Astrophysical ices as a source of molecular diversity in gas and solid phases

Grégoire DANGER

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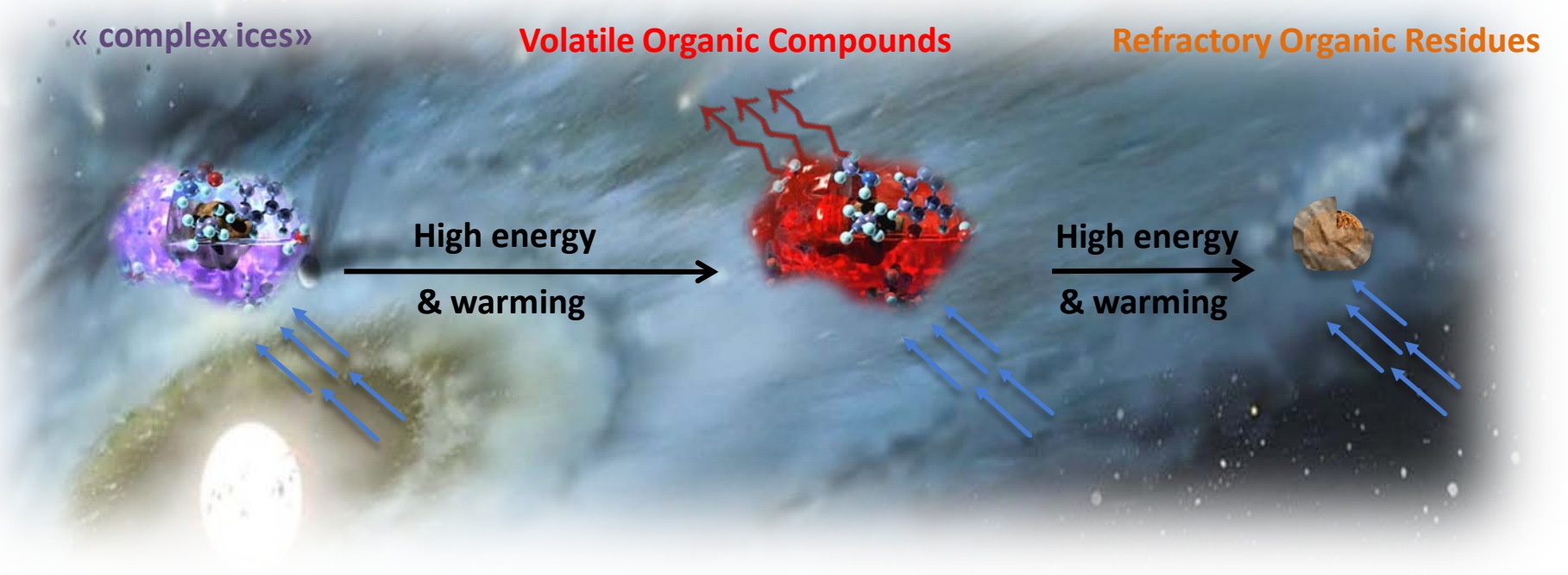
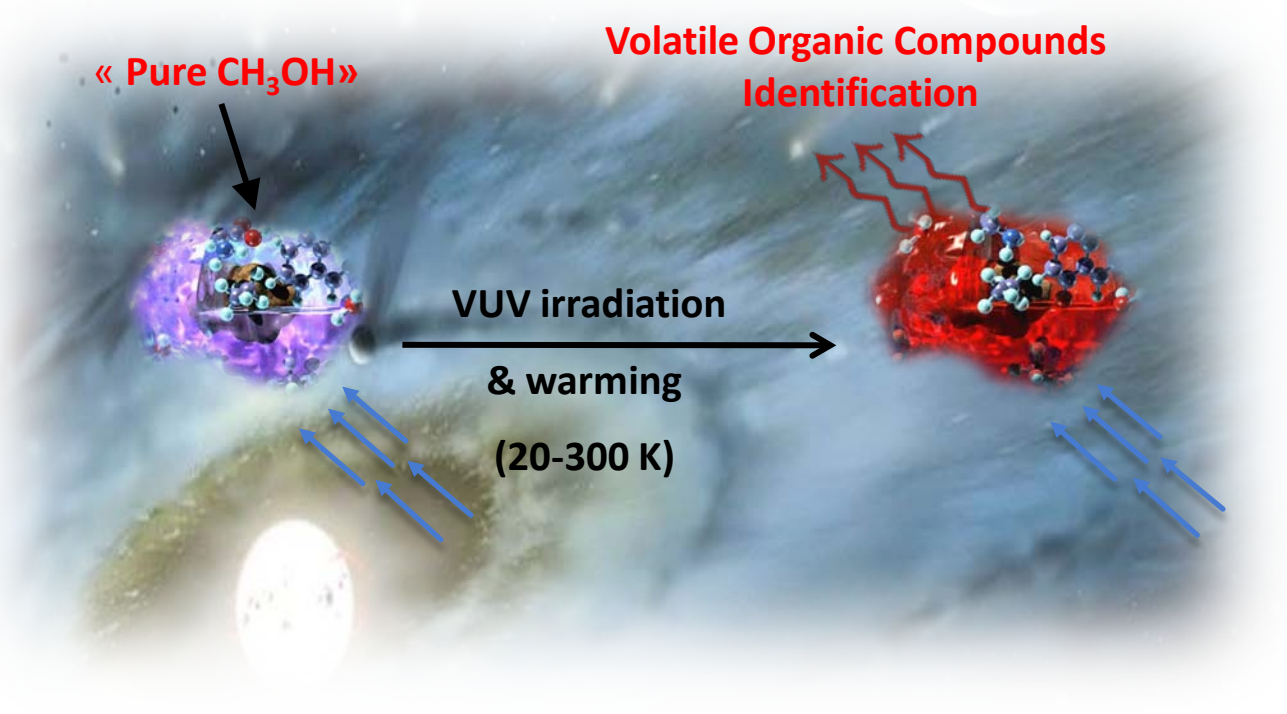
Collaborations:

Astrophysical ices as a source of molecular diversity



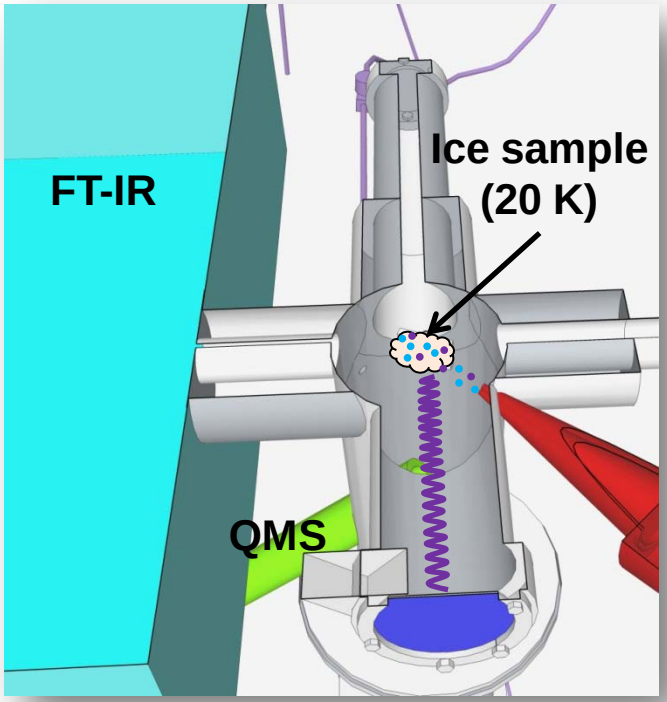
Methanol CH_3OH
An abondant source of reduces carbon in interstellar and cometary ices



