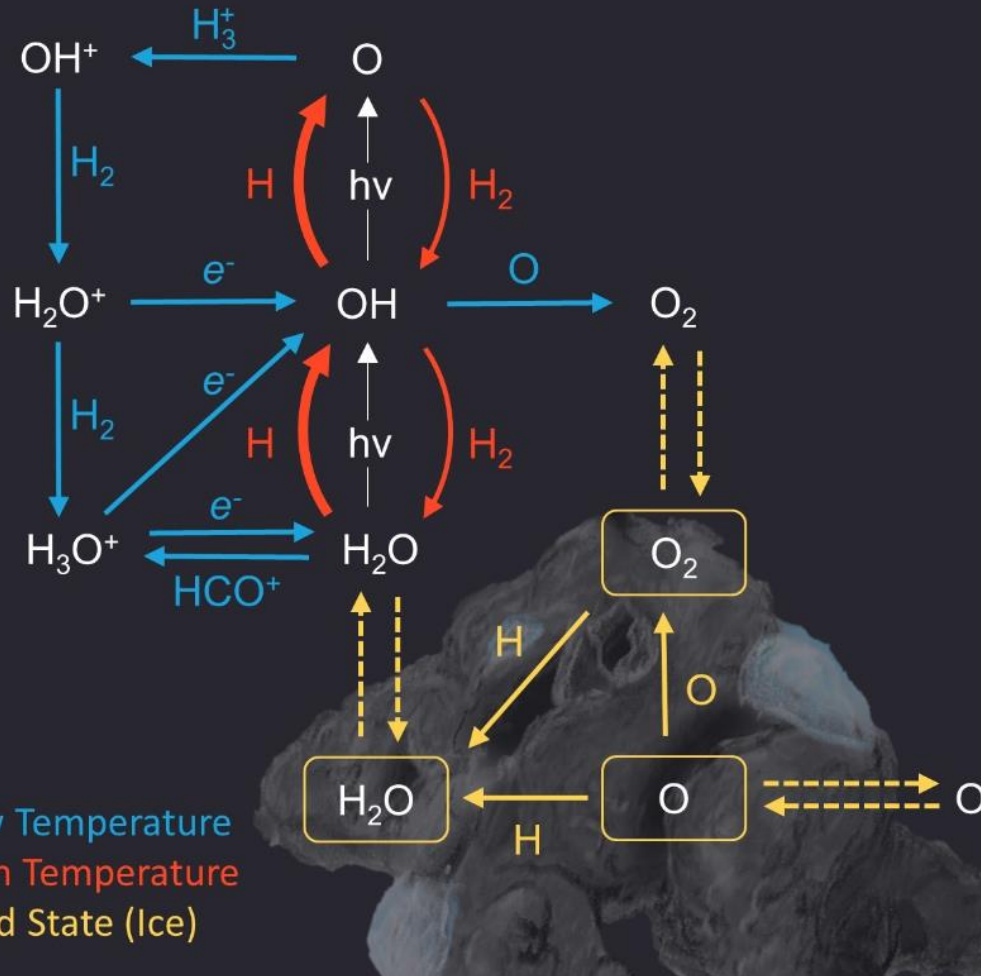


Prof. Ewine van Dishoeck



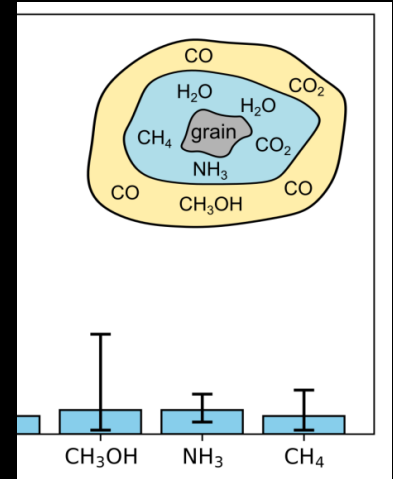
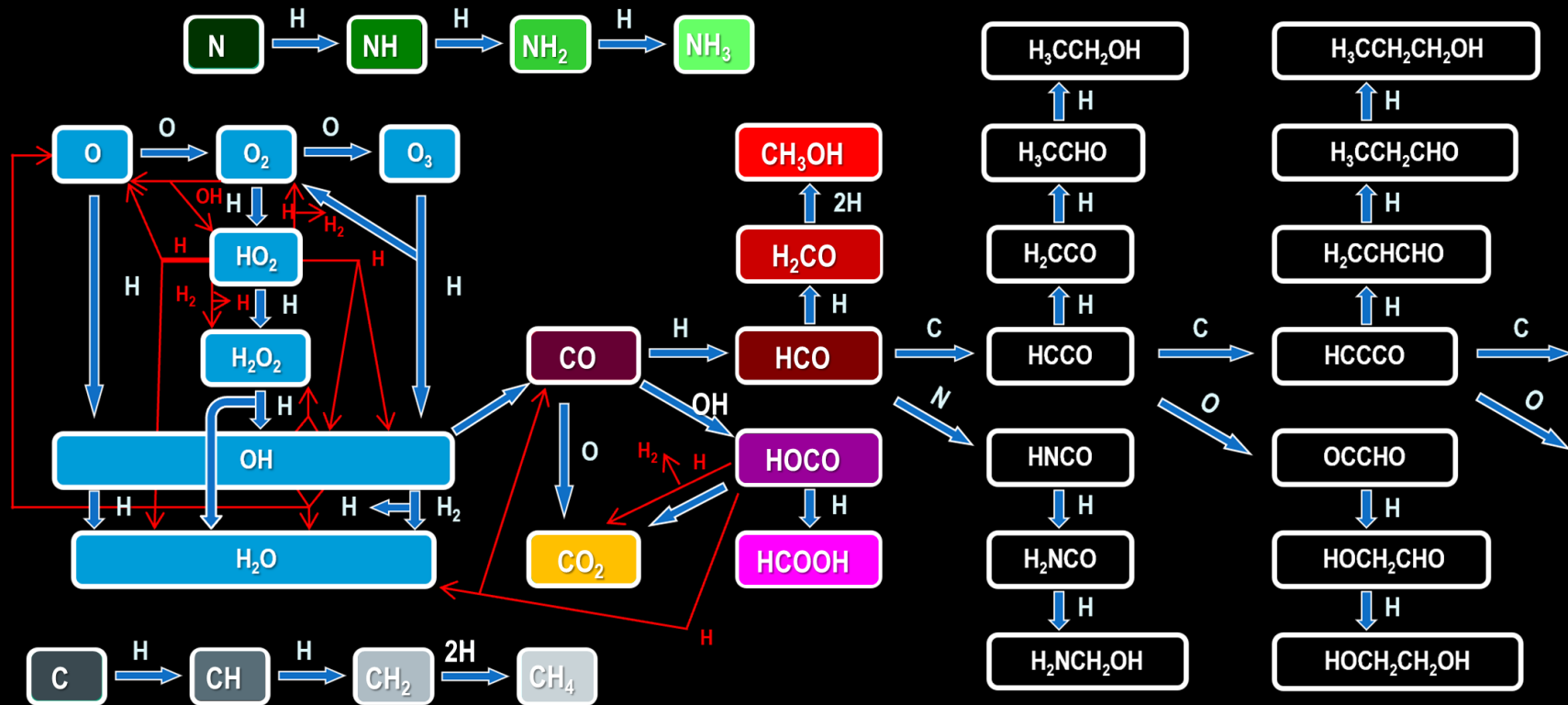
Prof. Herma Cuppen

Molecules form via Dark Chemistry



Öberg, Chem. Rev. (2016)

Molecules form via Dark Chemistry



erg, Chem. Rev. (2016)

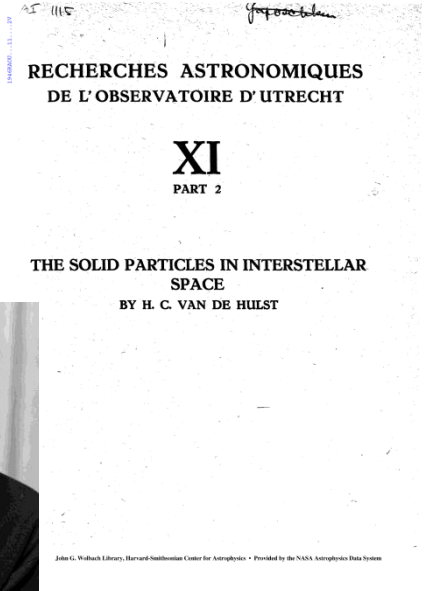
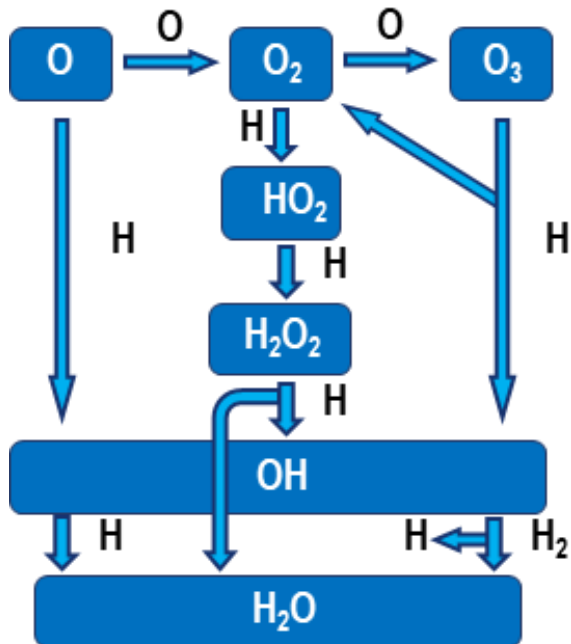
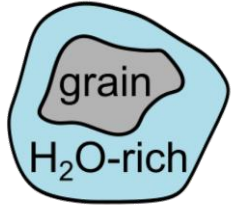


Linnartz, Ioppolo & Fedoseev, *IRPC* (2015)

Ioppolo *et al.*, *MNRAS* (2011b)
Chamley *et al.*, *A&A* (2001)
Fedoseev *et al.*, *MNRAS* (2015)

Qasim *et al.*, *Nature Astron.* (2020)

Water forms via Dark Chemistry



van de Hulst, RAOU (1946)

ASTRONOMY AND ASTROPHYSICS
Model Calculations of the Molecular Composition of Interstellar Grain Mantles
A. G. G. M. Tielens* and W. Hagen**
Laboratory Astrophysics Group, Rijksuniversiteit, 3300 RA Leiden, The Netherlands
Received February 1, accepted May 19, 1982

Summary. The chemical composition of mantles accreting on interstellar grains has been calculated numerically with a chemical reaction scheme which comprises gas phase as well as grain surface reactions. The equilibrium abundances of the molecules in the gas are calculated using gas phase reactions except for H_2 formation. The composition of the growing grain mantle is determined on the basis of the relative accretion rates of the gas phase molecules and diffusion controlled surface reactions of the molecules on the grain surface. The results show that in most circumstances grain mantles consist of the molecules H_2O , H_2CO , SiO , CO , CS , C_2H_2 , H_2C_2 , and NH_3 . The relative concentrations of these species depend strongly on the physical conditions in the gas. The formation of H_2 on grain surfaces is examined in detail. We conclude that it proceeds through hydrogen abstraction from molecules like H_2CO , H_2N , N_2H , and N_2H_2 . In some cases these molecules act as radical trapping sites for H atoms.

Introduction. The first detection of interstellar extinction provided definite evidence for the existence of interstellar dust (Trompeter, 1930), and the composition of the grains has been a very uncertain quantity since the proposed grain materials are a "dirty ice" mixture, water and silicates (see de Haan, 1959; Cassinelli and Schumann, 1964; Hayakawa and Wickramasinghe, 1962; Karijis, 1963). The dust (the fine solid fraction of a solid mixture) of CaF_2 , $CaCl_2$, NH_4Cl , H_2O with embedded impurities containing other elements all properties to their elemental abundances (van de Hulst, 1946), an alternative answer to A. G. G. M. Tielens. Present address: NASA Ames Research Center, M.S. 245-6, Moffett Field, CA 94035, USA. ** Present address: Koninklijke Shell Laboratorium, Amsterdam, The Netherlands.

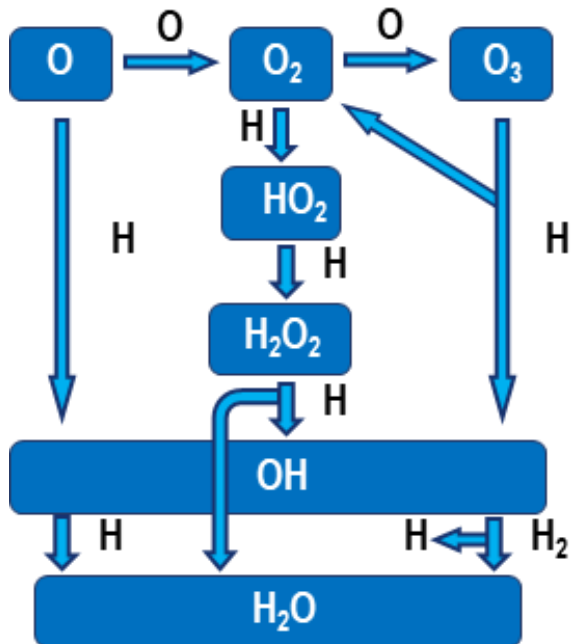
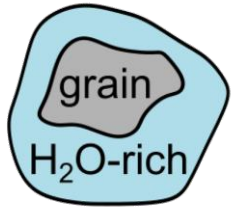


Tielens & Hagen, A&A (1982)

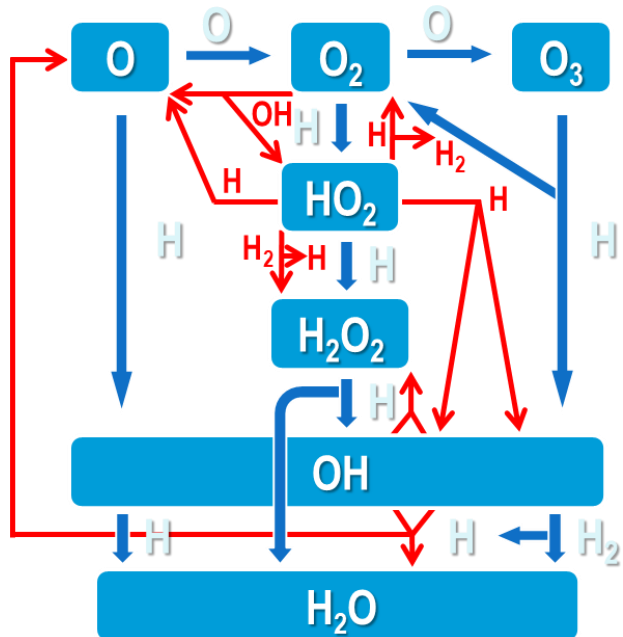
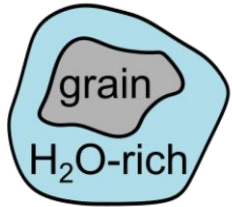


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Water forms via Dark Chemistry



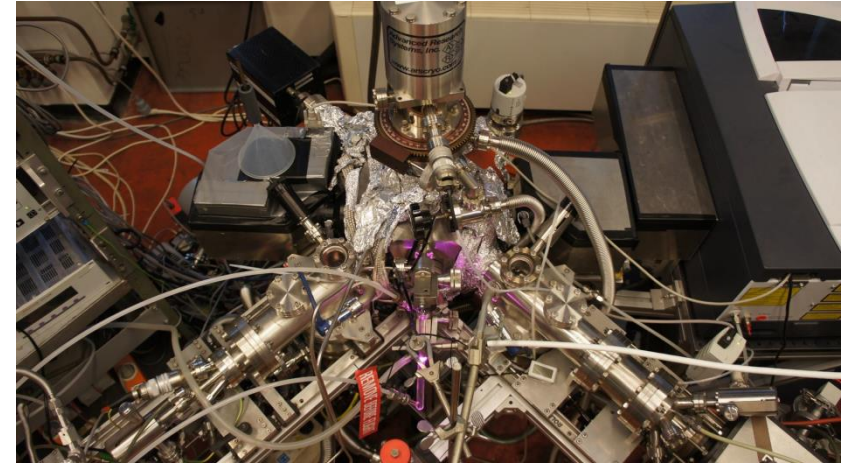
Water forms via Dark Chemistry



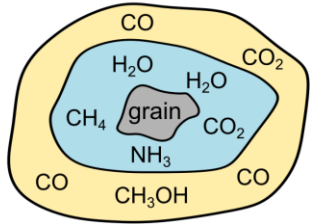
Dulieu et al. 2010; Jing et al. 2011

Miyauchi et al. 2008; Ioppolo et al. 2008, 2010; Matar et al. 2008; Oba et al. 2009, 2012, 2014; Cuppen et al. 2010; Chaabouni et al. 2012; Lamberts et al. 2013, 2014a; 2014b; 2015; 2016

Mokrane et al. 2009; Romanzin et al. 2011



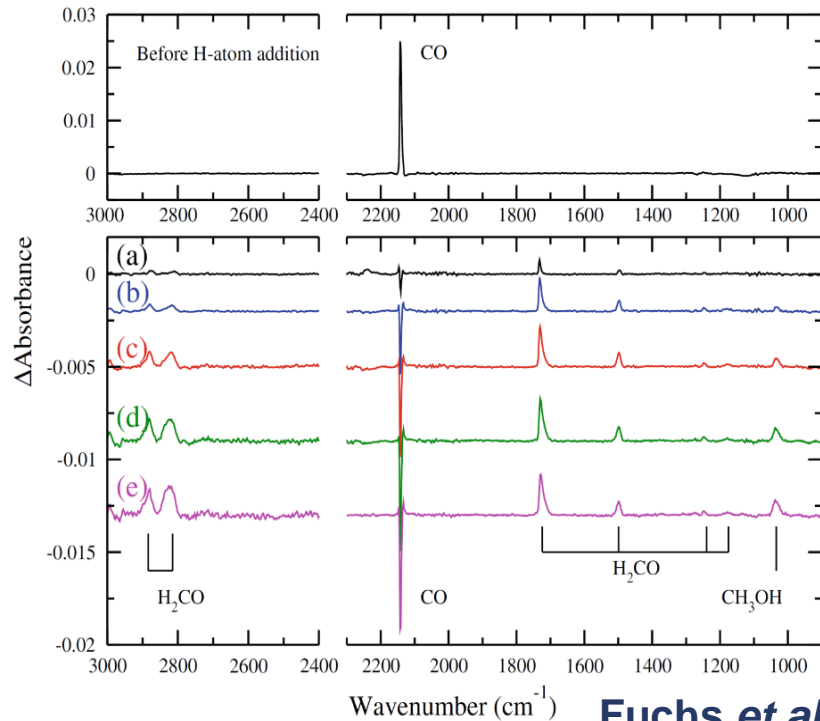
MeOH forms via Dark Chemistry



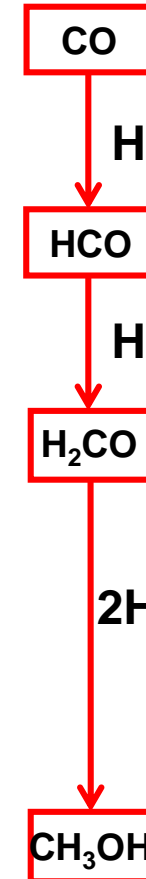
Watanabe et al., *ApJ* (2004)

Hidaka et al., *ApJ* (2004)

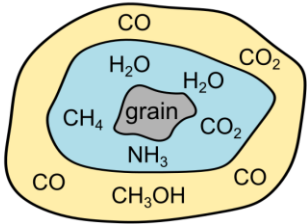
Hiraoka et al., *ApJ* (2002)



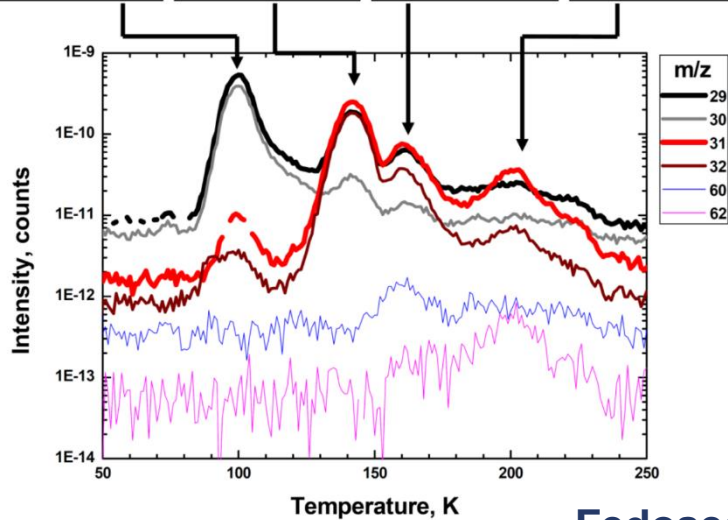
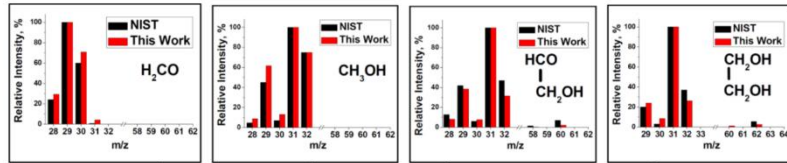
Fuchs et al., *A&A* (2009)