Principle of the VAHIIA device
Recovery and analysis of VOC by GC-MS

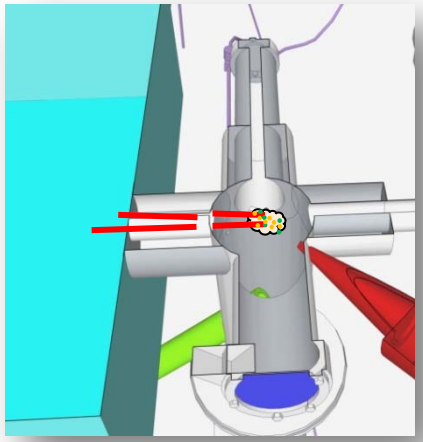
ANR-12-JS08-0001
2012-2015

Vacuum chamber (10^{-9} mbar)



GC-MS

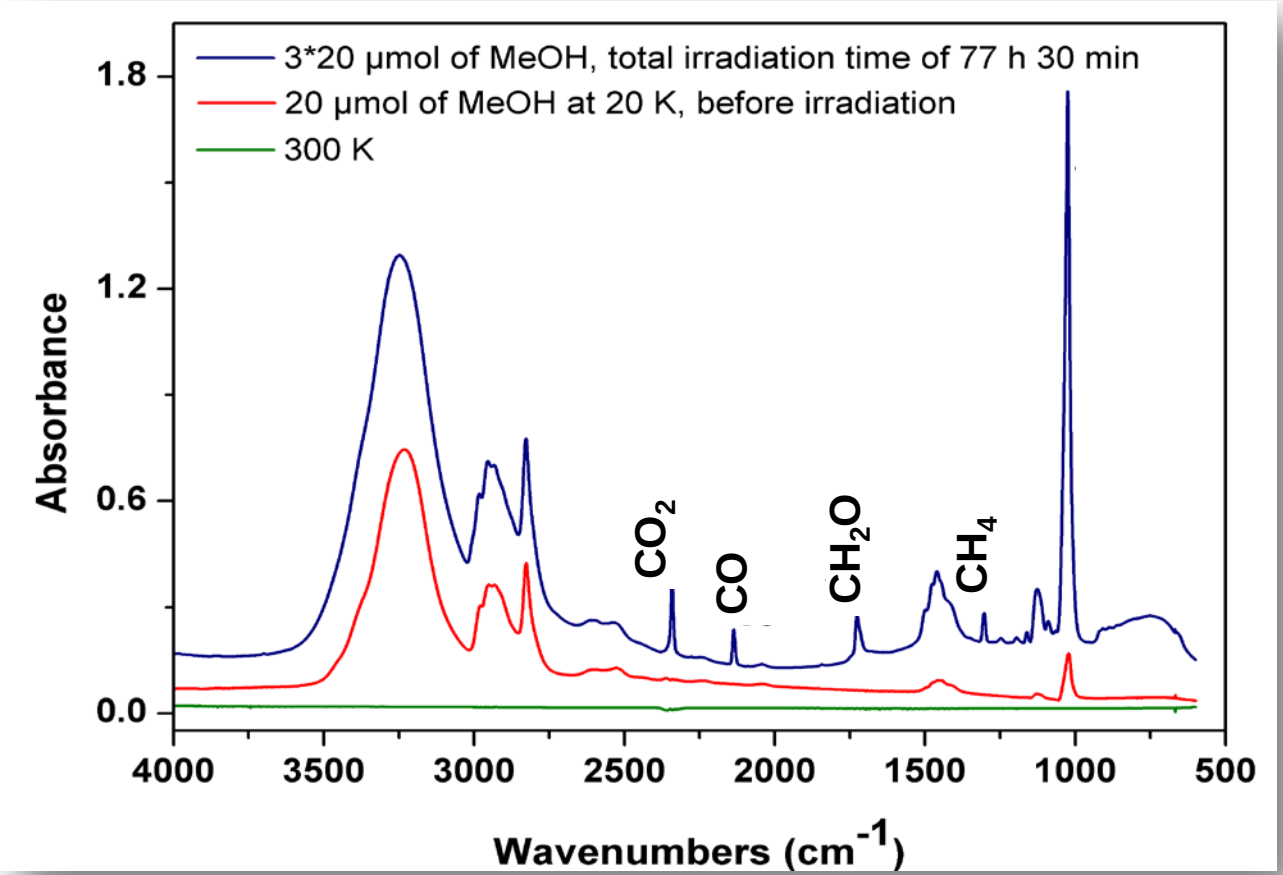
FTIR



Ice formation in simulated conditions

Abou Mrad et al., Anal. Chem., 2014, 86, 8391

Methanol CH_3OH
Analysis with the VAHIIA system



Infrared spectroscopy at 20K:

Non ambiguous Identification of CH_4, CO, CO_2 & formaldehyde

Abou Mrad et al., MNRAS, 2016, 458,1234

Methanol CH_3OH
Analysis with the VAHIIA system – products identified

C_1
CO
Carbon monoxide
CO_2
Carbon dioxide
CH_2O
Formaldehyde
HCOOH
Formic acid
CH_4
Methane

C_2
Ethanol
Acetaldehyde
Dimethylether
Glycolaldehyde
Acetic acid
Methyl formate
C_2H_6
Ethane
Ethylene glycol

C_3
Propan-1-ol
Methyl acetate
Propan-2-ol
Propionaldehyde
Dimethoxymethane
Acetone
Glycerol

C_4
2-methyl-1-propanol
Butan-1-ol
2-butanol
Ethyl acetate
Butyraldehyde
2-butanone
Methyl propionate

35 molecules identified

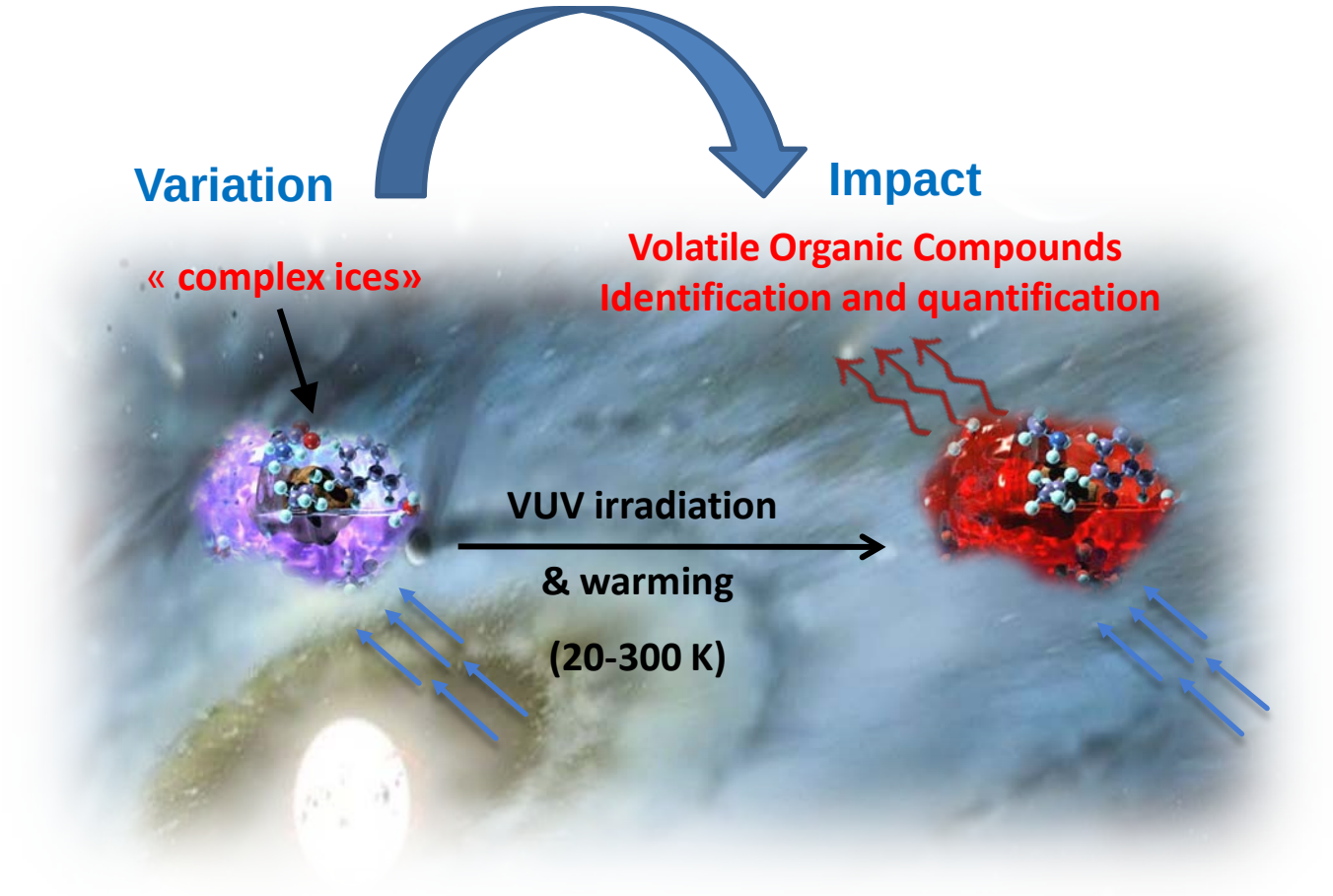
Gerakines et al., A&A, 1996, 312, 289
Oberg et al., A&A, 2009, 504, 891
Henderson et al., ApJ, 2015, 800, 66
Maity et al., PCCP, 2015, 17, 3081
Kaiser, Angew. Chem., 2015, 54, 195