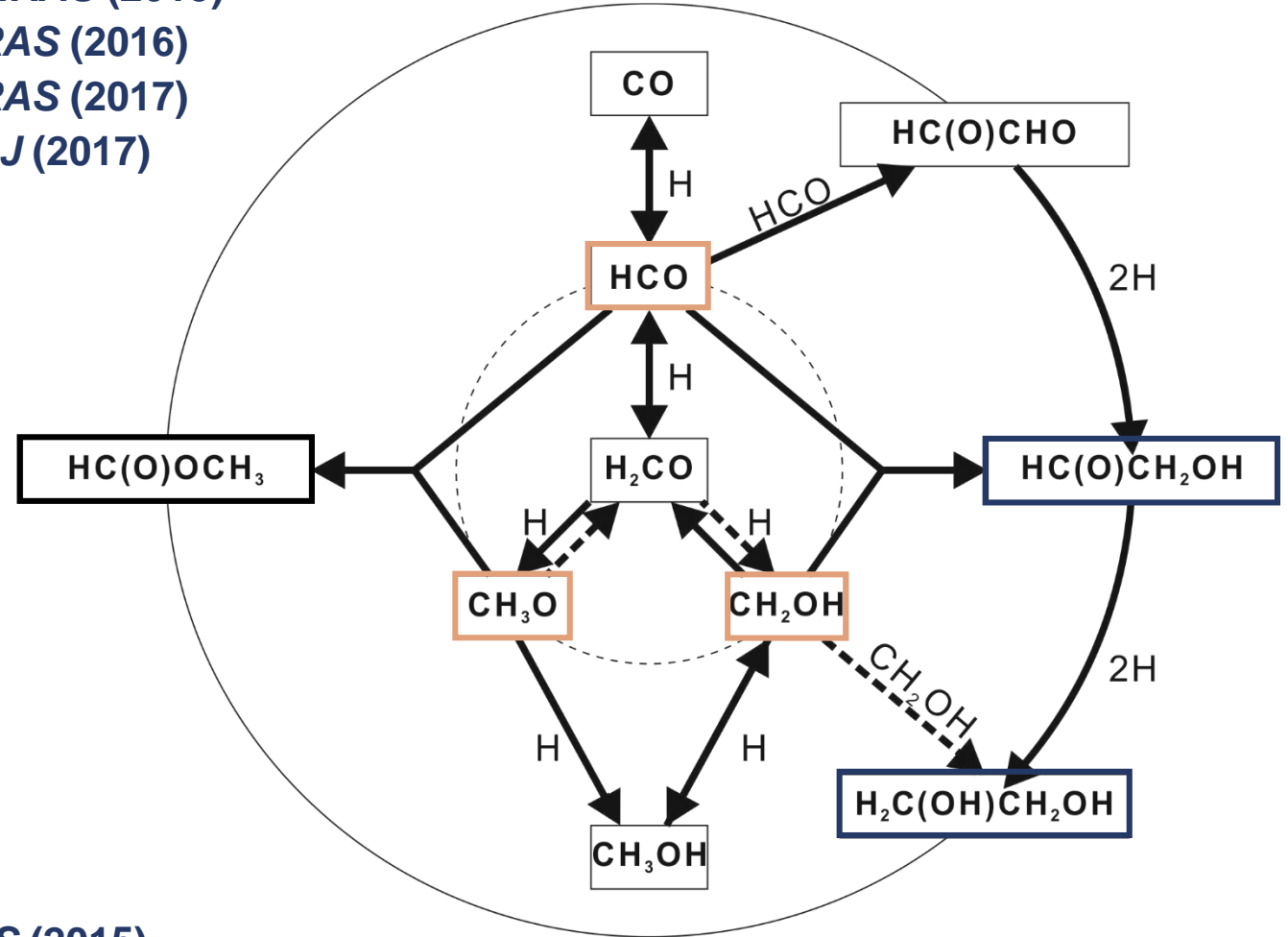
COMs form via Dark Chemistry



Fedoseev *et al.*, *MNRAS* (2015)
Chuang *et al.*, *MNRAS* (2016)
Chuang *et al.*, *MNRAS* (2017)
Fedoseev *et al.*, *ApJ* (2017)



Fedoseev *et al.*, *MNRAS* (2015)

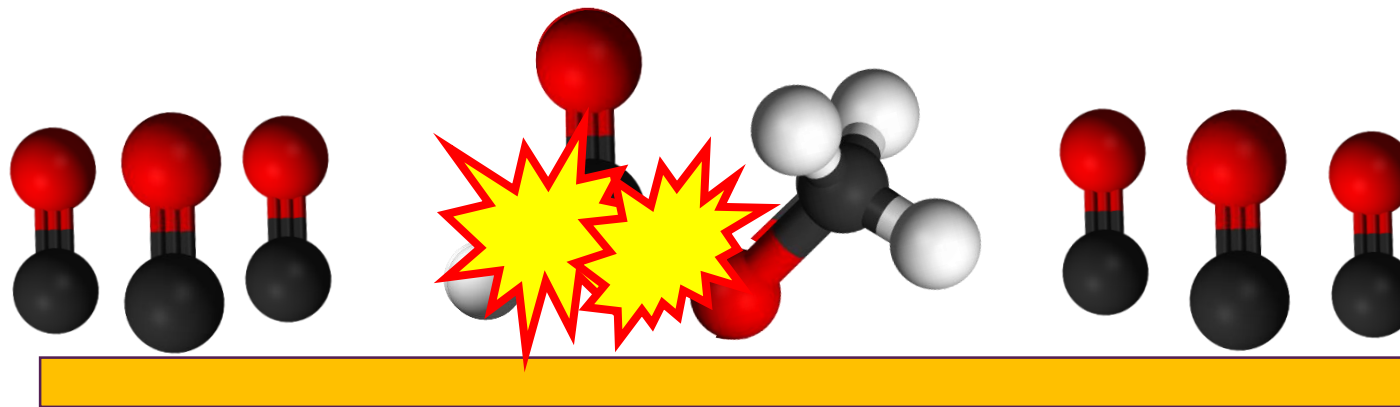
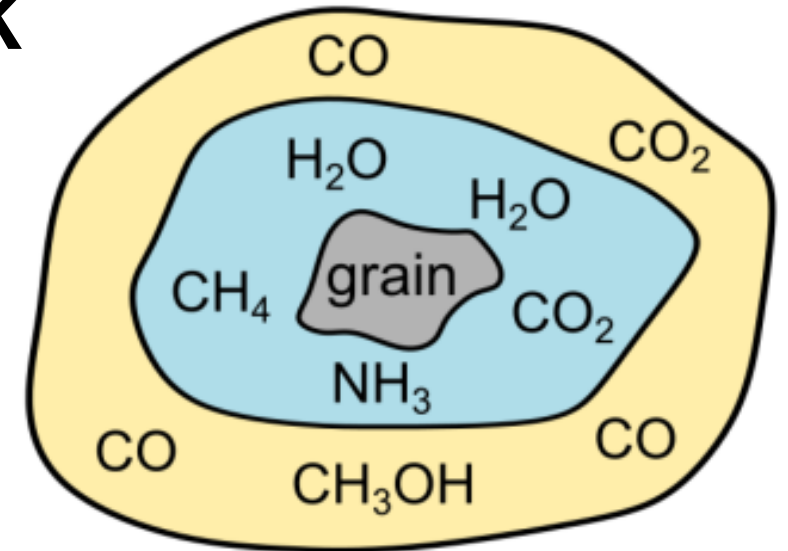


COMs form via Dark Chemistry

A non-diffusive reaction mechanism at 10 K

Fedoseev *et al.*, *MNRAS* (2015)
Chuang *et al.*, *MNRAS* (2016)
Chuang *et al.*, *MNRAS* (2017)
Fedoseev *et al.*, *ApJ* (2017)

Qasim *et al.*, *A&A* (2019)
Chuang *et al.*, *A&A* (2020)
Qasim *et al.*, *Nat. Astron.* (2020)
Ioppolo *et al.*, *Nat. Astron.* (2021)



10 K

COMs form via Dark Chemistry

A non-diffusive reaction mechanism at 10 K

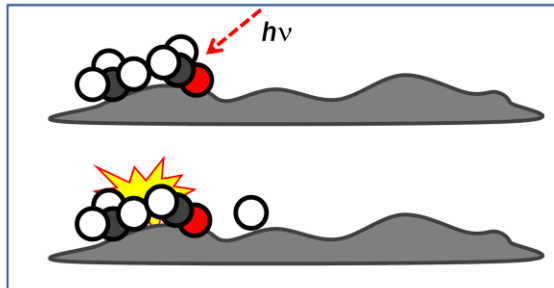
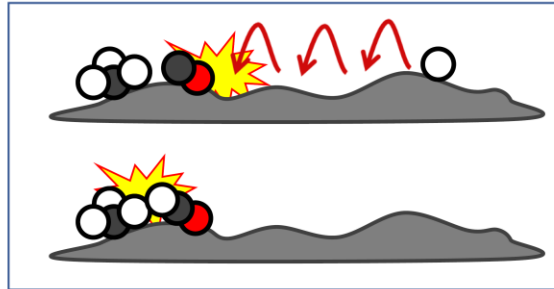
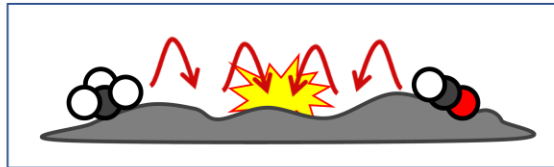
- *Diffusive:* $\text{CH}_3 + \text{HCO} \rightarrow \text{CH}_3\text{CHO}$
(very slow at low temps)

- *Non-diffusive (3-body reaction, 3B):*



⇒ only H needs to move!

- *Non-diffusive (photodissociation-induced, PDI):*

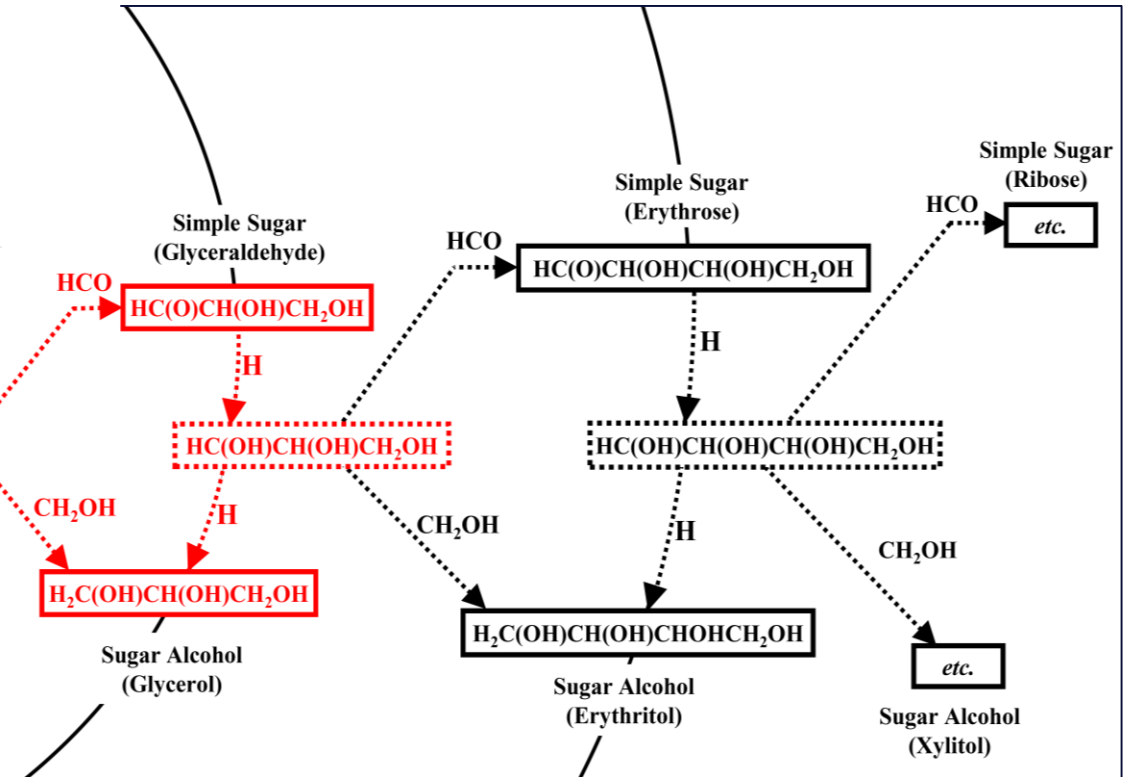
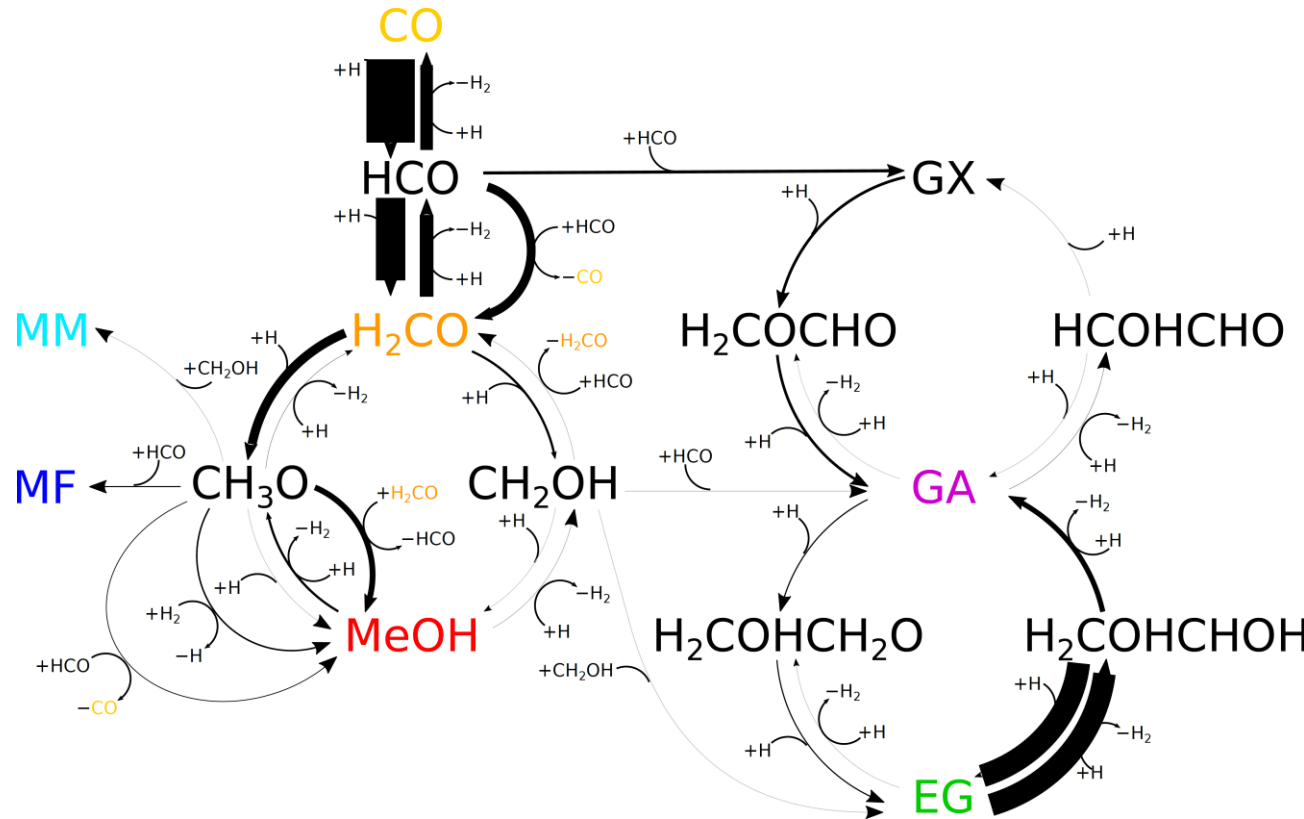
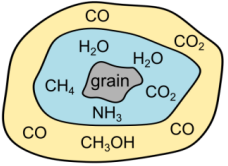


Jin and Garrod, *ApJS* (2020)
Garrod *et al.*, *ApJS* (2021)

First models of hot cores to use a **diffusive + non-diffusive** treatment.

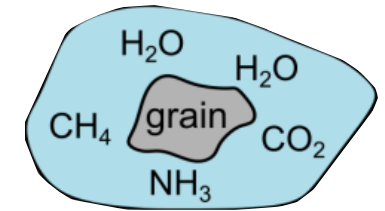
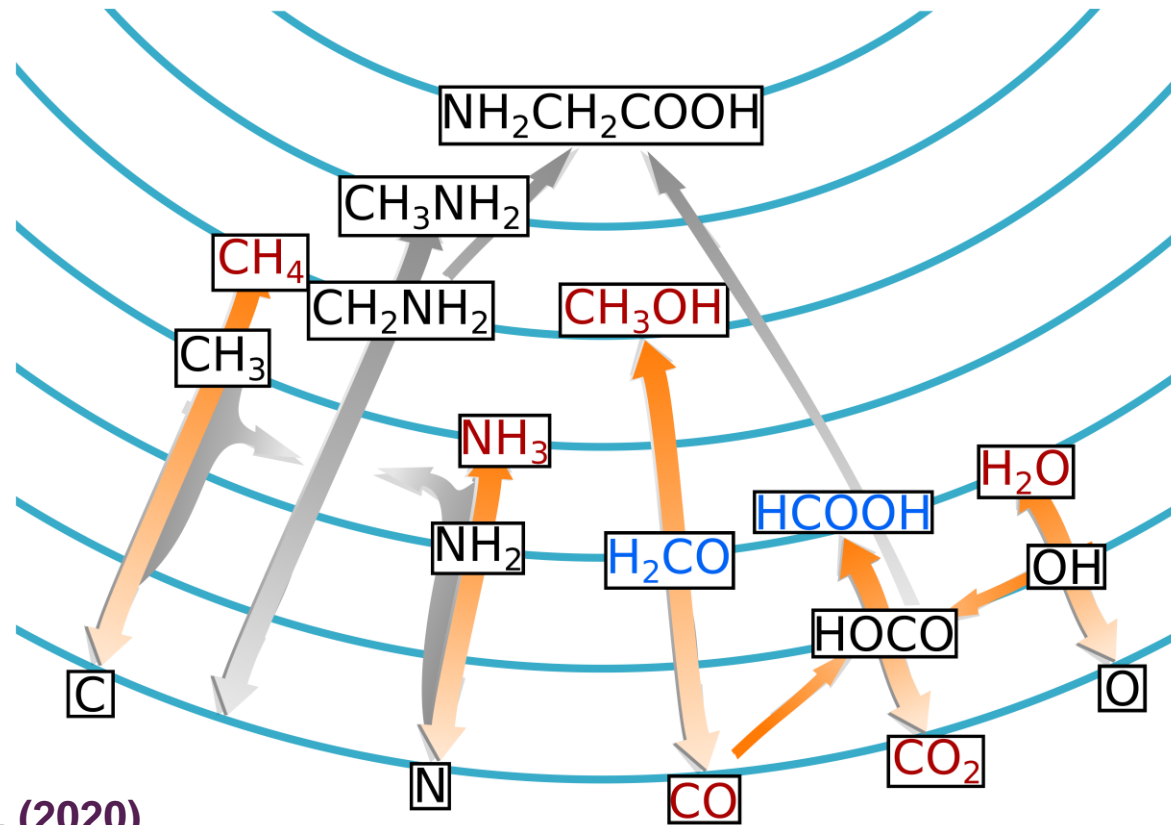
COM production shifted to much earlier times / lower temperatures.