C_5
2-methyl-1-butanol
2-pentanone
Methyl butyrate
3-methyl-1-butanol
Pentanal
3-methyl-2-butanol
2-2-dimethyl propanol
2-methyl butyraldehyde

C_6
2,2-dimethyl butanal
4-methyl-2-pentanone
Hexanal
2-methyl pentanal

Abou Mrad et al., MNRAS, 2016, 458,1234

Complex ices
Impact of the ice composition on VOC abundances detected in the gas phase



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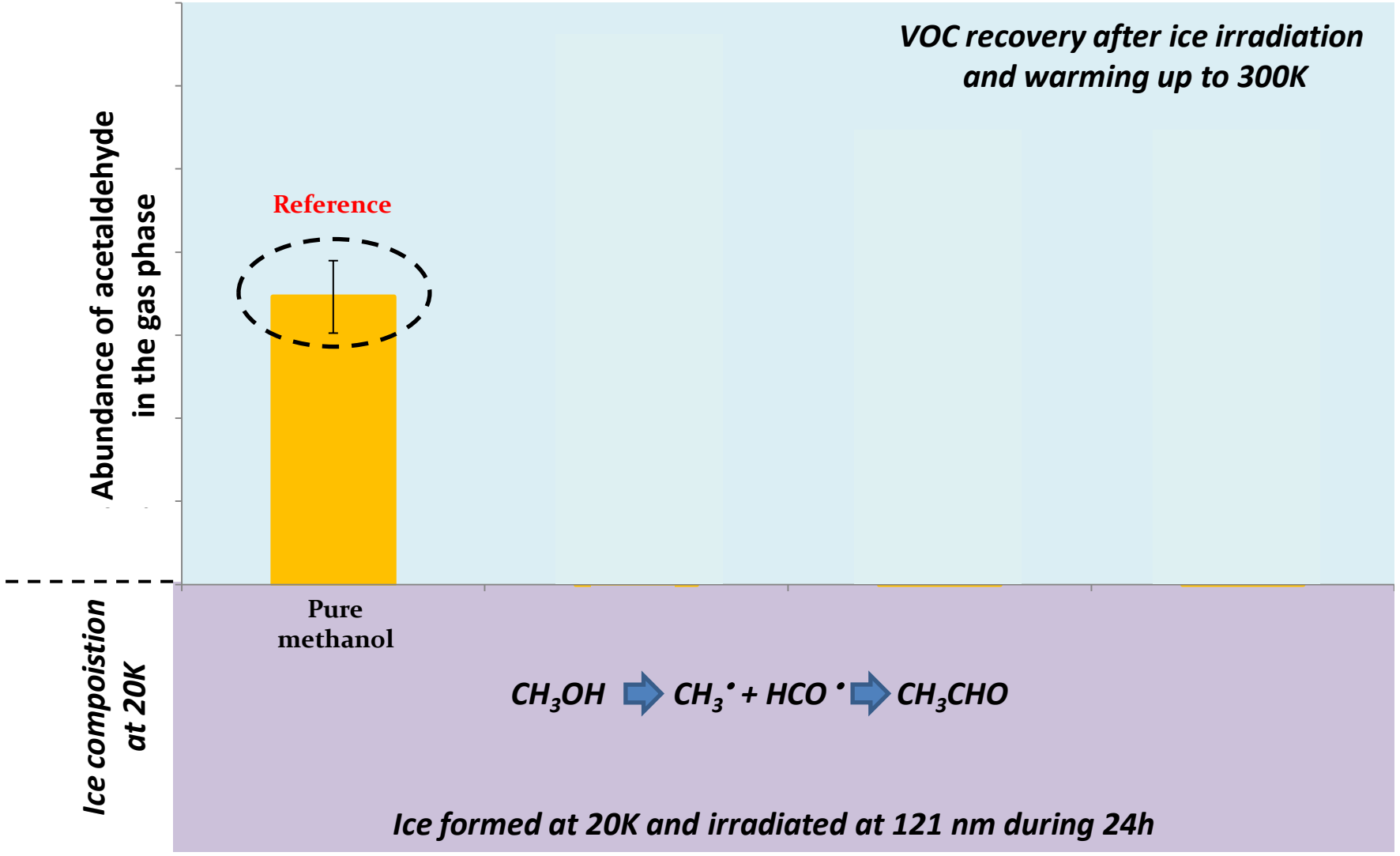
Impact of the ice composition on VOC abundances detected in the gas phase

Abou Mrad et al., ApJ, 2017, 846, 124

VOC example: Acetaldehyde



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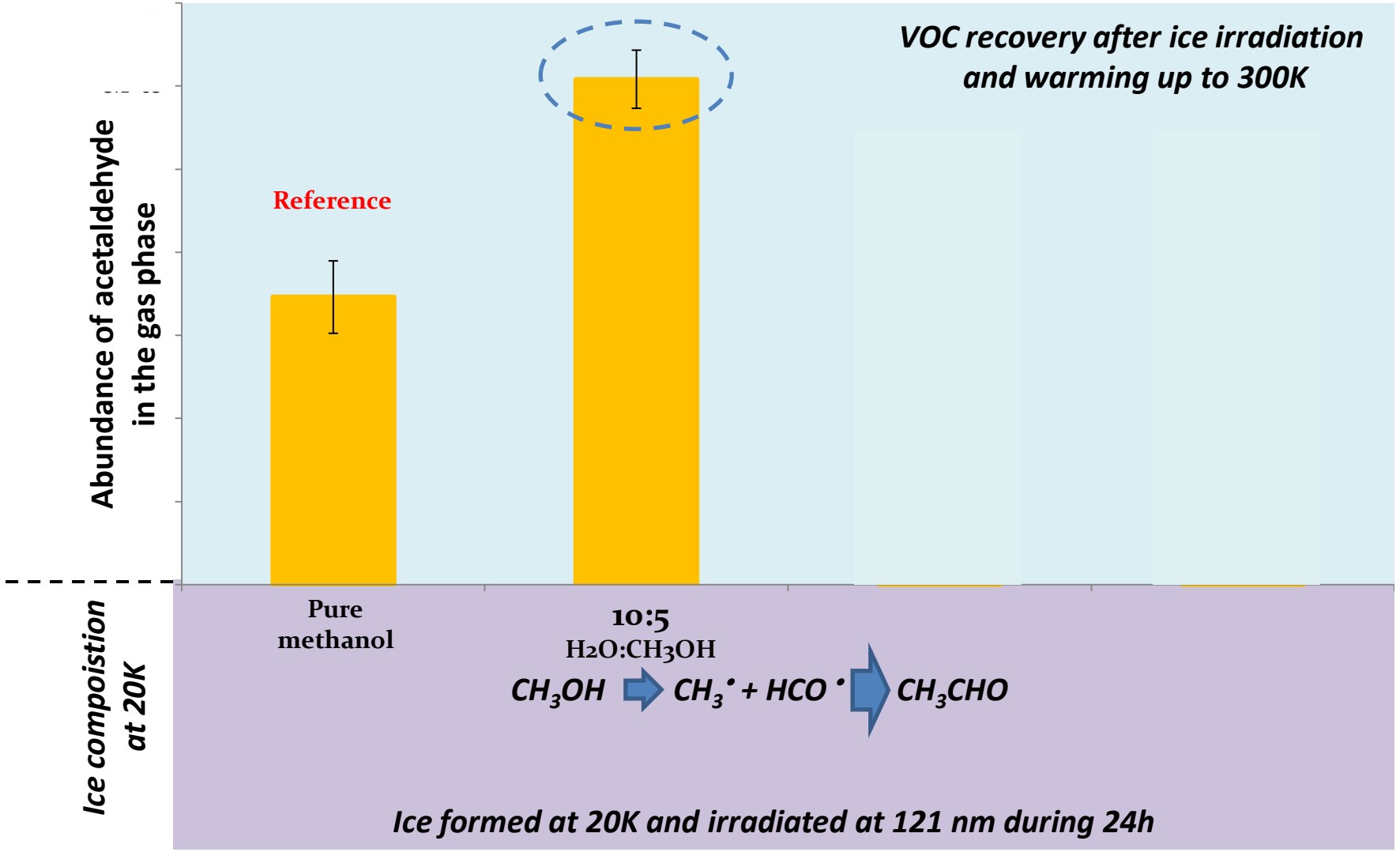

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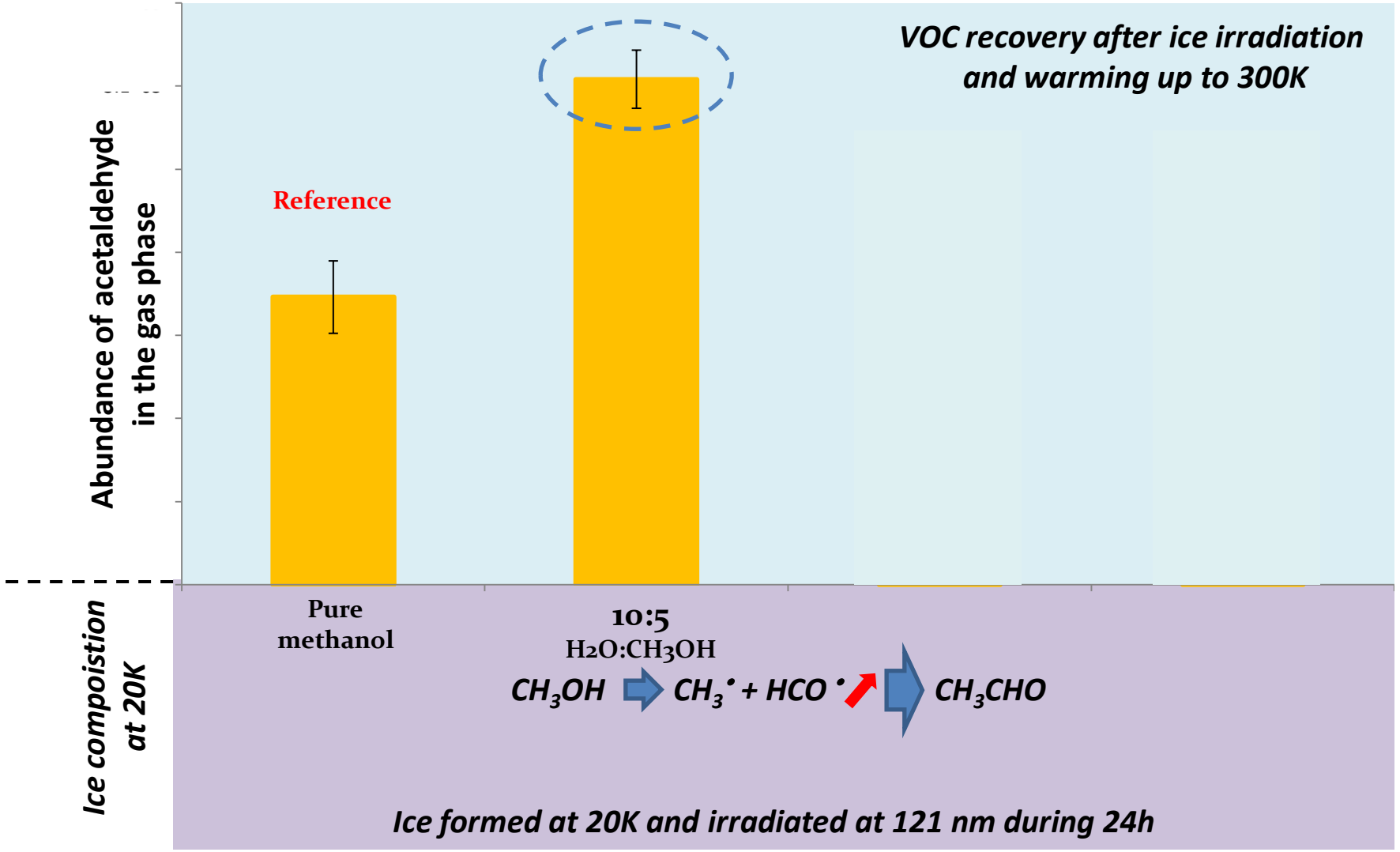

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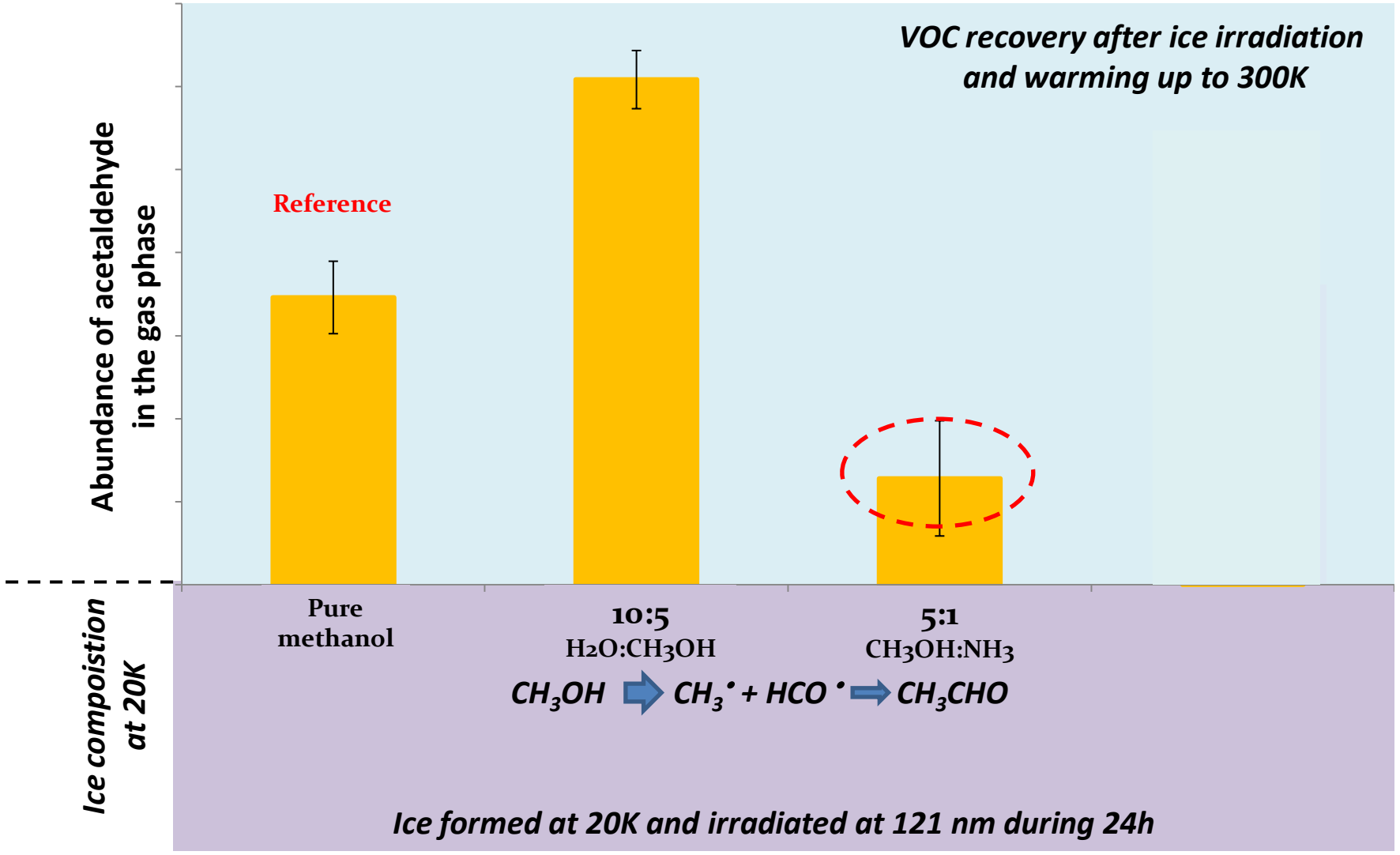