Sugars form via Dark Chemistry



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

Glycine forms via Dark Chemistry



Qasim *et al.*, *Nature Astron.* (2020)

Fedoseev *et al.*, *MNRAS* (2015)

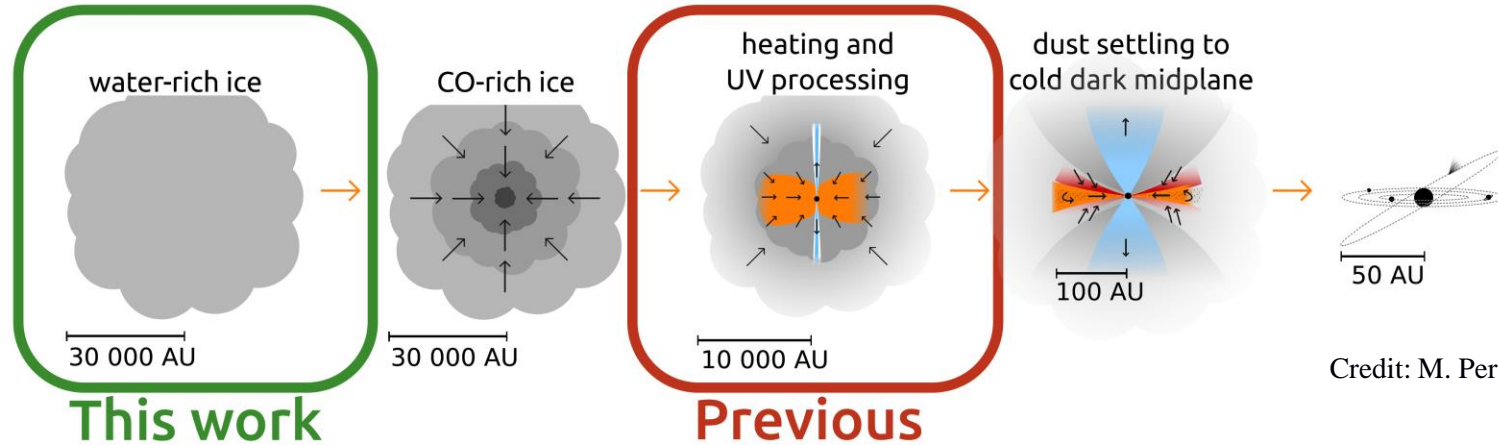
Fuchs *et al.*, *A&A* (2009)

Ioppolo *et al.*, *MNRAS* (2011a)

Ioppolo *et al.*, *MNRAS* (2011b)

Ioppolo *et al.*, *ApJ* (2008)

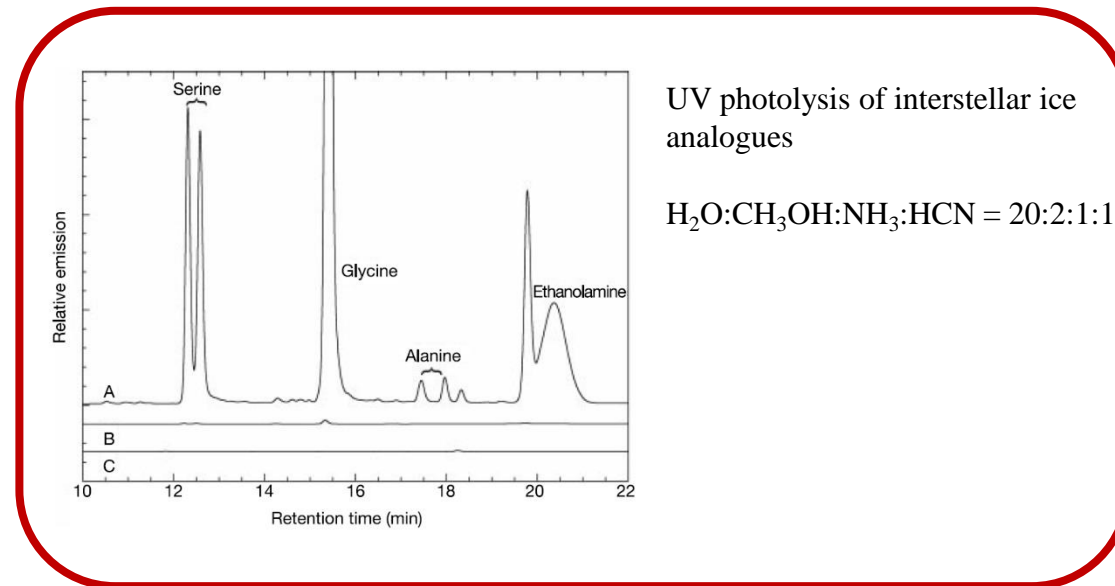
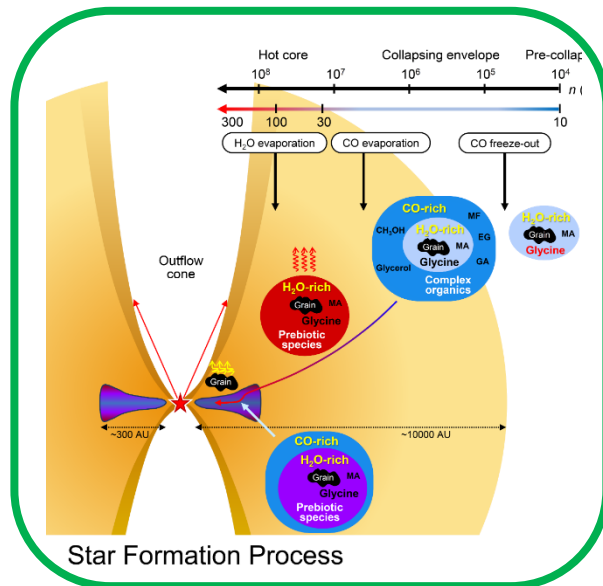
Glycine forms via Dark Chemistry



Credit: M. Persson

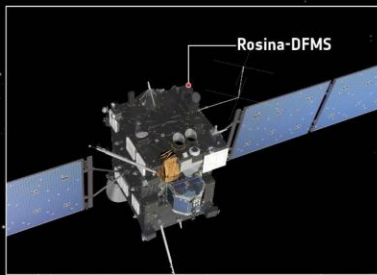
Ioppolo *et al.*, *Nature Astron.* (2021)

Bernstein *et al.*, *Nature* 416, 401 (2002)

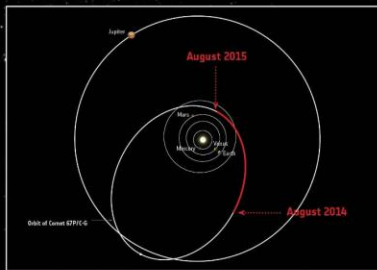


Glycine forms via Dark Chemistry

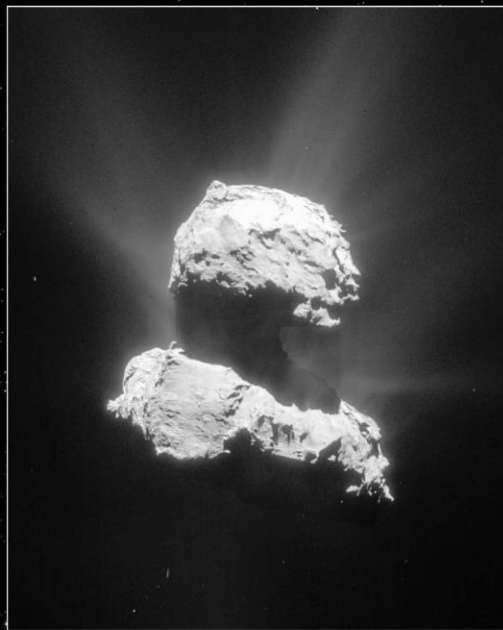
→ ROSETTA'S COMET CONTAINS INGREDIENTS FOR LIFE



The measurements were made with the Rosetta Orbiter Spectrometer for Ion and Neutral Analysis Double-Focusing Mass Spectrometer (ROSINA-DFMS).

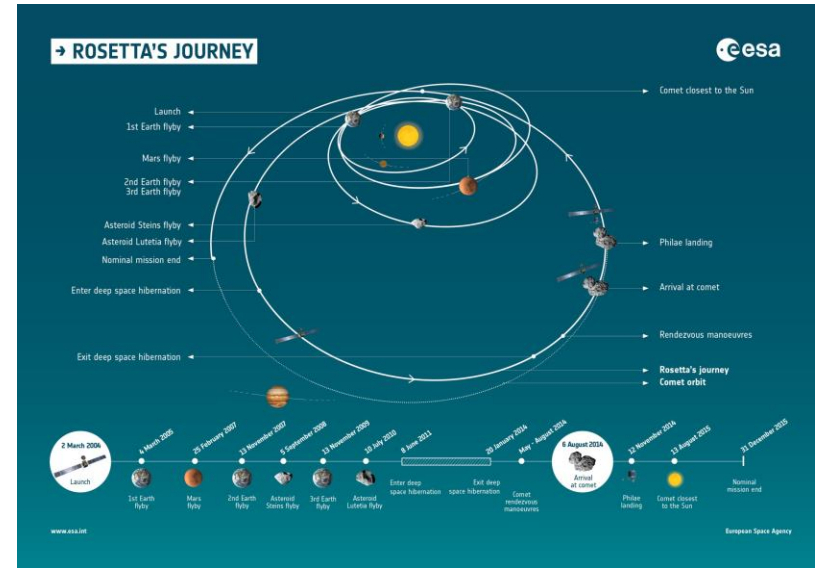
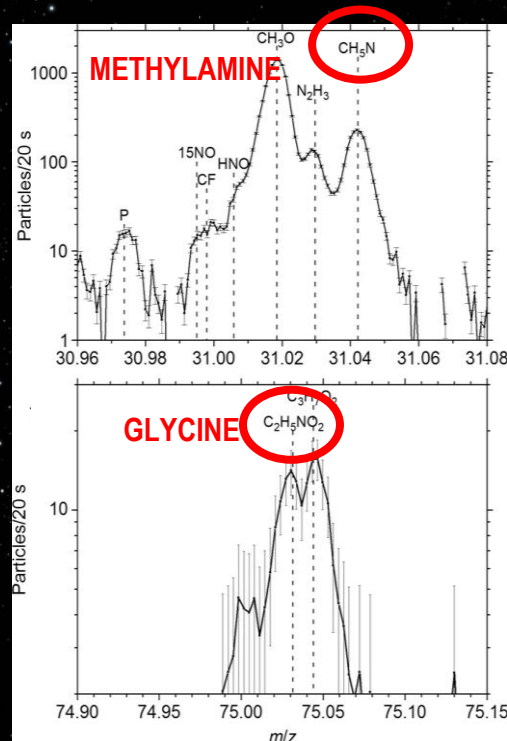


The data were collected between August 2014 and August 2015.

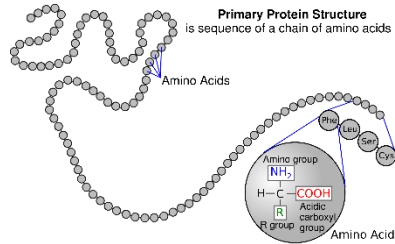


The measurements were made when Rosetta was between 10 and 200 km from the comet.

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

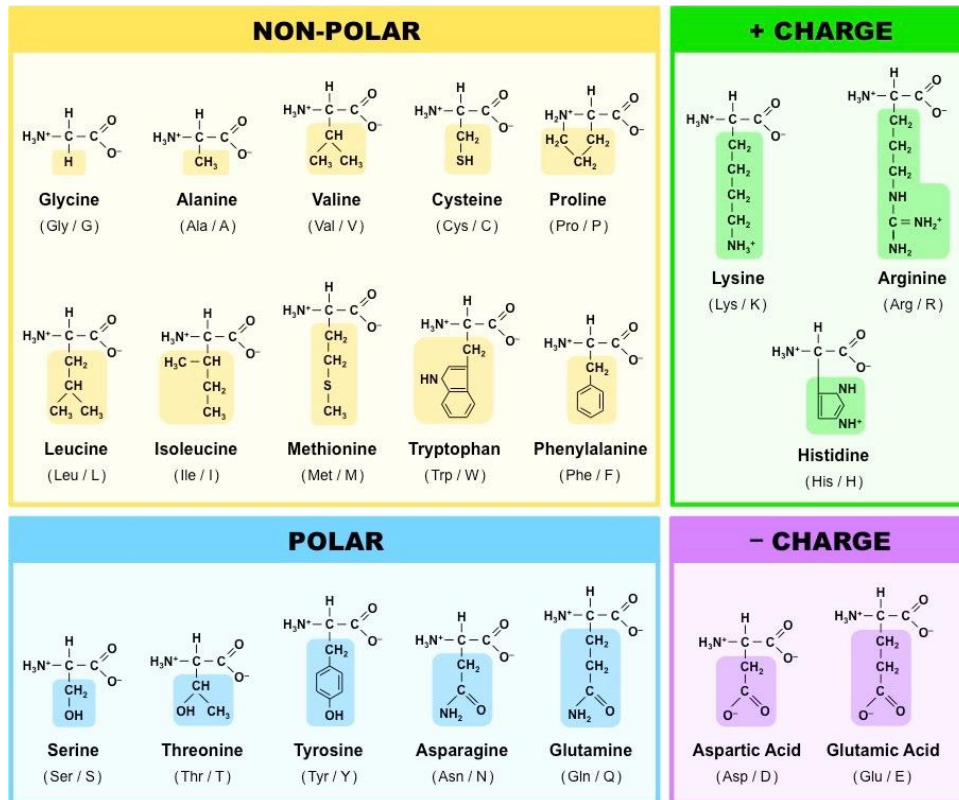
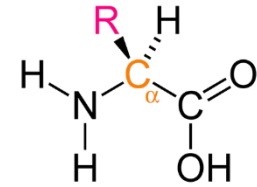


Amino acids formation via Dark Chemistry

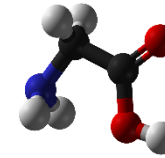


Oba *et al.*, *CPL* (2015) showed
H-abstraction on R-group

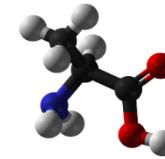
Formation of proteinogenic α -amino acids?



α -glycine

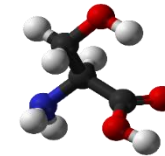


α -alanine



?

α -serine



?

...

...

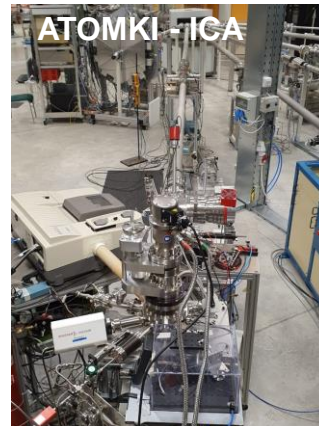
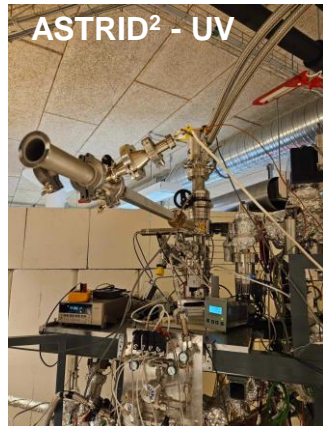
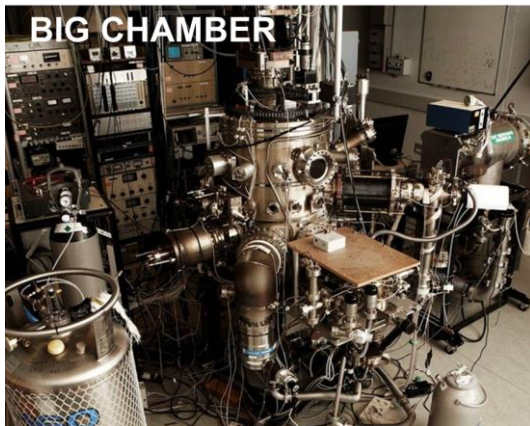
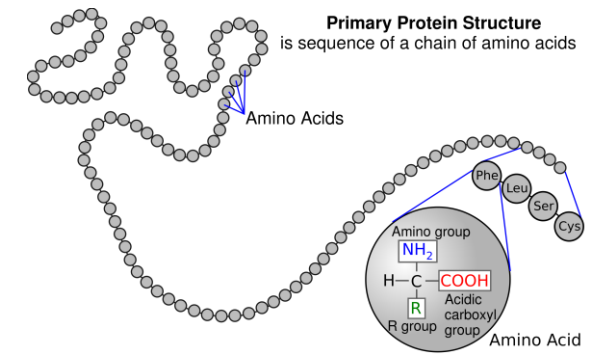
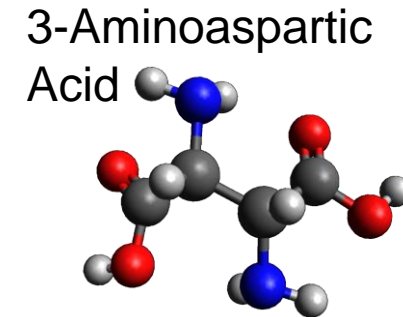
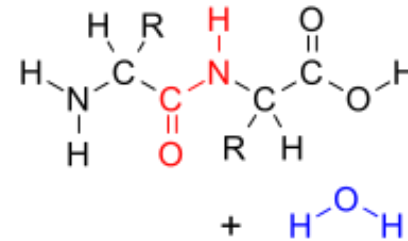
InterCat: Shedding Light on the Formation of the Building Blocks of Life in Space

Investigation of peptide bond formation

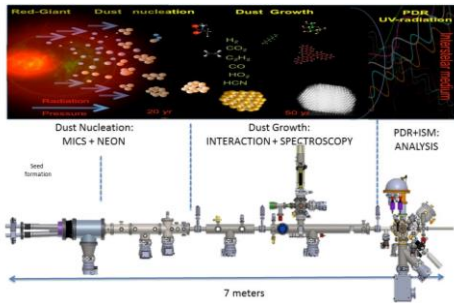


Alfred Hopkinson

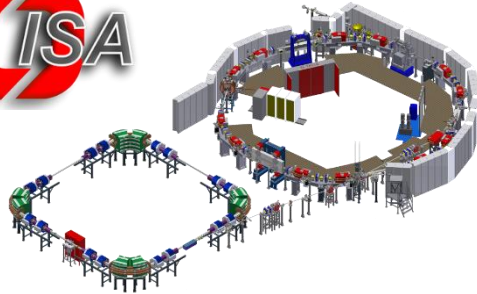
- 1) **Hydrogenation/Deuteration of Gly on cold grain analogs**
Deuterium exchange observed
Formation of **larger species**
- 2) **1 keV e⁻ irradiation of Gly**
- 3) **20 keV H⁺ irradiation of Gly**
- 4) **1 MeV H⁺ irradiation of Gly**
Peptide-like bonds



Astrochemistry at Large-Scale Facilities



STARDUST MACHINE

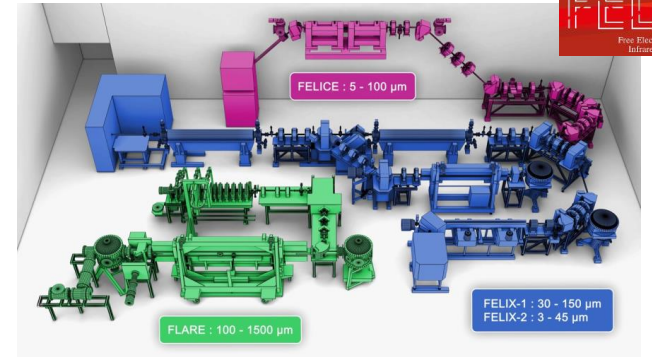


**ICE
CHAMBER**

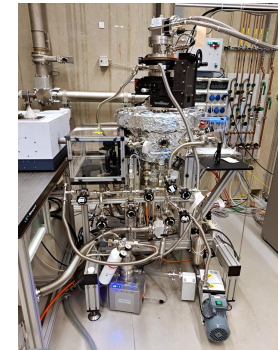
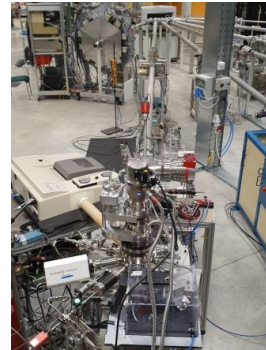
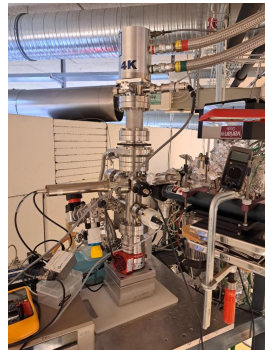
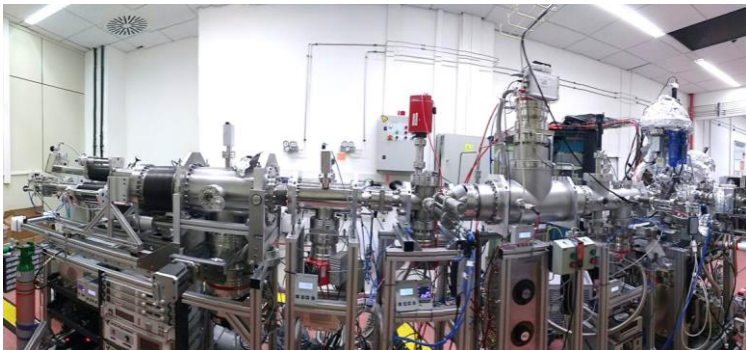