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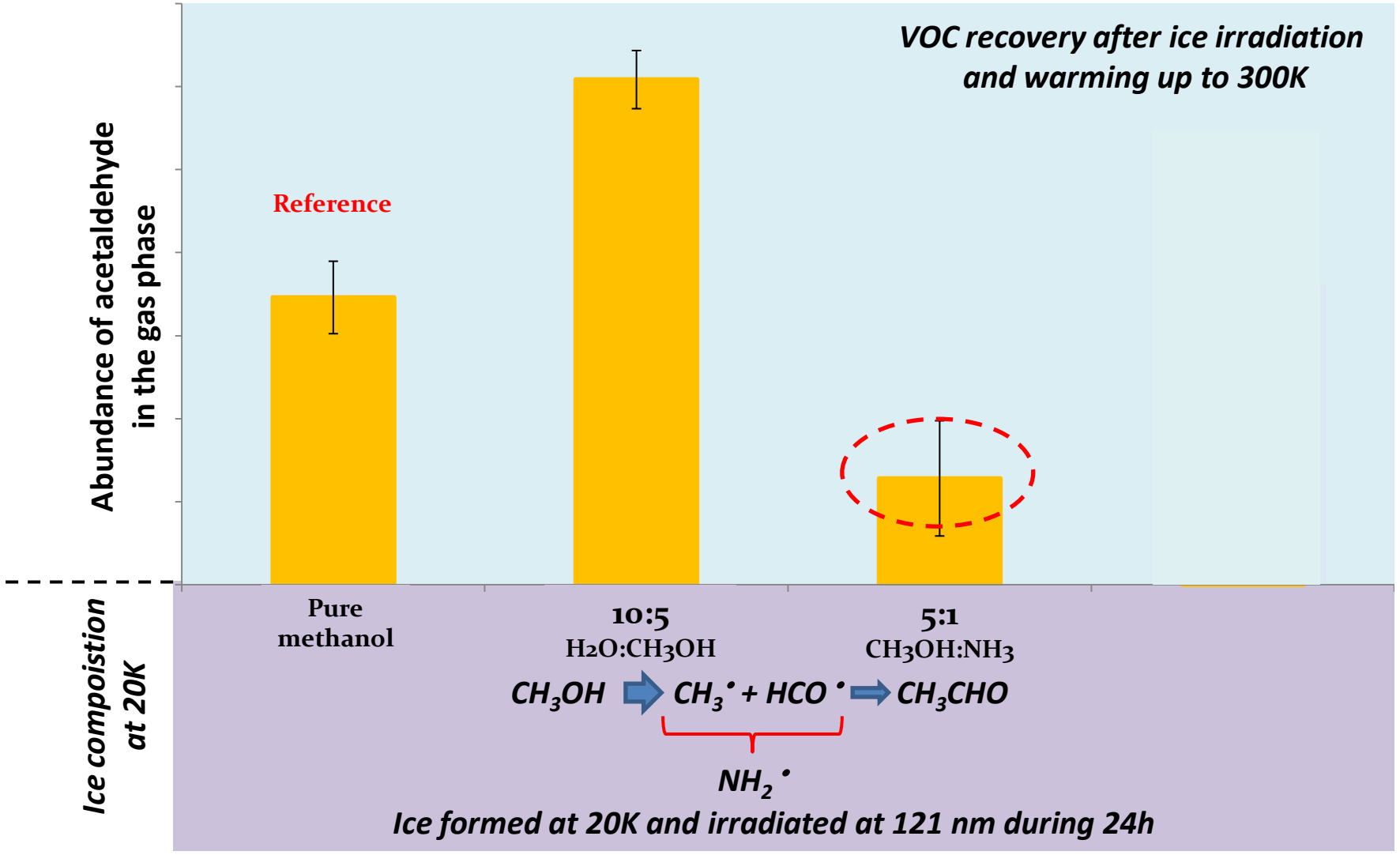

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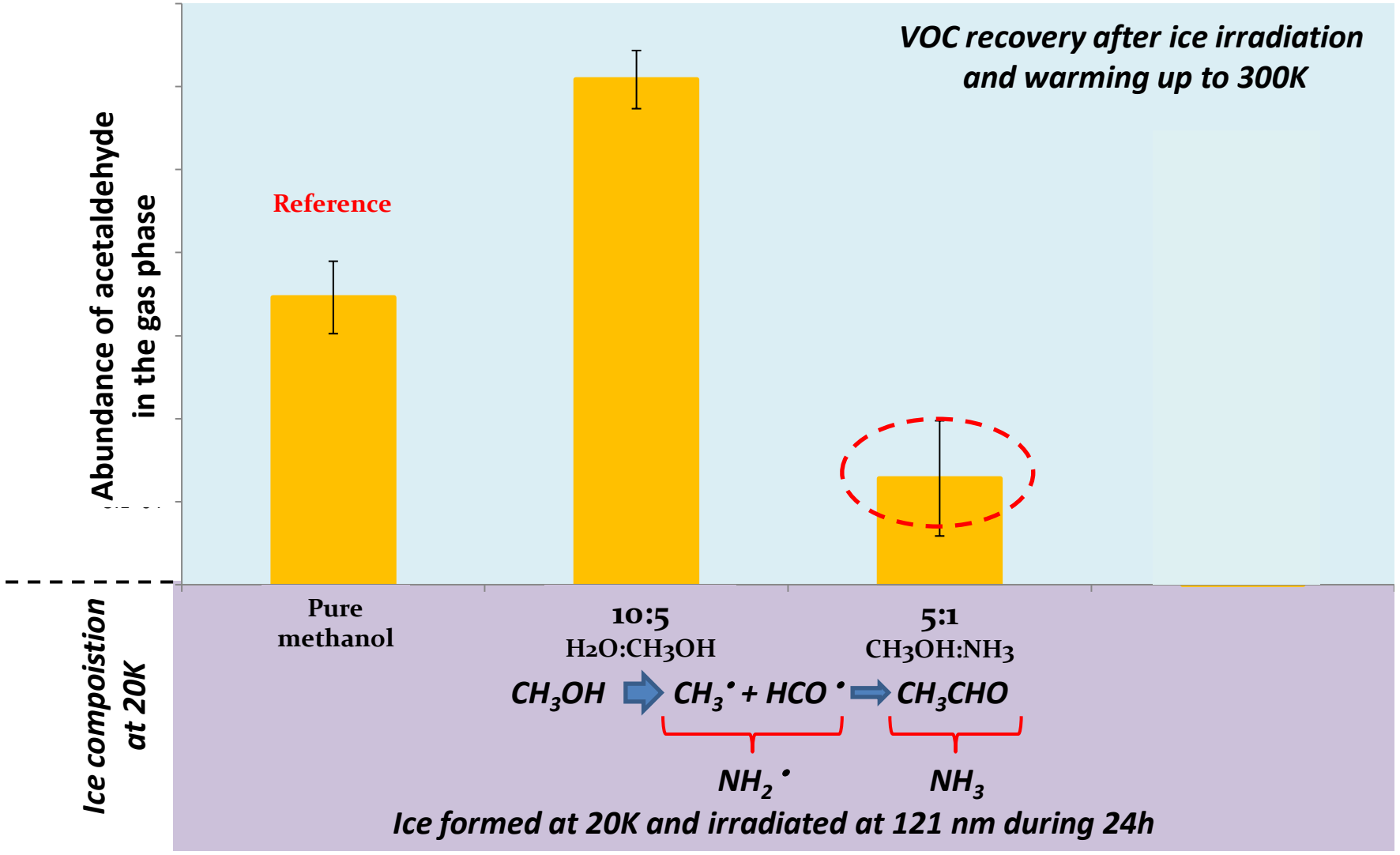

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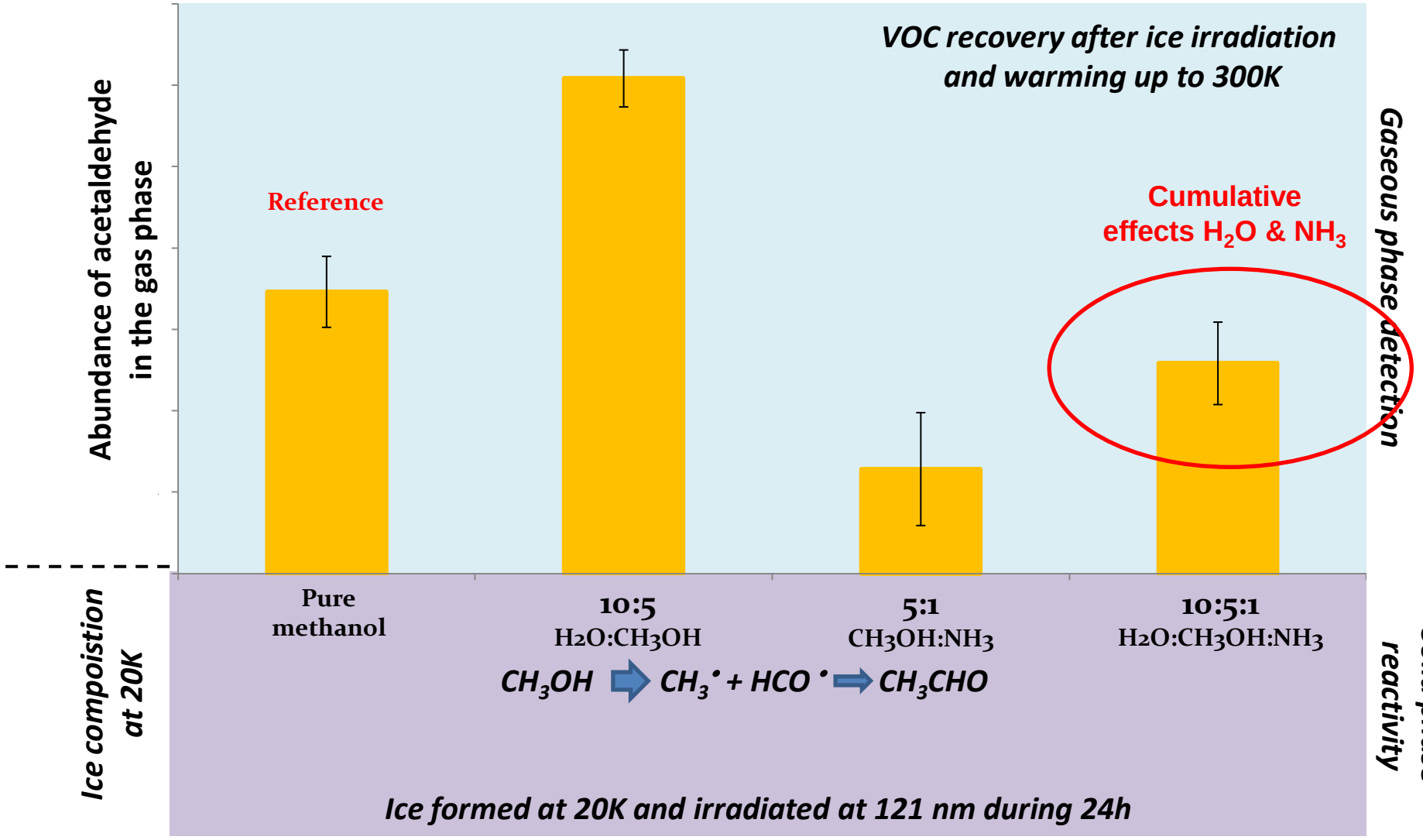
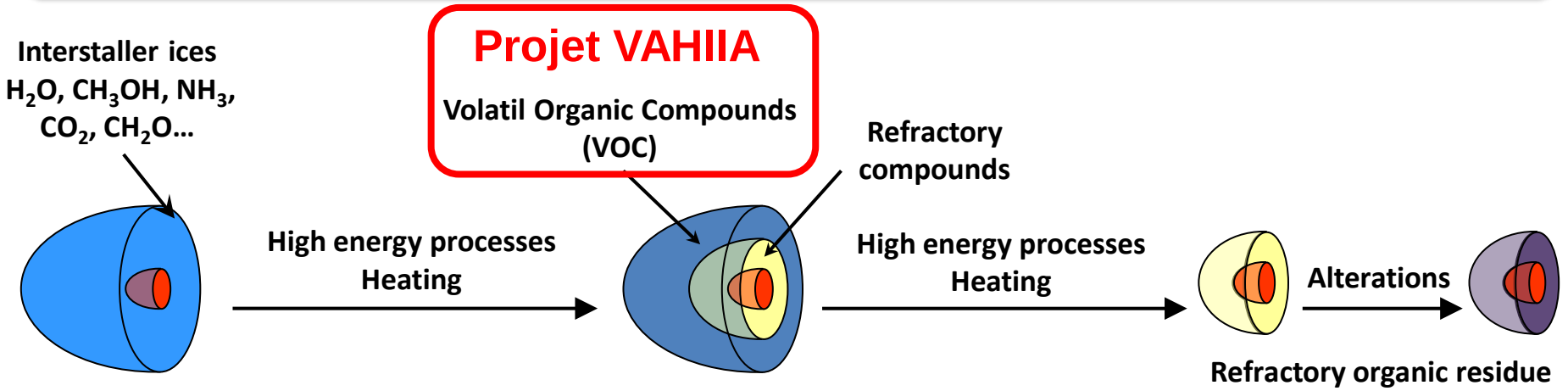


Evolution of interstellar icy grains
Toward the formation of complex organic matter in interplanetary bodies



Chemistry in diluted environment
20 K – 150 K

Radical and Thermal reactivities in water ice

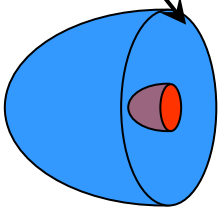
Formation of small complex organic molecules

Water matrix restructuration and water desorption
150 K – 185 K

① Main desorption of VOCs

Evolution of interstellar icy grains
Toward the formation of complex organic matter in interplanetary bodies

Interstaller ices
H_2O, CH_3OH, NH_3,
CO_2, CH_2O…

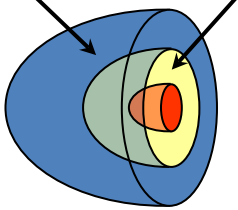


High energy processes
Heating

Projet VAHIIA

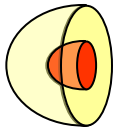
Volatil Organic Compounds
(VOC)