ICA

AQUILA



LISA



ATOMKI

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



ICA

$P < 1 \times 10^{-9}$ mbar

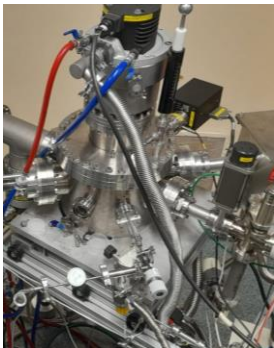
$T_{\text{surf}} = 20 - 300$ K

$E_{\text{ions}} = 200 \text{ keV} - 4 \text{ MeV } H^+$

$H^+, He^+, He^{++}, C^+, C^{++}, O^+, O^{++}, S^+, S^{++}$

Current = nA - μ A

- 2 keV electron gun
- Effusive Cell



AQUILA

$P < 1 \times 10^{-9}$ mbar

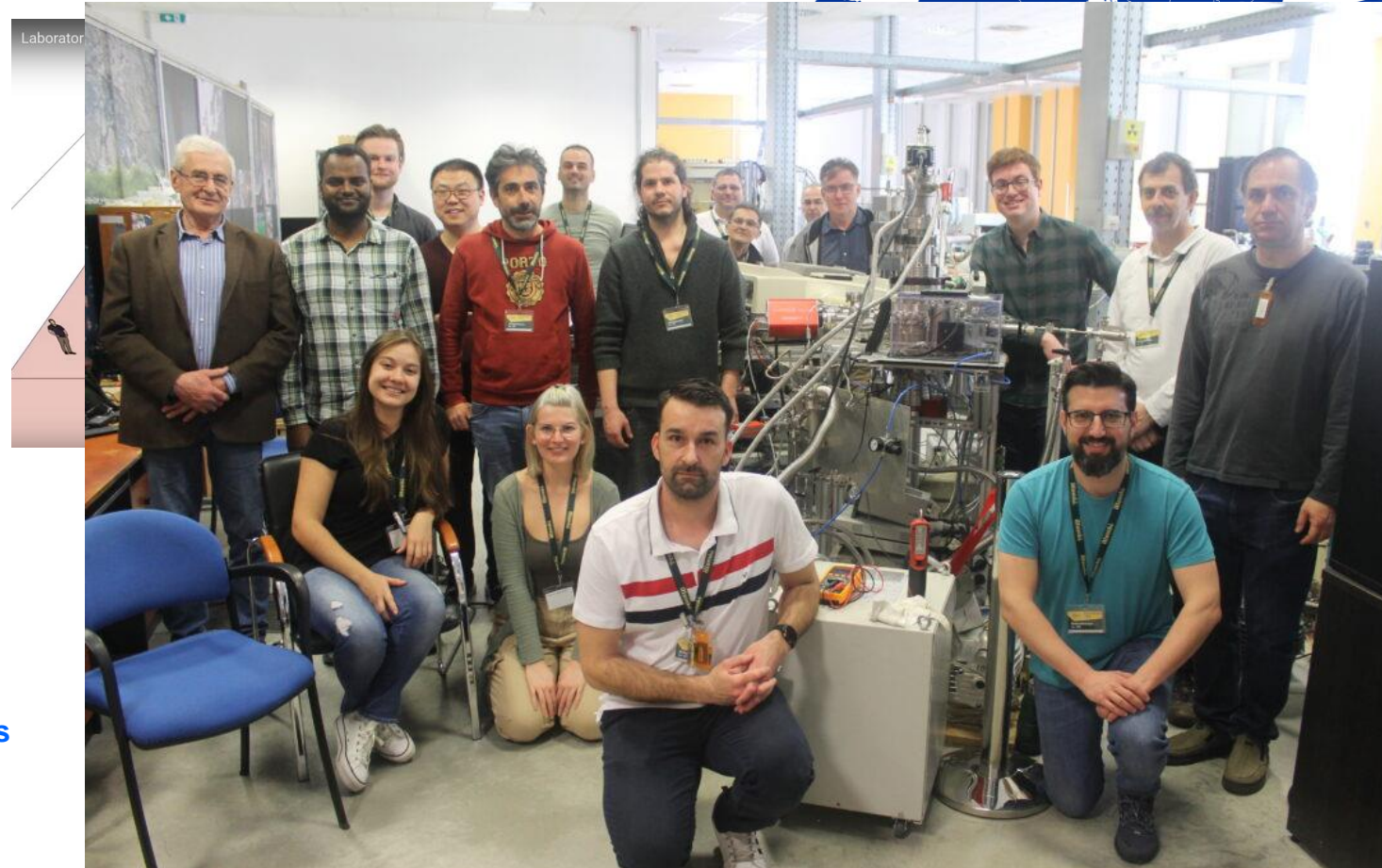
$T_{\text{surf}} = 20 - 300$ K

$E_{\text{ions}} = 100\text{s eV} - 10\text{s keV}$

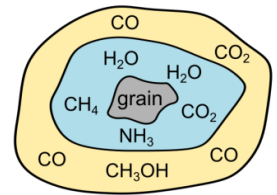
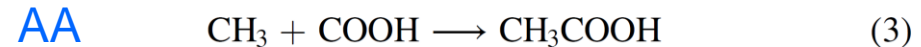
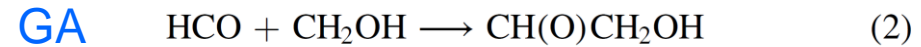
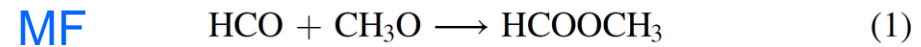
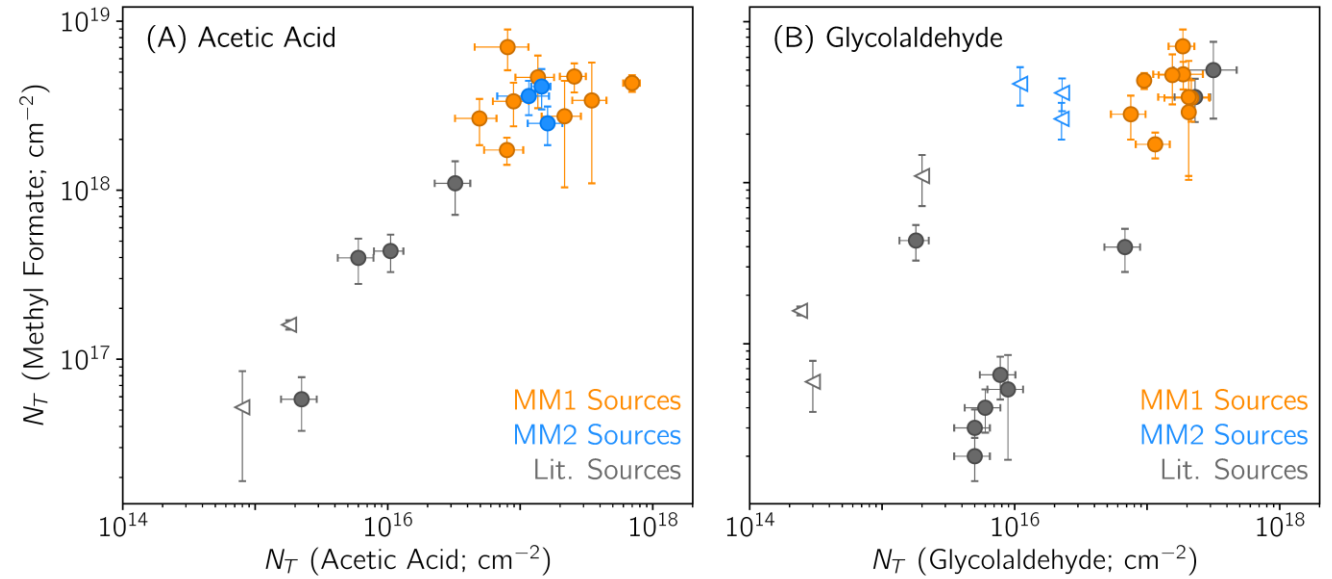
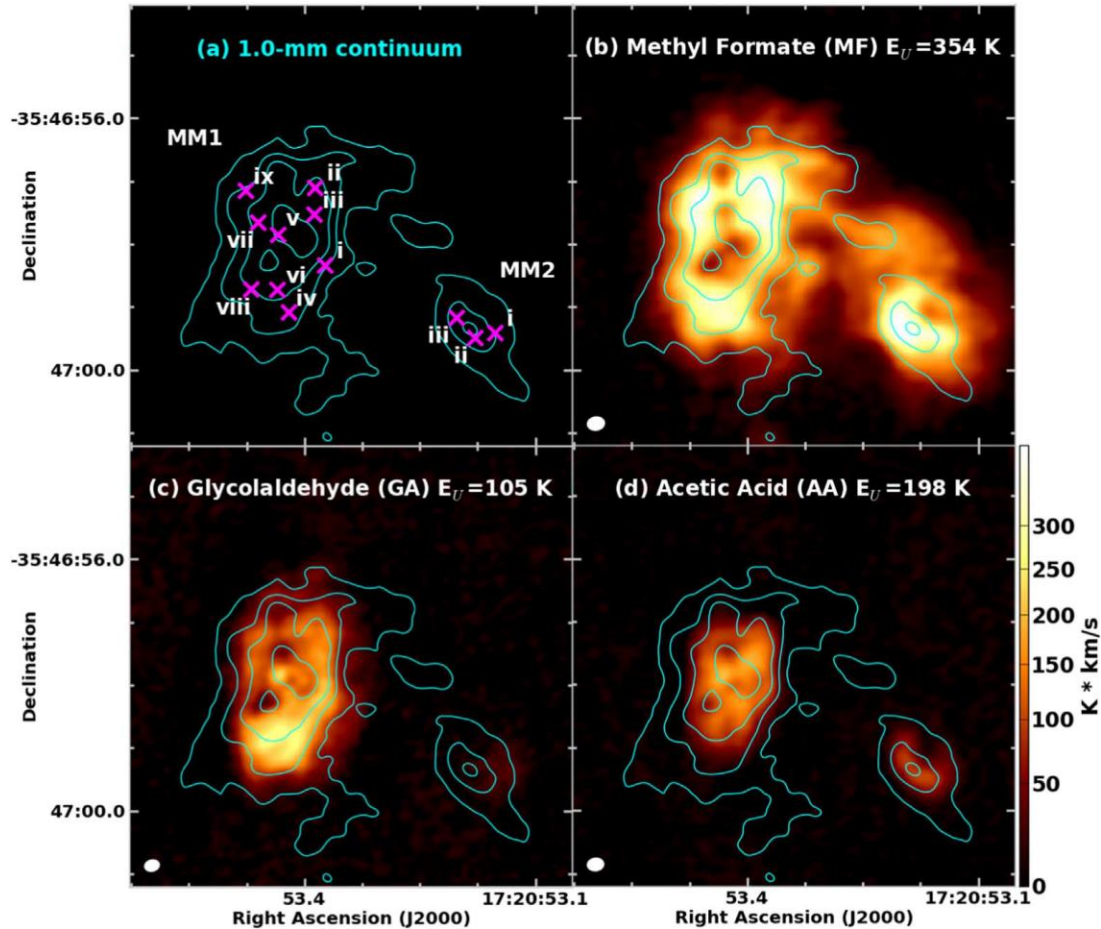
Solar Wind: H, He, C, O, Si, Fe, Ni ions

High charge state of ions

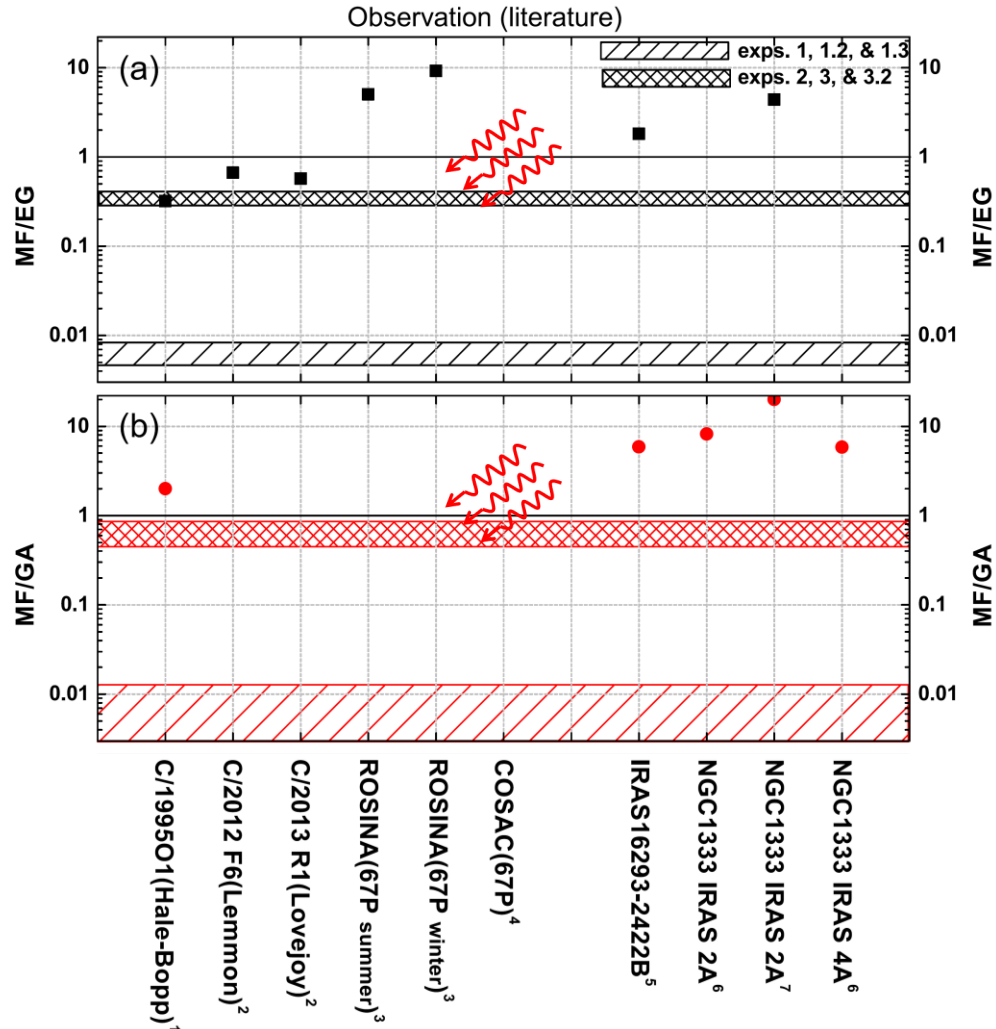
Positive/negative ions or molecular ions



Detection of MF Isomers in space



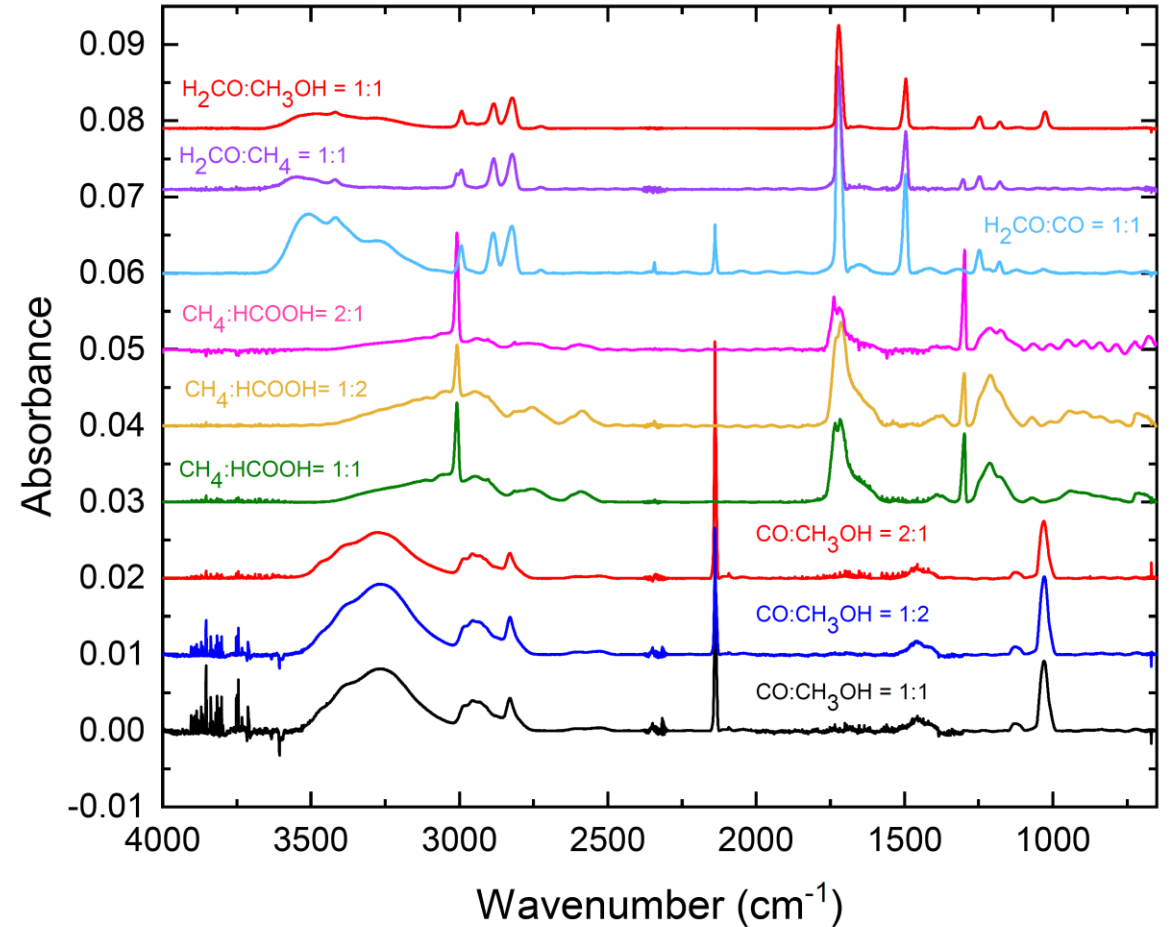
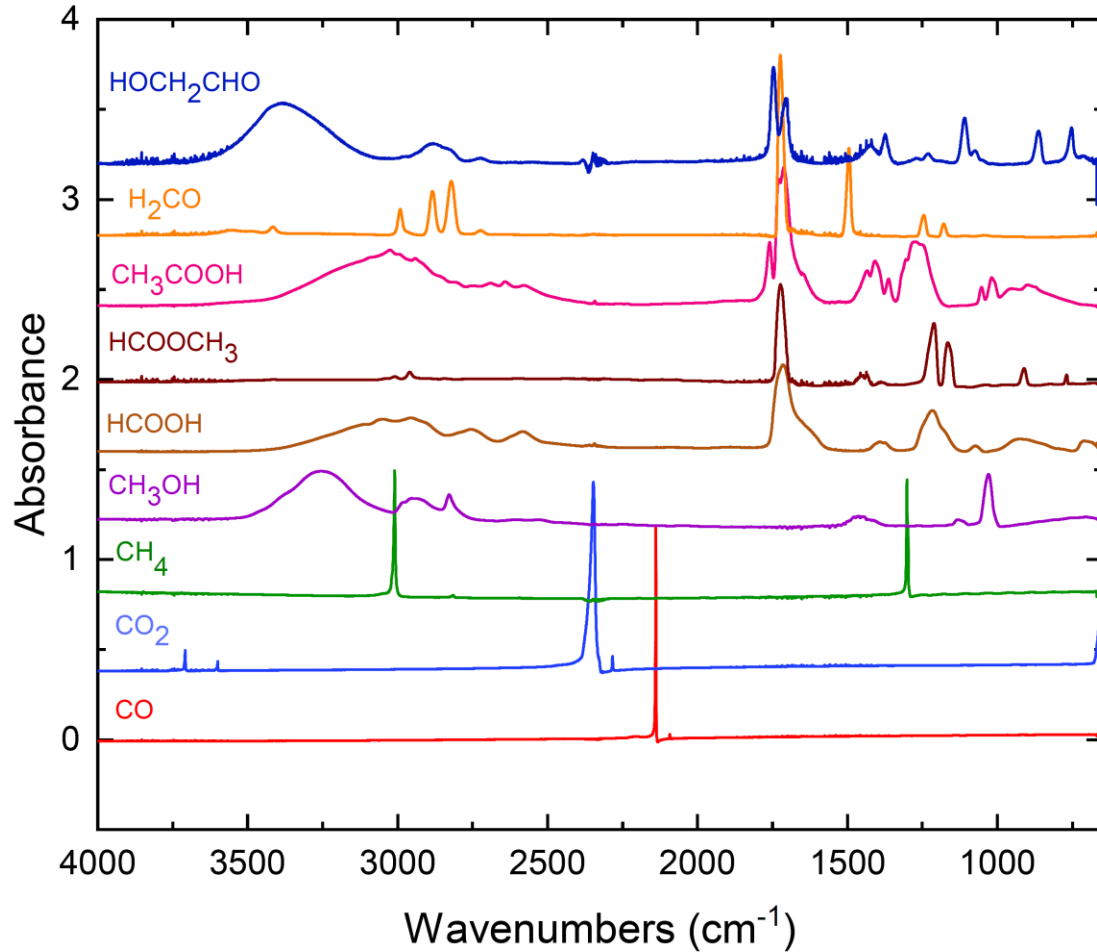
Formation of MF Isomers in space