Refractory
compounds

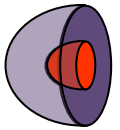


High energy processes
Heating

Projet RAHIIA



Alterations



Refractory organic residue

ANR RAHIIA_SSOM (2016-2021)

Chemistry in diluted environment
20 K – 150 K

Radical and Thermal reactivities in water ice

Formation of small complex organic molecules

Water matrix restructuration and water desorption
150 K – 185 K

① Main desorption of VOCs

② Some VOCs trapped and react in the water matrix

Chemistry in concentrated environment
> 185 K

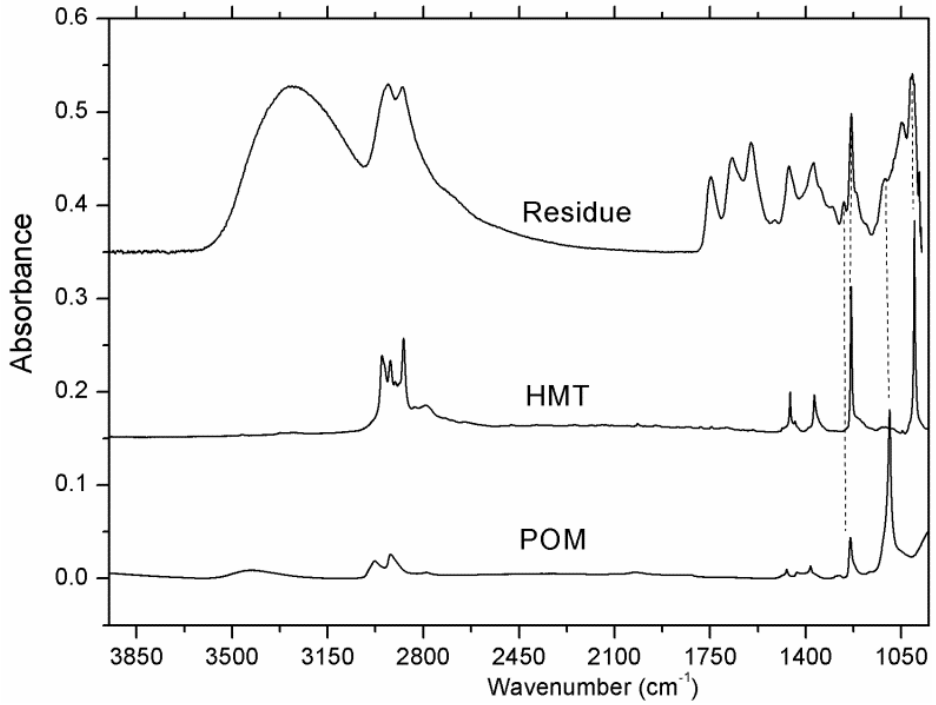
Reactivity in absence of water

Formation of « macromolecules »

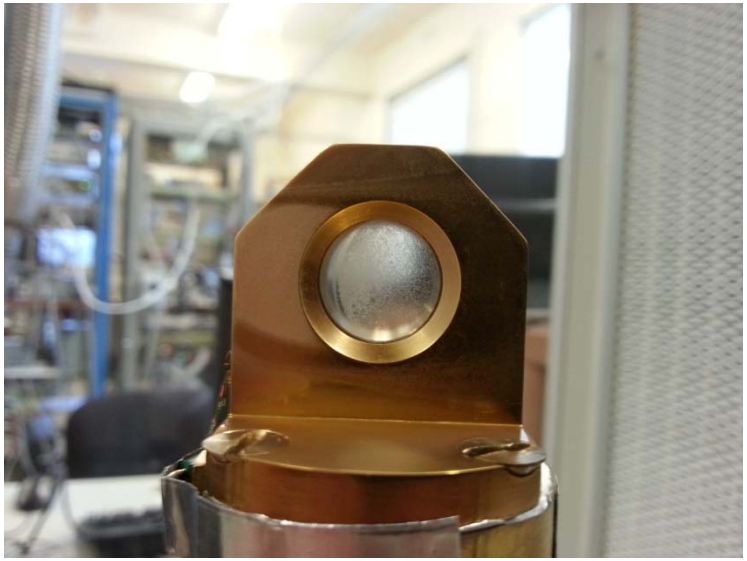
Organic residue from ice processing

ANR-16-CE29-0015
2016-2021

Most abundant molecules



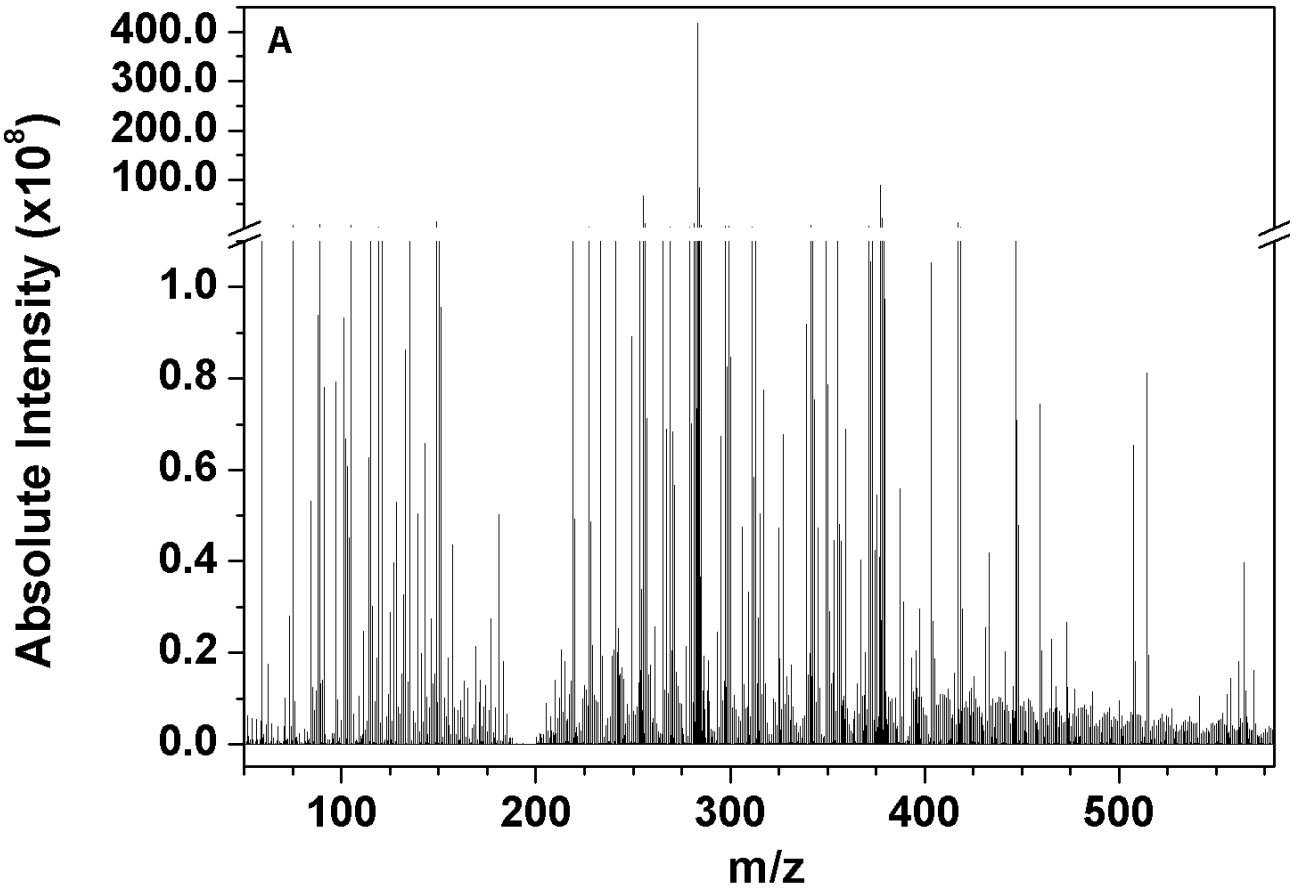
FT-IR analysis of an organic residue coming from a H_2O:CH_3OH:NH_3 ice