No.	Experiments	T_{sample} (K)	Ratio (CO:CH ₃ OH)	$\text{Flux}_{\text{CO+CH}_3\text{OH}}$ ($\text{cm}^{-2}\text{s}^{-1}$)	Flux_{H} ($\text{cm}^{-2}\text{s}^{-1}$)	Flux_{UV} ($\text{cm}^{-2}\text{s}^{-1}$)	Time (s)
1	CO + CH ₃ OH + H	14	4:1	1.2E13	6.0E12	–	3600
2	CO + CH ₃ OH + $h\nu$	14	4:1	1.2E13	–	4.0E12	3600
3	CO + CH ₃ OH + H + $h\nu$	14	4:1	1.2E13	6.0E12	4.0E12	3600
No.	Control experiments	T_{sample} (K)	Ratio (CO:CH ₃ OH)	$\text{Flux}_{\text{CO+CH}_3\text{OH}}$ ($\text{cm}^{-2}\text{s}^{-1}$)	Flux_{H} ($\text{cm}^{-2}\text{s}^{-1}$)	Flux_{UV} ($\text{cm}^{-2}\text{s}^{-1}$)	Time (s)
1.1	CO + CH ₃ OH + H ₂	14	4:1	1.2E13	–	–	3600
1.2	CO + CH ₃ OH + H	14	4:1	2.0E12	1.0E12	–	21600
1.3	CO + CH ₃ OH + H	14	4:1	2.0E12	6.0E12	–	21600
3.1	CO + CH ₃ OH + H ₂	14	4:1	1.2E13	–	–	3600
3.2	CO + CH ₃ OH + H ₂ (100%) + $h\nu$	14	4:1	1.2E13	–	4.0E12	3600
3.3	CO + CH ₃ OH + H ₂ (70%) + $h\nu$	14	4:1	1.2E13	–	4.0E12	3600
4.1	CO + CH ₃ OH + Ar(100%) + $h\nu$	14	4:1	1.2E13	–	4.0E12	3600
4.2	CO + CH ₃ OH + Ar(70%) + $h\nu$	14	4:1	1.2E13	–	4.0E12	3600
4.3	CO + CH ₃ OH + Ar(30%) + $h\nu$	14	4:1	1.2E13	–	4.0E12	3600

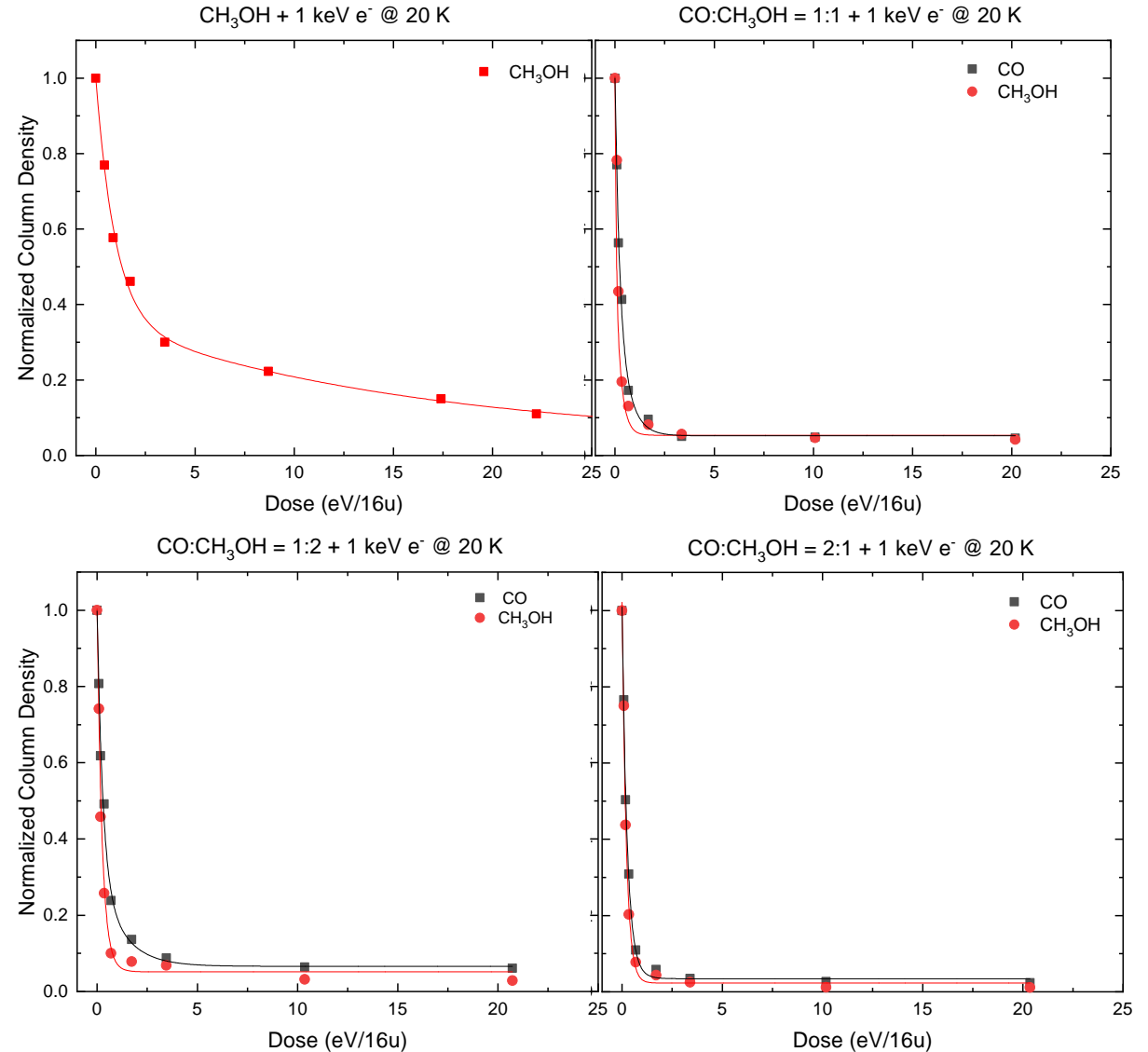
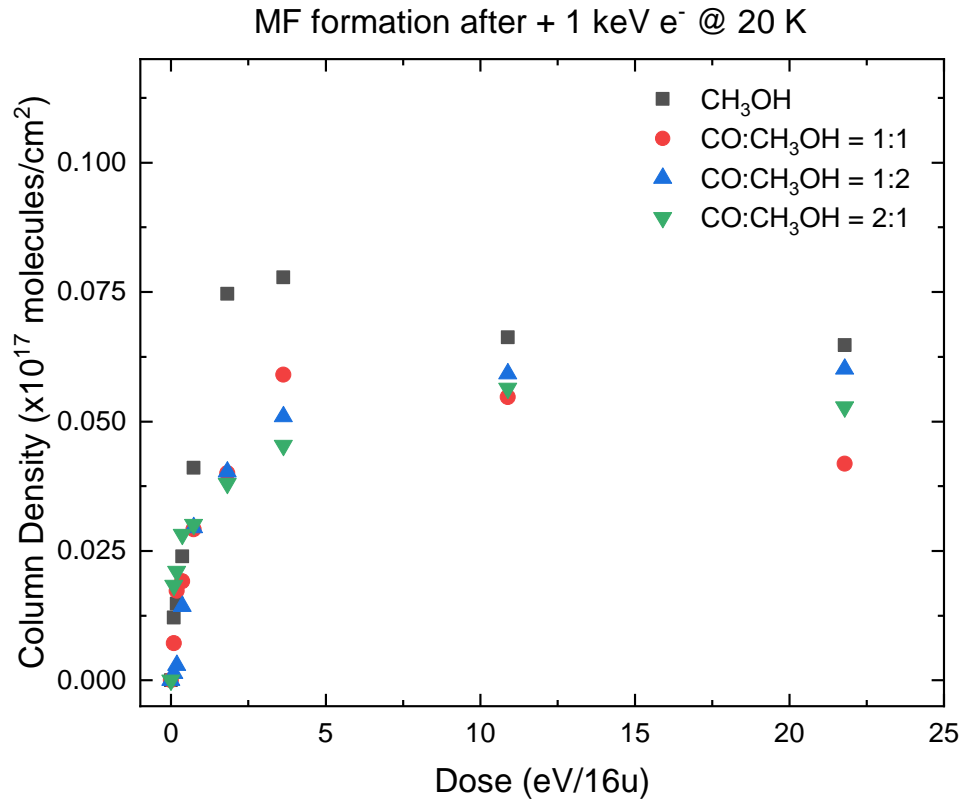
Formation of MF Isomers in space

Ices + 0.2 & 1 MeV H⁺ / 1 keV e⁻



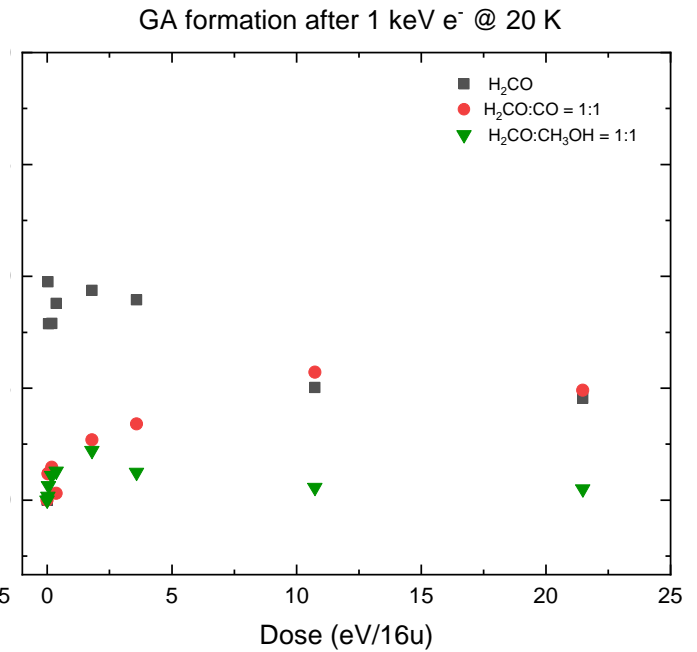
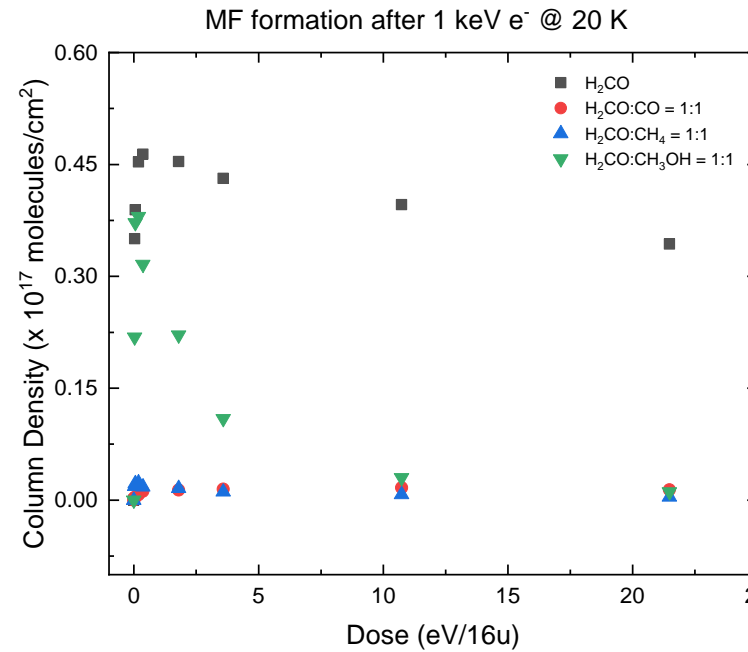
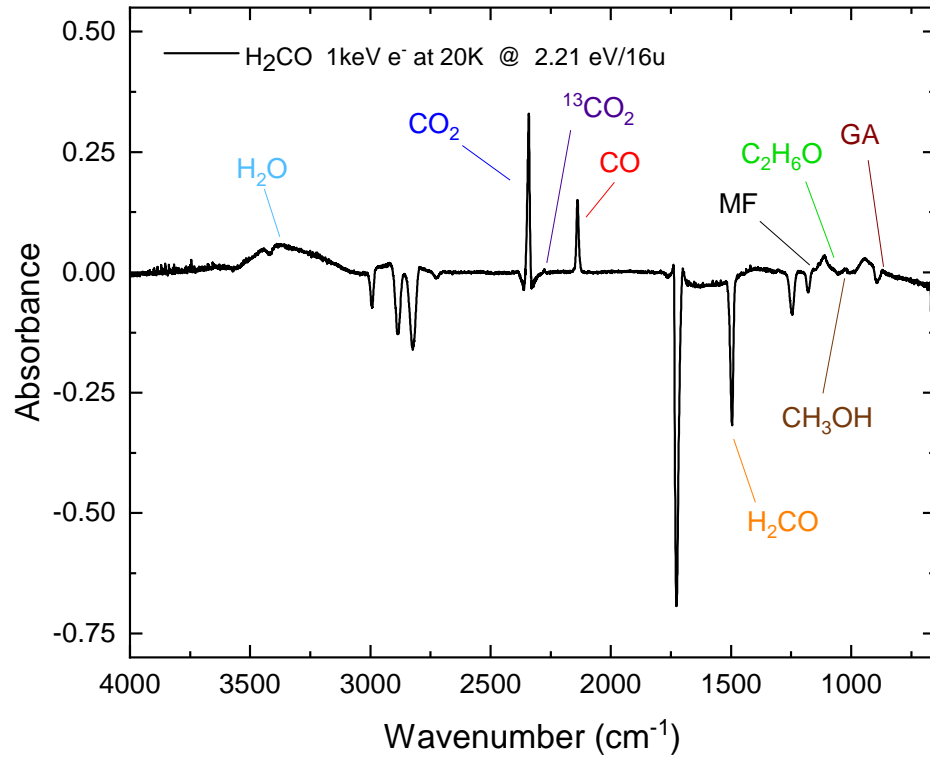
Formation of MF Isomers in space

MeOH-rich + 1 keV e⁻



Formation of MF Isomers in space

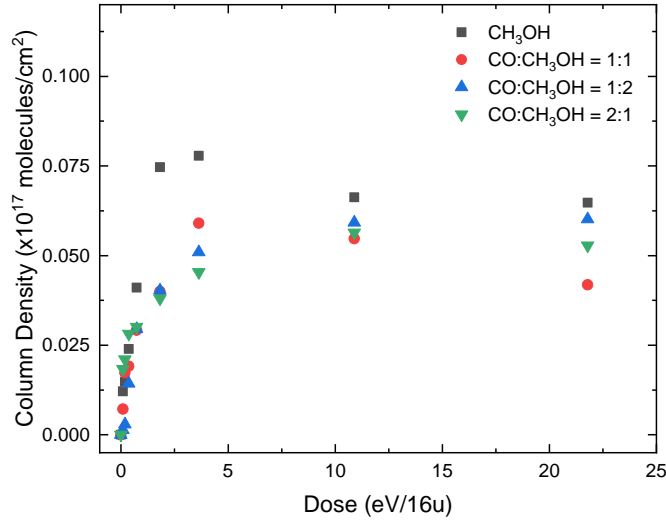
H₂CO-rich + 1 keV e⁻



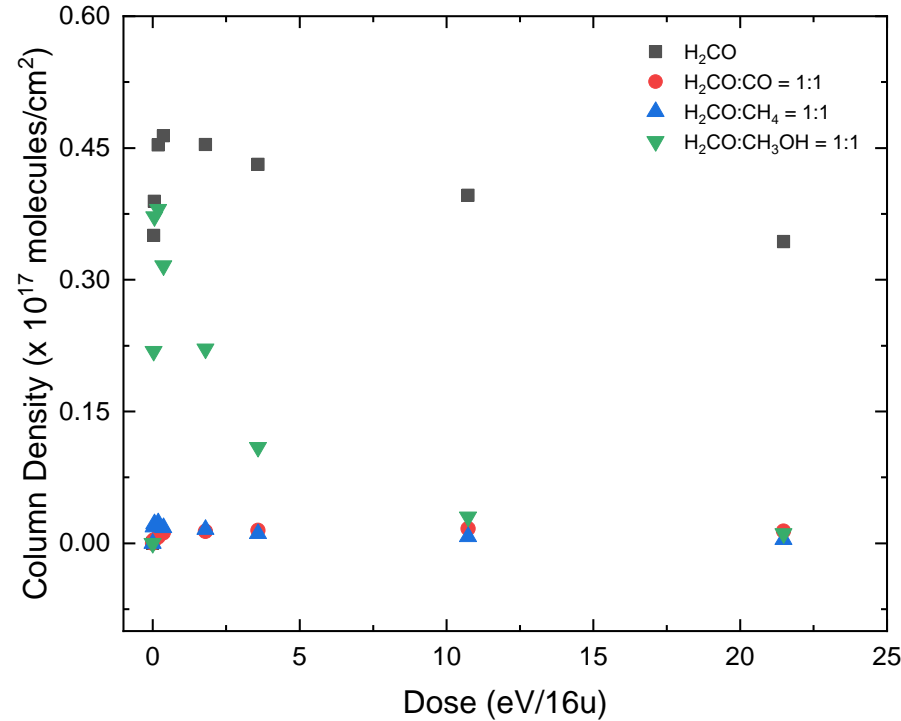
Formation of MF Isomers in space

H₂CO-rich + 1 keV e⁻

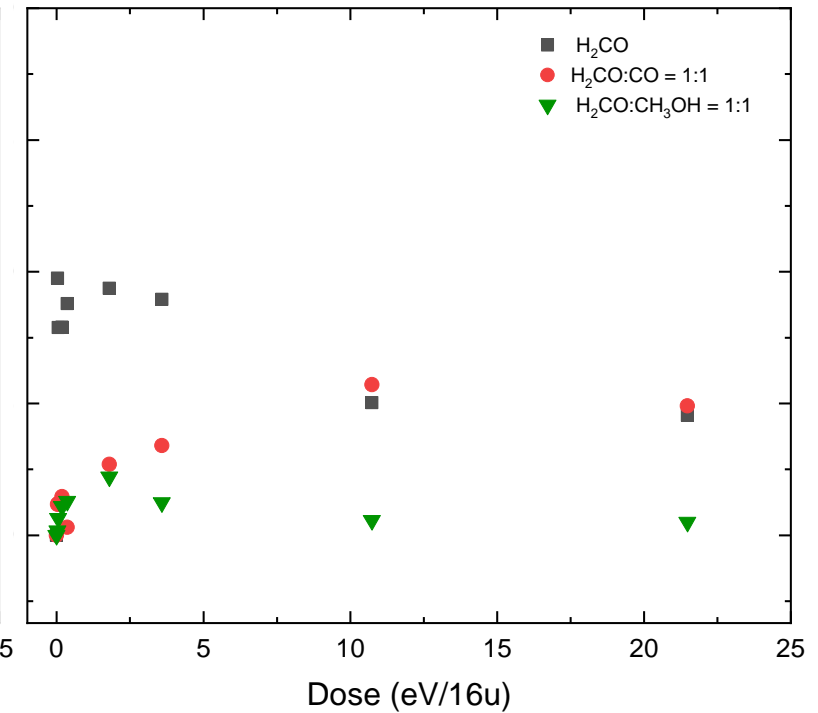
MF formation after + 1 keV e⁻ @ 20 K



MF formation after 1 keV e⁻ @ 20 K



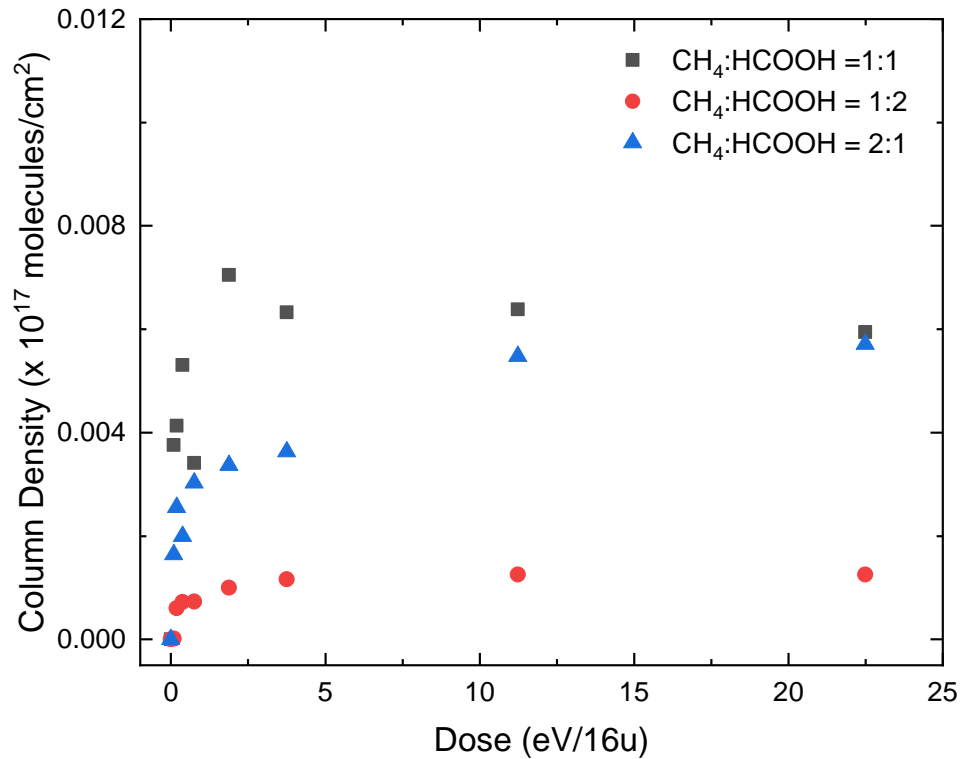
GA formation after 1 keV e⁻ @ 20 K



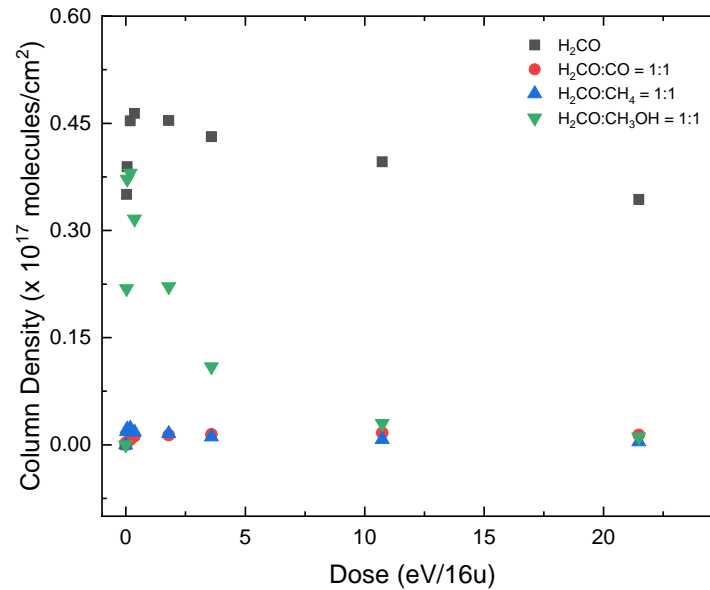
Formation of MF Isomers in space



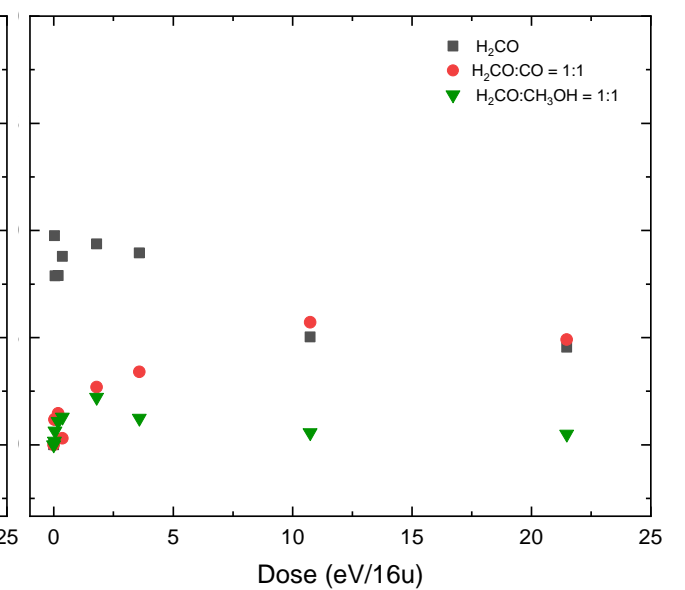
AA formation after 1 keV e^- @ 20 K



MF formation after 1 keV e^- @ 20 K



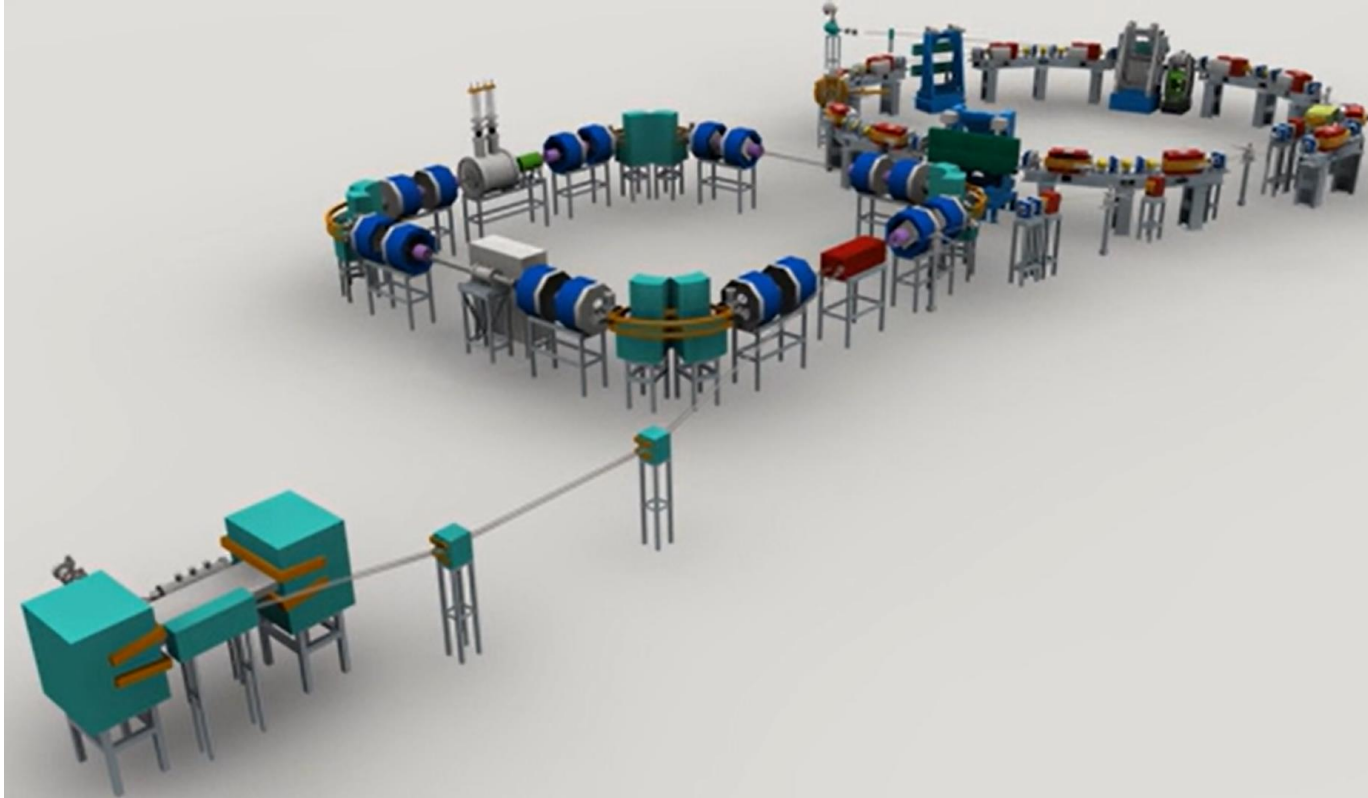
GA formation after 1 keV e^- @ 20 K



Observed MF-AA and MF-GA correlations probably due to warm surface and gas phase chemistry

Balucani et al. (2015); Ascenzi et al. (2019); Garrod et al. (2022)

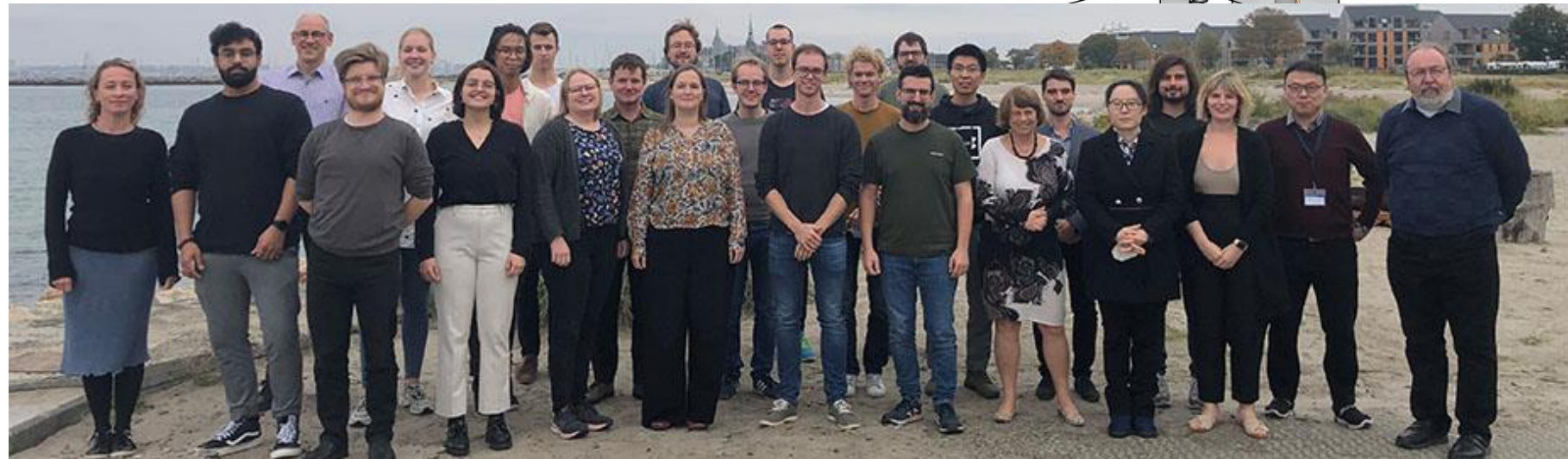
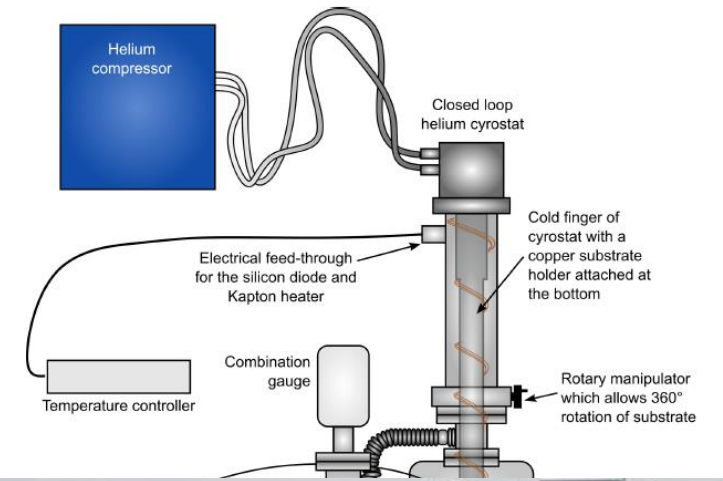
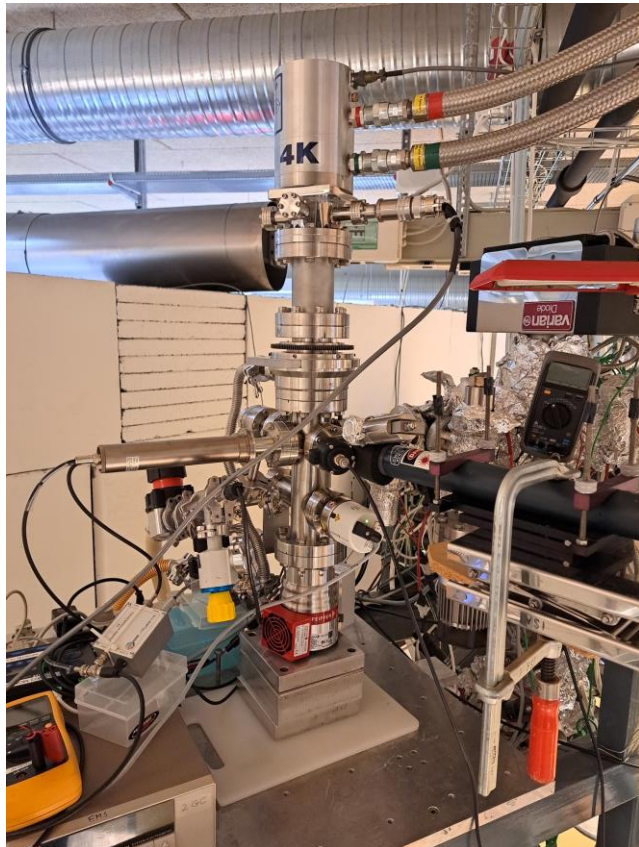
ASTRID²



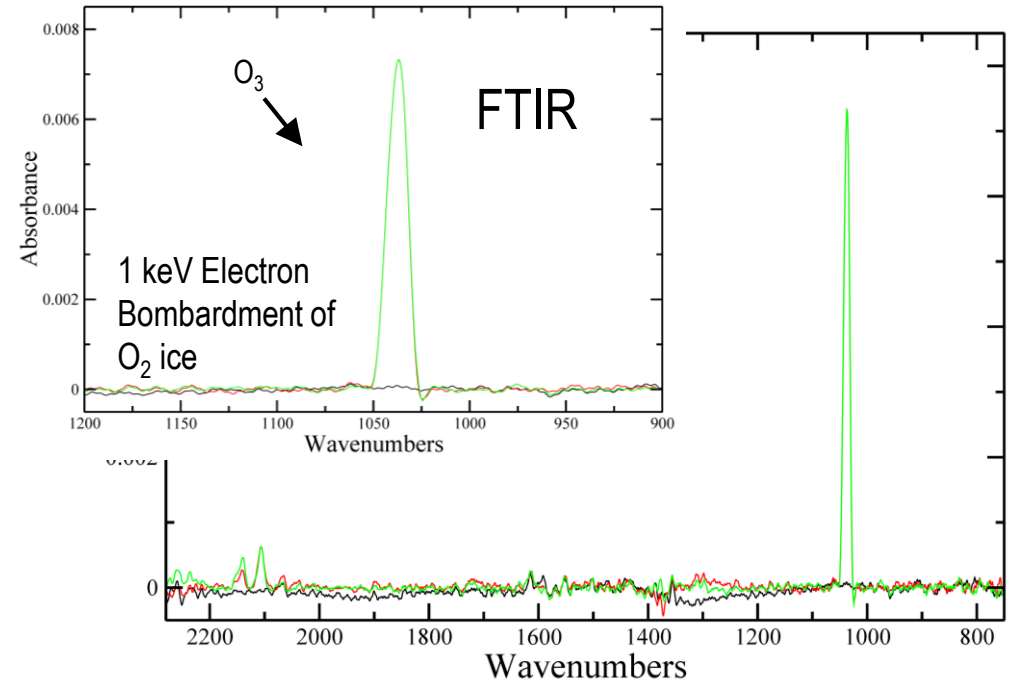
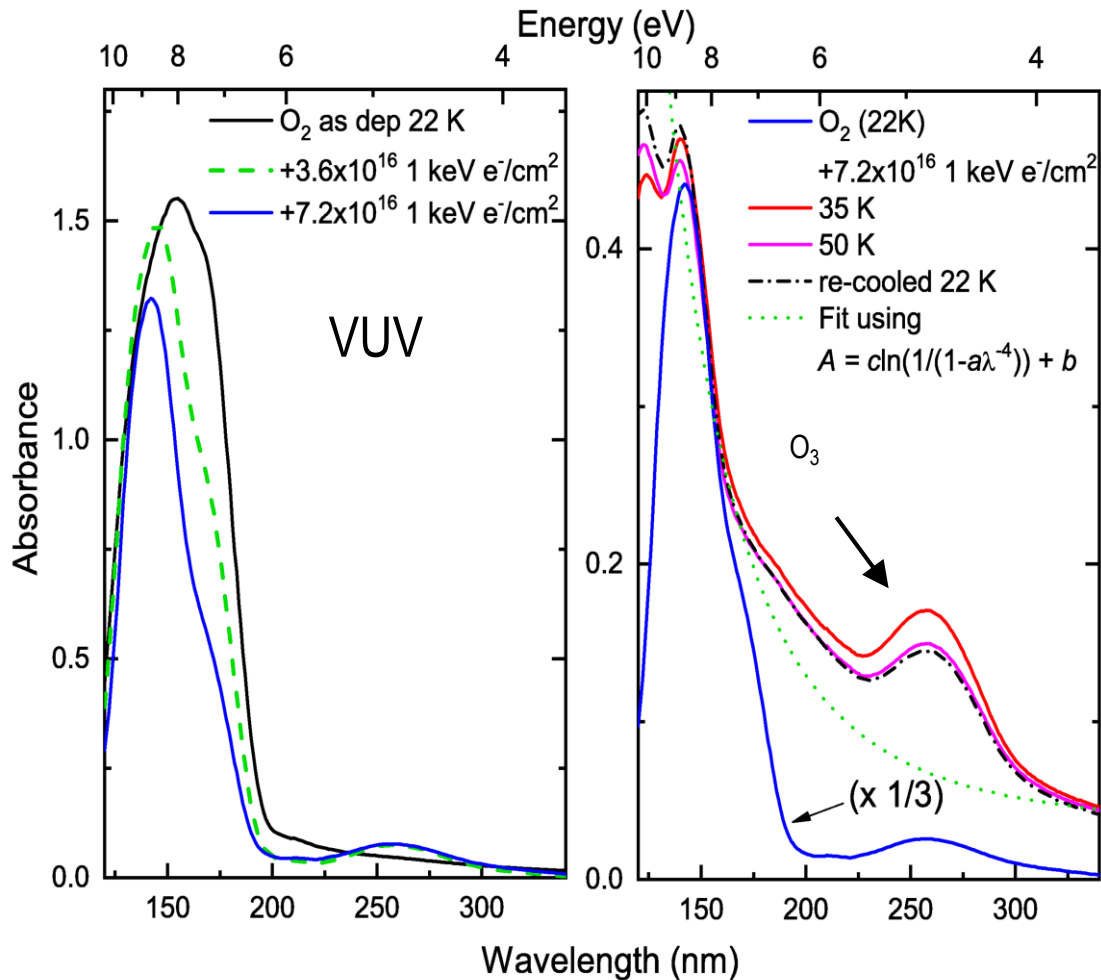
Ice Chamber (IC)



VUV and UV-vis spectroscopy of ices and electron irradiation



VUV vs IR Spectroscopy

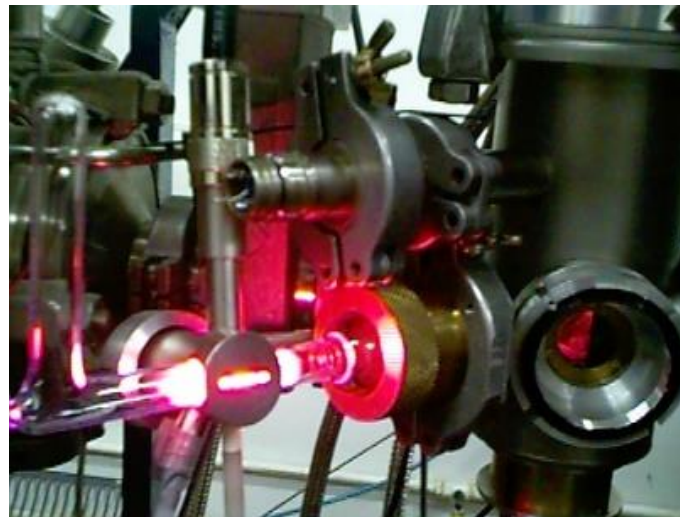


VUV ice Database

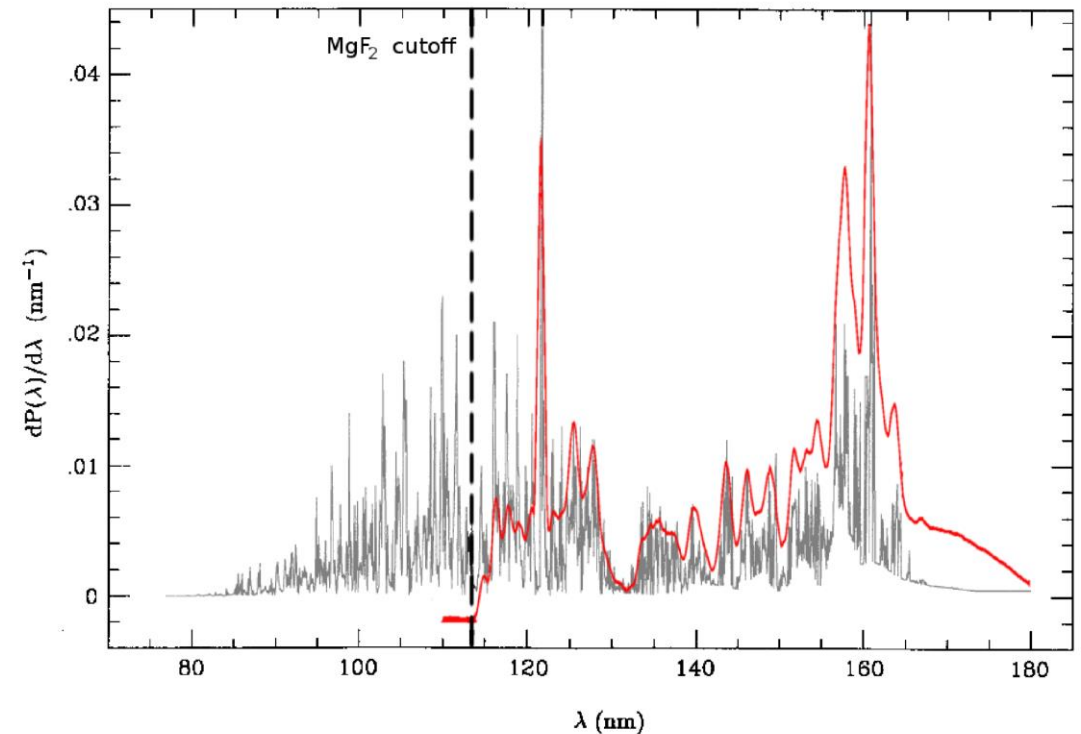


A comprehensive large VUV/UV-vis ice database to

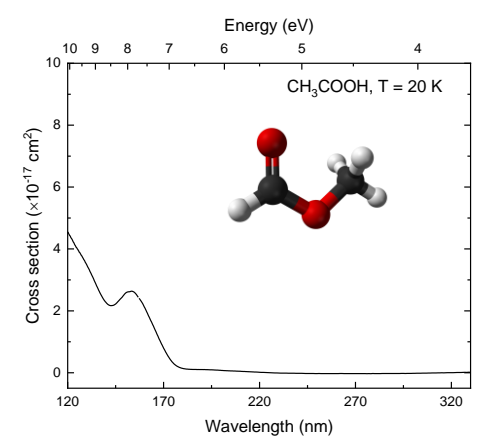
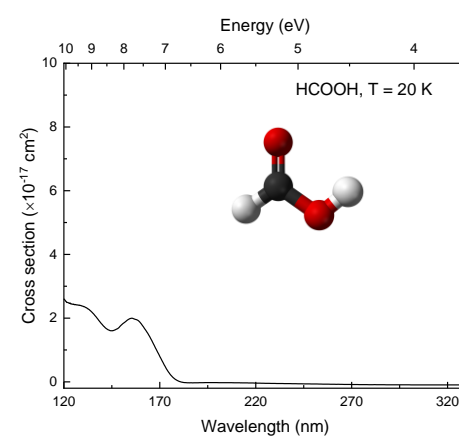
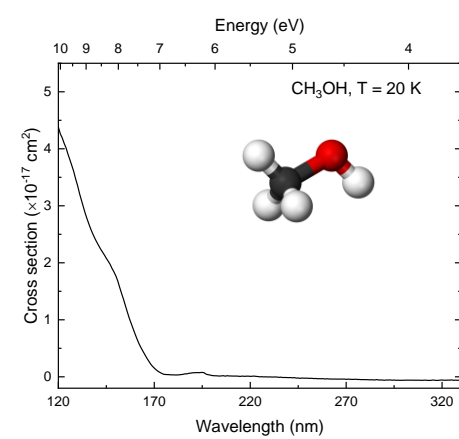
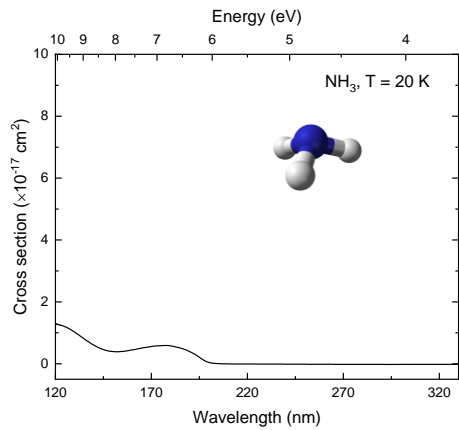
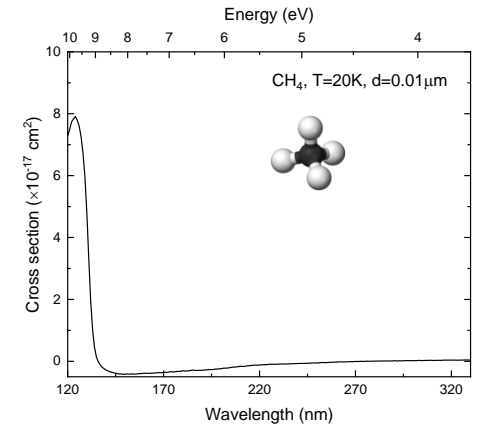
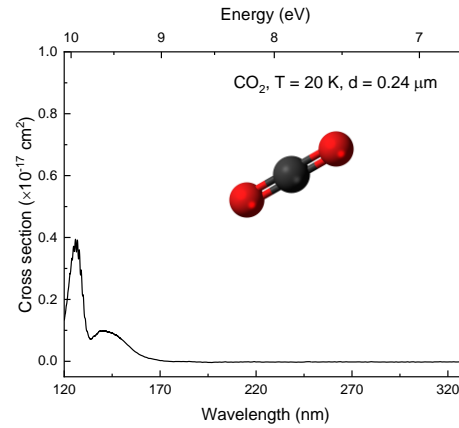
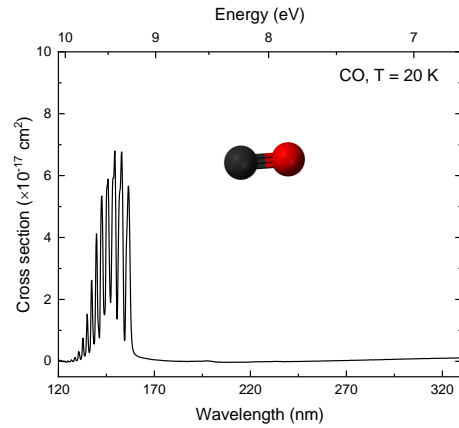
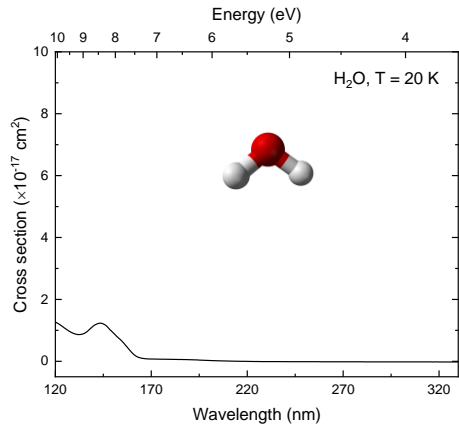
- Identify simple & complex molecules (e.g., prebiotic species) in the Solar System.
- Aid the study of UV photoprocesses.



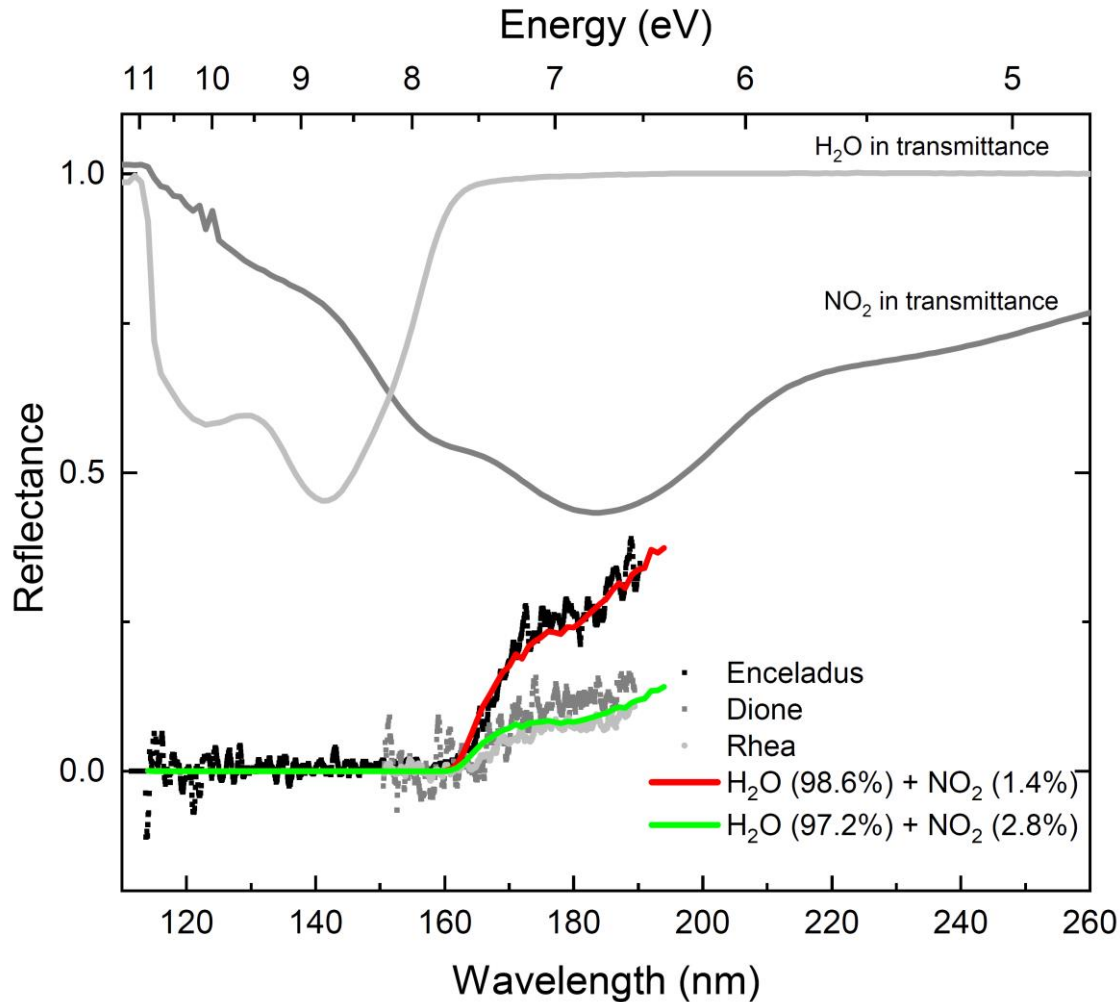
LASP INAF-Catania



VUV ice Database



Ices in the Solar System



JUICE (JUperiter ICy moons Explorer)

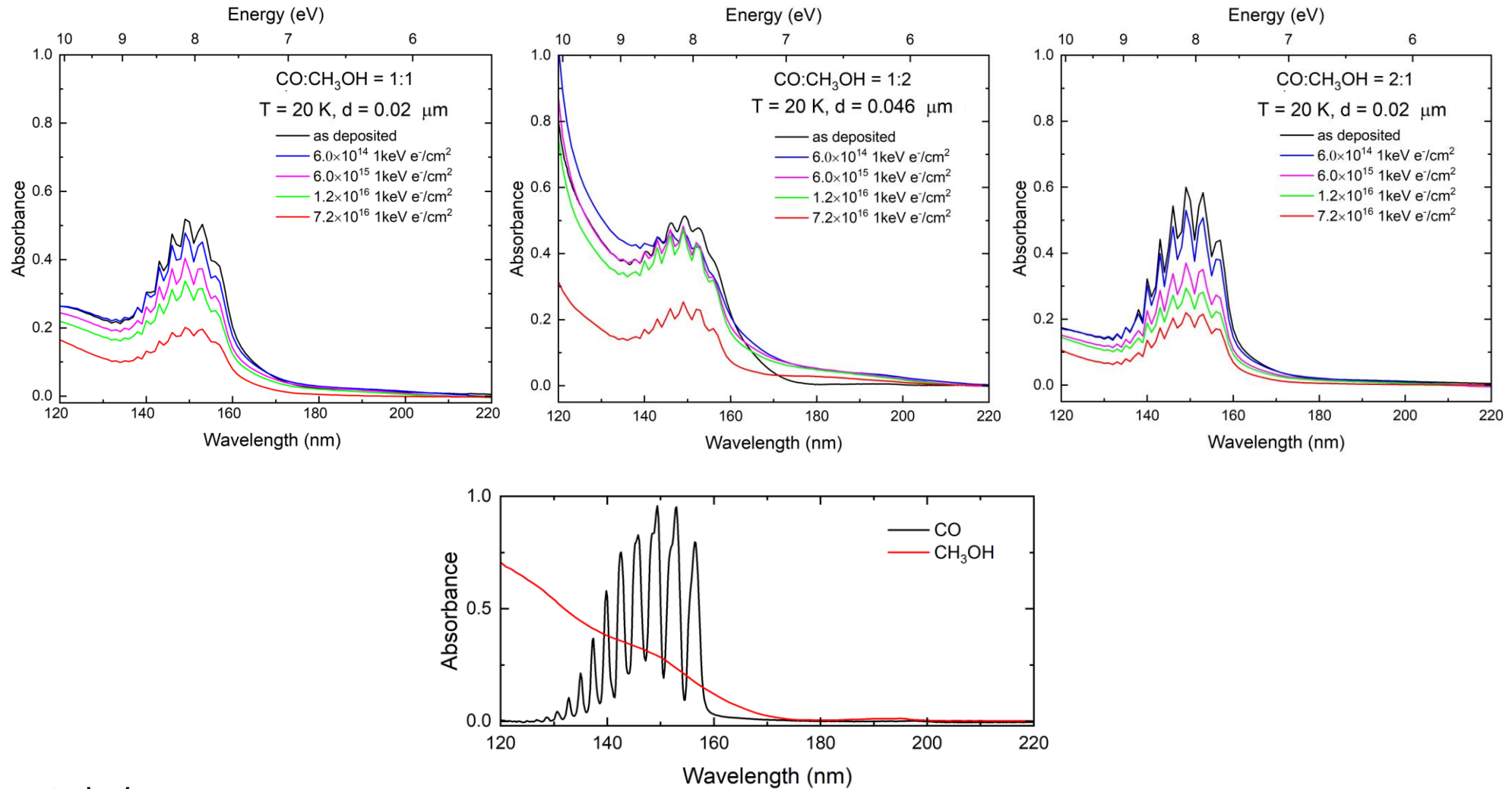
Exploring the emergence of habitable worlds around gas giants

The diagram illustrates the JUICE mission. It shows Earth, Europa, Ganymede, and Callisto. Below each moon is a cross-section showing its internal structure. A key indicates the composition: ice (white), water (blue), rock (grey), and metal (black). The JUICE spacecraft is shown orbiting Jupiter.

Credit: ESA

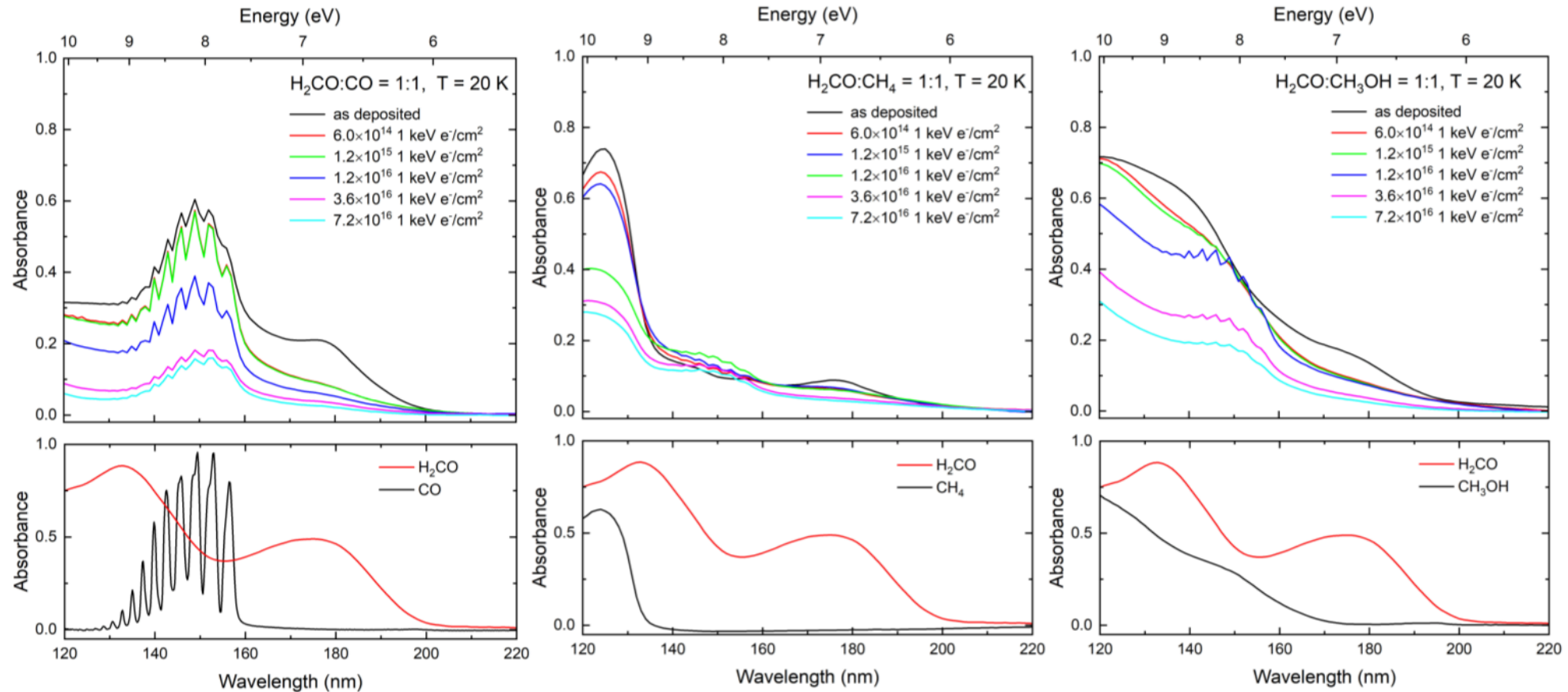
Formation of MF Isomers in space

MeOH-rich + 1 keV e⁻



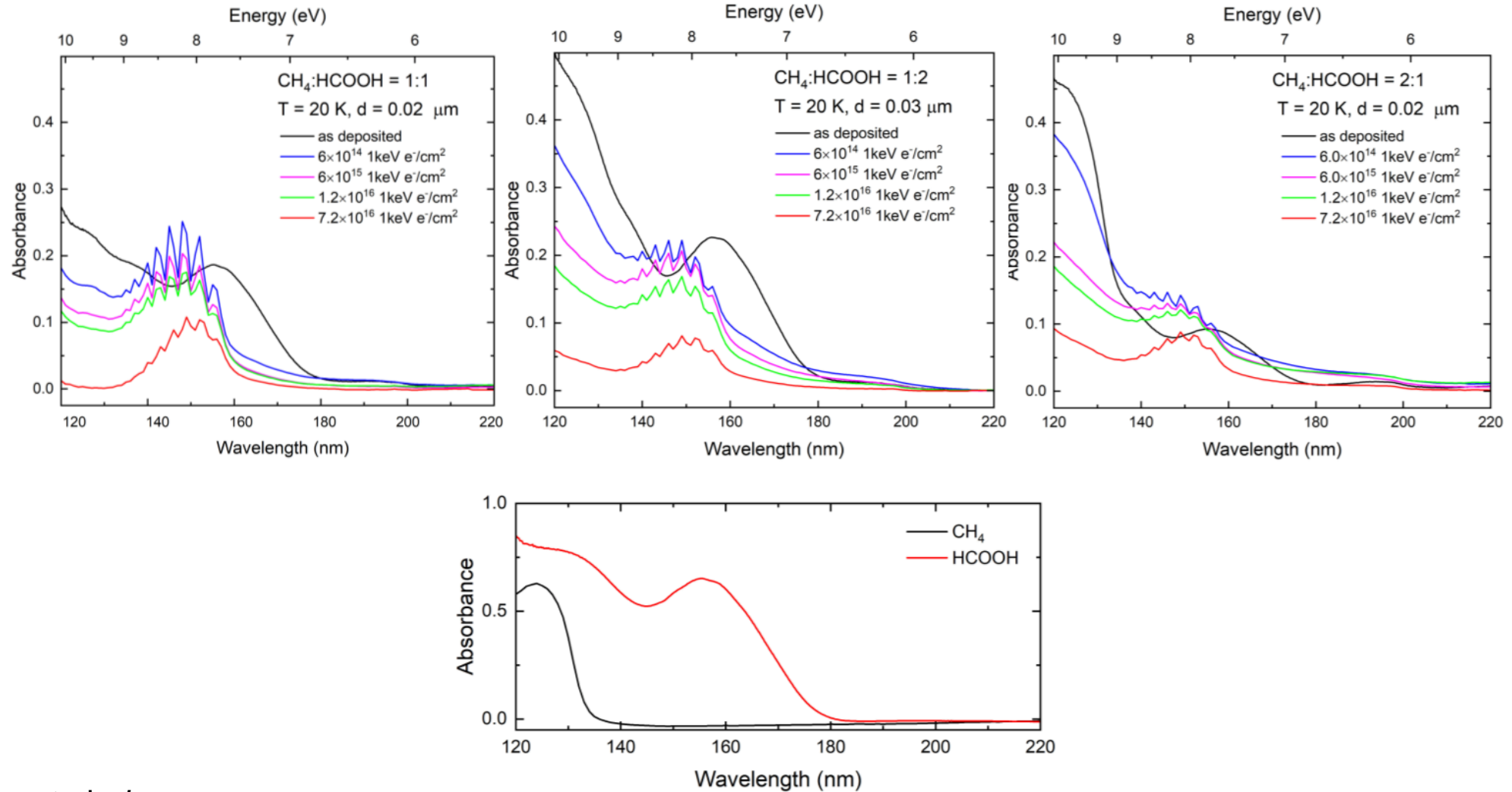
Formation of MF Isomers in space

H_2CO -rich + 1 keV e^-



Formation of MF Isomers in space

$\text{CH}_4:\text{HCOOH} + 1 \text{ keV } e^-$



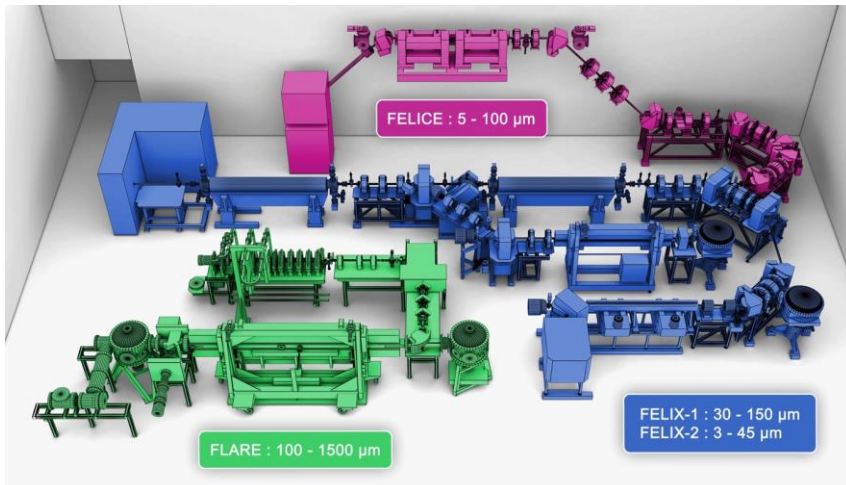
HFML-FELIX



Radboud Universiteit Nijmegen



Radboud University
Nijmegen, The Netherlands



Lab Ice Surface Astrophysics (LISA)

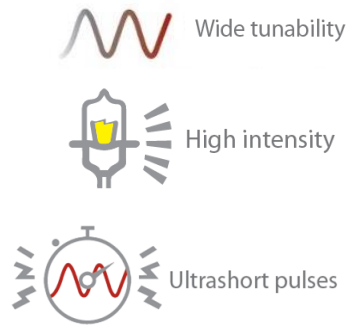
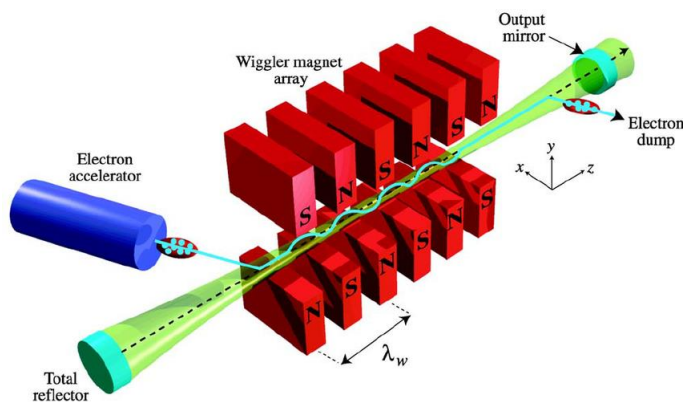
End Station at FEL-1 & FEL-2 (2.7 – 150 μm):

UHV Chamber ($P = 1 \times 10^{-10}$ mbar $T = 8 - 450$ K)

Analytical Tools (FTIR & QMS)

Sample Manipulation (Rotation + XYZ)

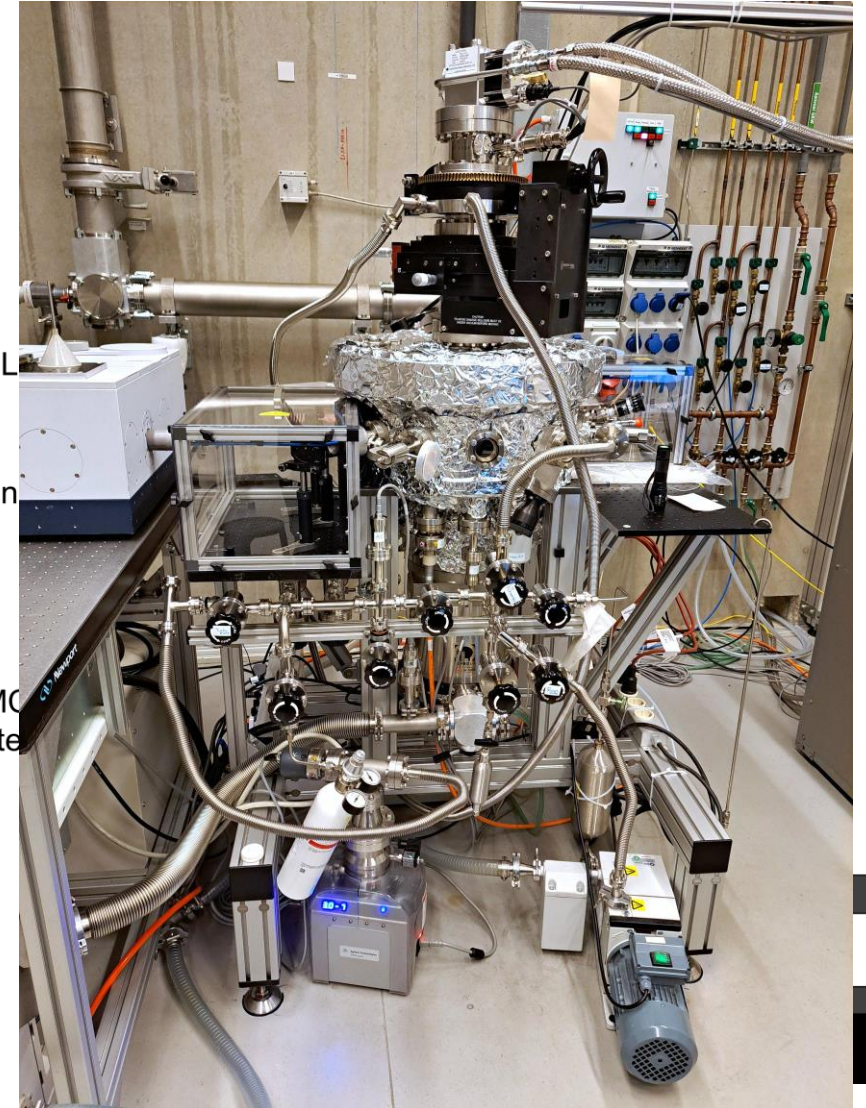
Source (5 keV electron gun)



Dosing L

5 keV
electron gun

MO
Dete



Lab Ice Surface Astrophysics (LISA)

LISA is open to internal and external users:

Selective IRFEL-induced Changes in Ices

Simulating: IR radiation, exothermic surface reactions,
CRs heating, ice grain collisions, and shocks

Selective IR-induced Phase Changes in Ices (India)

Selective IR-induced Diffusion of Molecules (UK)

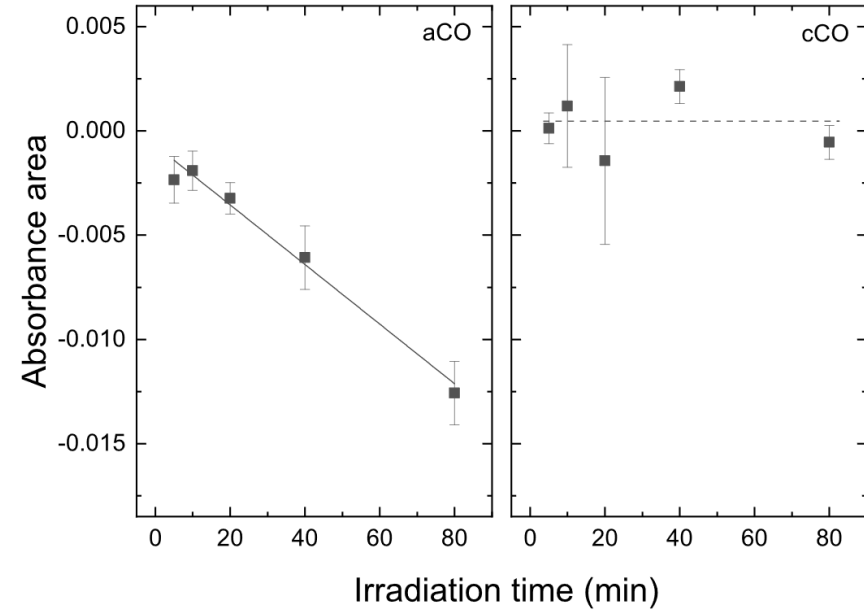
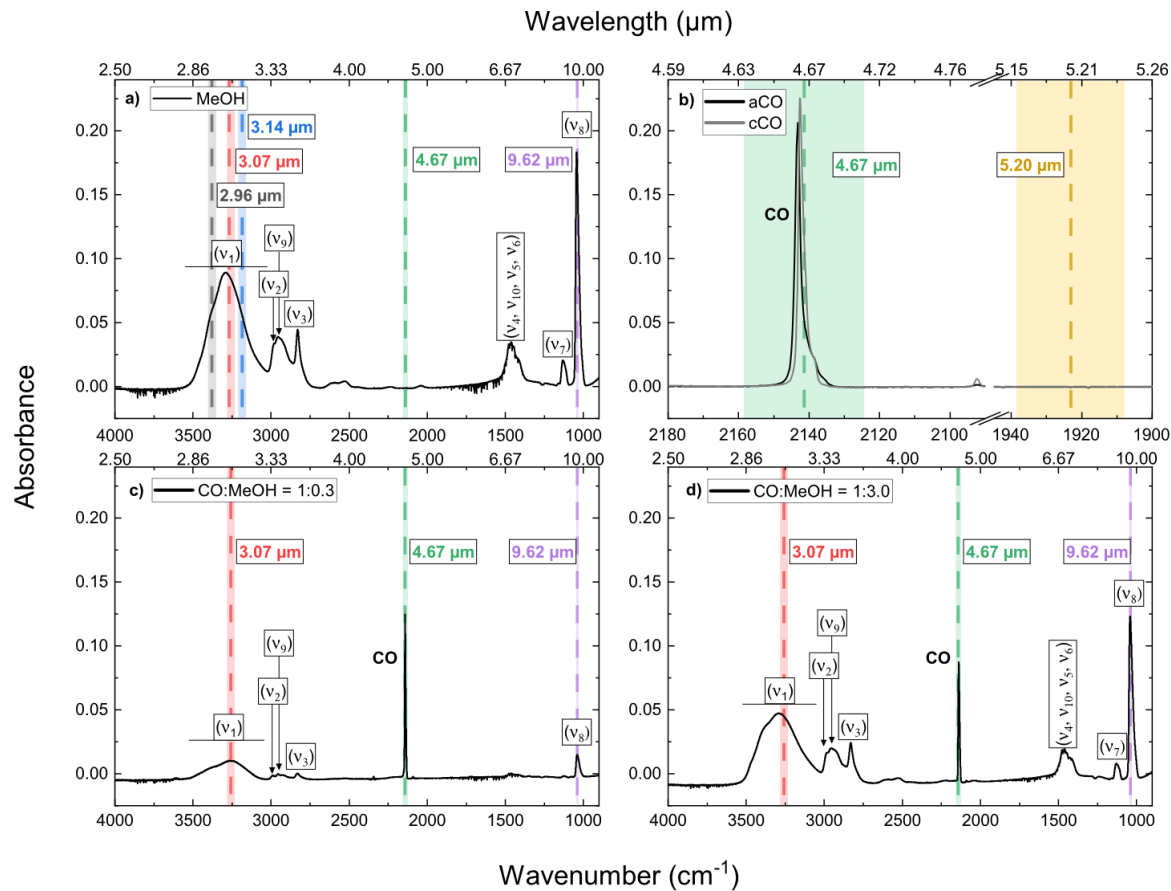
Desorption Induced upon Vibrational Excitation (NL)

Selective IR-induced Chemistry in PAHs (DK)



Desorption Mechanisms

IR Photodesorption



Desorption Mechanisms

IR Photodesorption

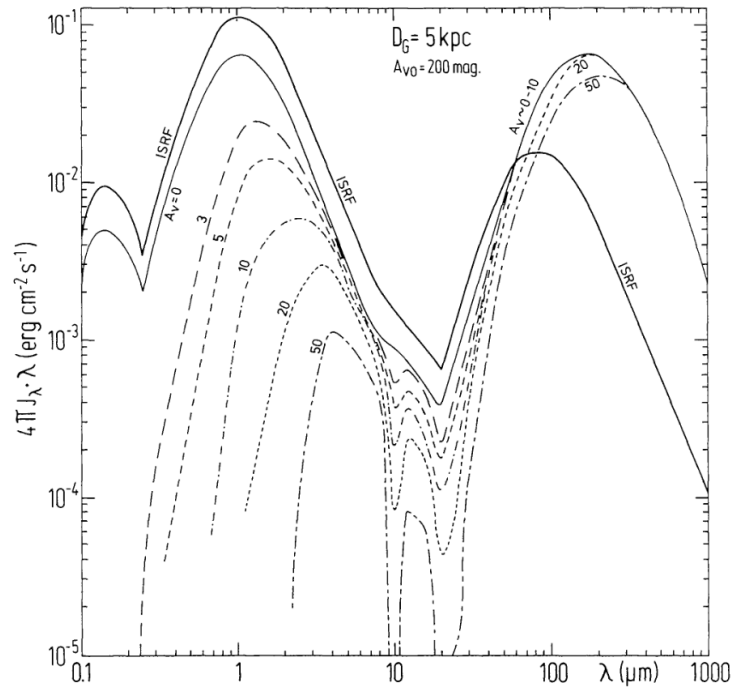


Fig. 4. The radiation field inside a giant molecular cloud, located at $D_G = 5$ kpc and with a visual extinction to its center of $A_{V_0} = 200$ mag. ISRF refers to the radiation field at far distances from the cloud, $A_V = 0$ is the radiation field at the surface of the cloud, $A_V = 3, 5, 10$ etc. is the radiation field inside the cloud at distances $A_V = 3, 5, 10$ etc. mag from the surface of the cloud

Table 2. Comparison of the estimated fluxes, desorption rates, and desorption efficiencies of CH_3OH and CO species induced by IR and UV photons.

		Interstellar flux (photons $\text{cm}^{-2} \text{s}^{-1}$)	Rate (molecules photon^{-1})	Estimated efficiency (molecules $\text{cm}^{-2} \text{s}^{-1}$)
CO	IR	$> 3 \times 10^9$ ^(a)	$\lesssim (1.1 \pm 0.3) \times 10^{-8}$ ^(c)	$\sim 3.3 \times 10^1$
	UV	$\sim 1 \times 10^4$ ^(b)	$\sim (0.14\text{--}8.9) \times 10^{-2}$ ^(d)	$\sim (1.4\text{--}89) \times 10^1$
CH_3OH	IR	$> 4 \times 10^8$ ^(a)	$\lesssim (3 \pm 1) \times 10^{-8}$ ^(c)	$\sim 1.2 \times 10^1$
	UV	$\sim 1 \times 10^4$ ^(b)	$\sim 1 \times 10^{-5}$ ^(e)	$\sim 1.0 \times 10^{-1}$

References. ^(a)Mathis et al. (1983). ^(b)Cecchi-Pestellini & Aiello (1992). ^(c)This work. ^(d)Öberg et al. (2007); Muñoz Caro et al. (2010); Fayolle et al. (2011); Chen et al. (2014); Paardekooper et al. (2016). ^(e)Bertin et al. (2016); Cruz-Diaz et al. (2016).

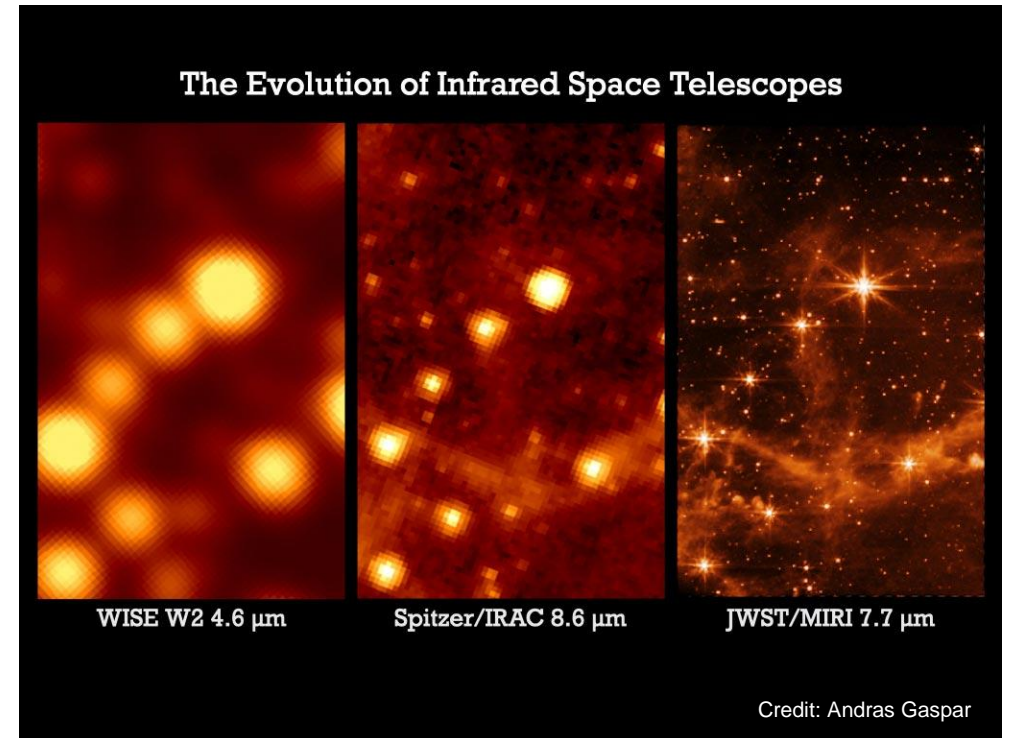
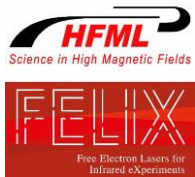
Conclusions

JWST is revolutionizing our understanding of star formation in the ISM

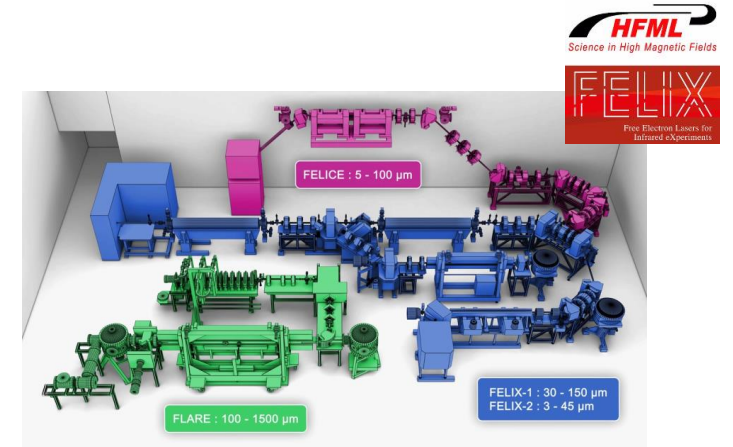
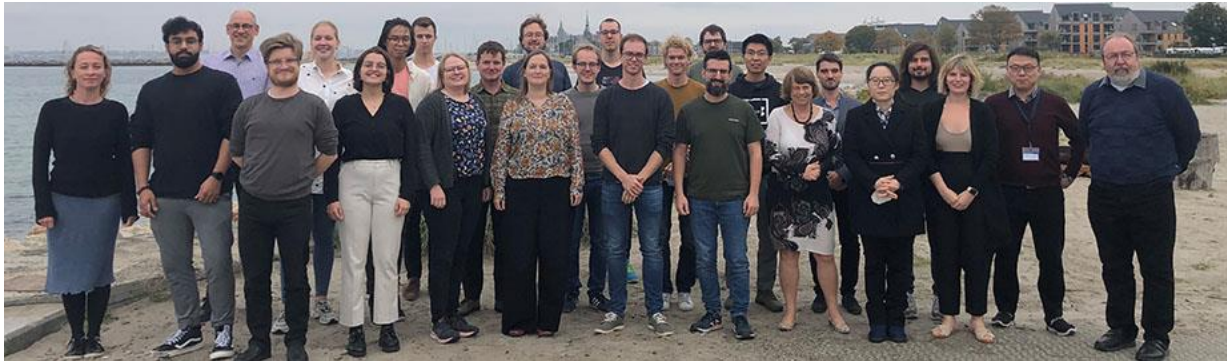
New systematic and consistent set of lab data are needed!

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

External users and new ideas are welcome!



Acknowledgements



Lab Ice Databases

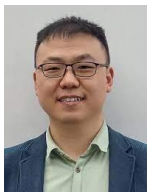
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Dr Duncan Mifsud



Dian Schrauwen