Images from Louis d'Hendecourt, IAS, Paris Orsay XI

http://piim.univ-amu.fr/Projet-RAHIIA

Organic residue from ice processing: untargeted analyses



FT-Orbitrap Analysis in Negative ESI mode = $[M-H]^-$ analysis

Molecules with proton donnor chemical functions (e.g. carboxylic acid –COOH)

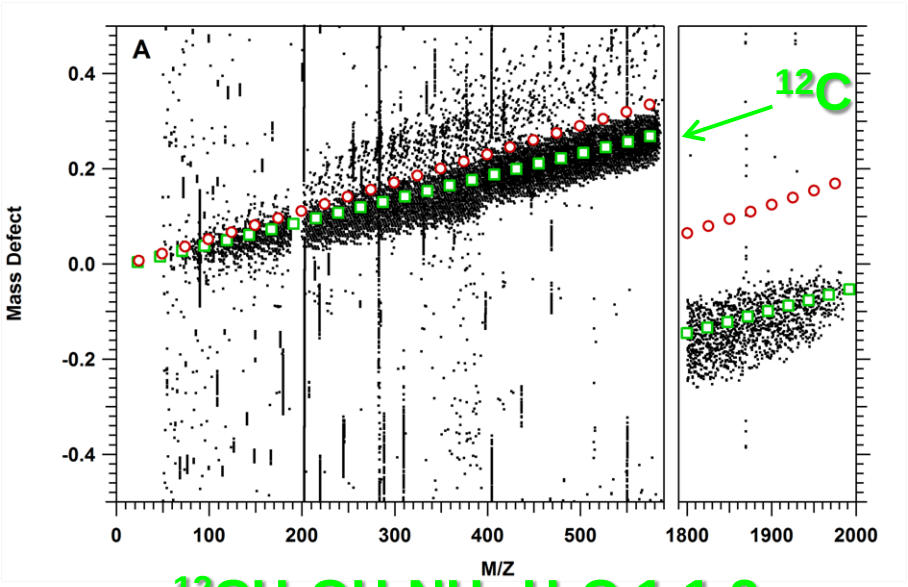
($H_2O/NH_3/CH_3OH$ =3/1/1)

Danger et al., Geochim.Cosmochim.Acta, 2013, 118 , 184-201

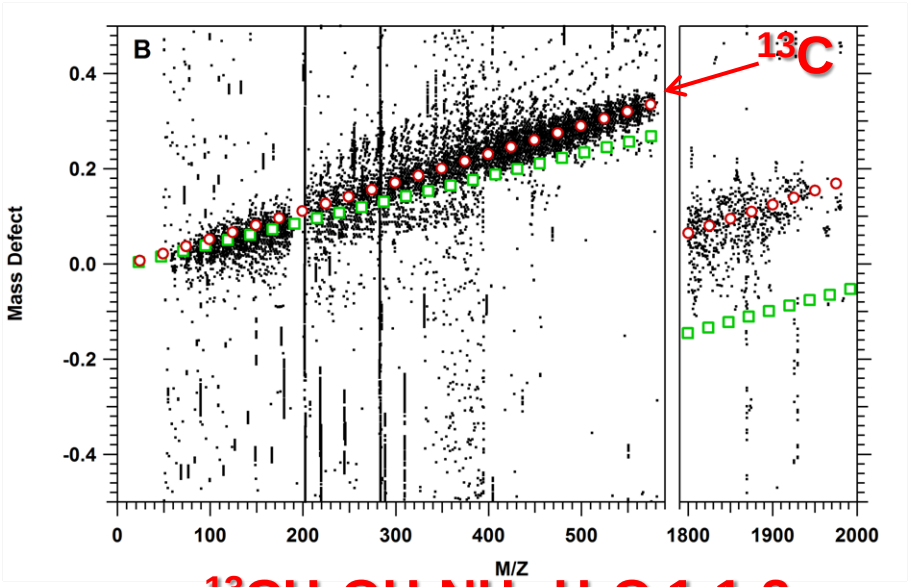
VHRMS (orbitrap) analyses of organic residues ($H_2O/NH_3/CH_3OH$ =3/1/1)

Mass Defect vs Exact Mass (MDvM)

Exact mass: 141.1128
Mass Defect: 141.1128-141= 0.1128



$^{12}CH_3OH:NH_3:H_2O$ 1:1:3



$^{13}CH_3OH:NH_3:H_2O$ 1:1:3

From an ice uniquely formed of $H_2O:CH_3OH:NH_3$
VUV + warming
=
Thousand of molecules with masses
up to 4,000 Da -> macromolecules
=
Complex and rich chemistry
=
Important molecular diversity

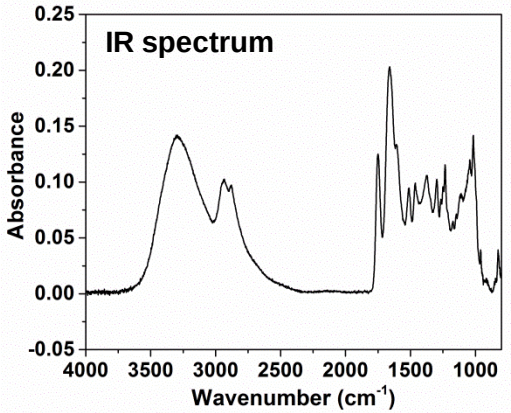
Danger et al., Geochim.Cosmochim.Acta, 2013, 118 , 184-201

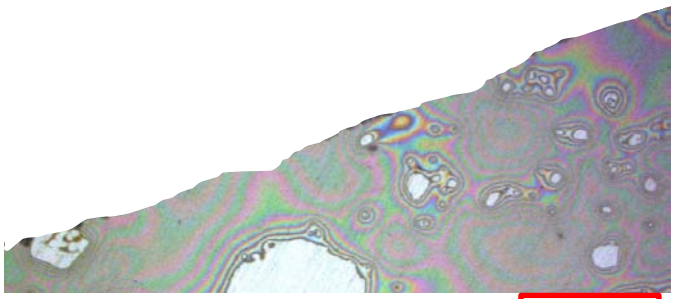
From soluble to insoluble matters

A scenario from extraterrestrial ices to soluble and insoluble materials

Residue (soluble)

300 K





residue

de Marcellus et al., MNRAS, 2017, 464, 114

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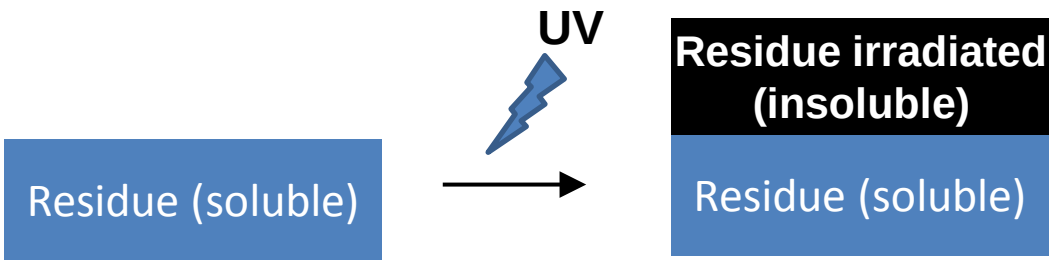
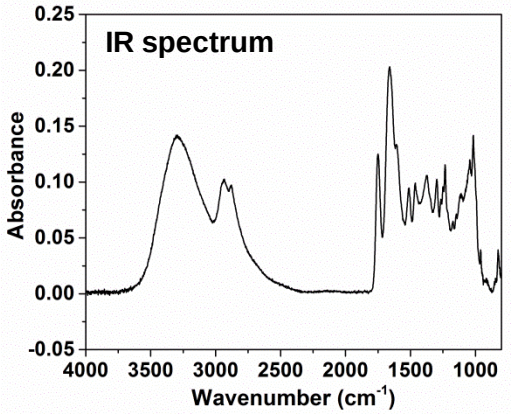


300 K



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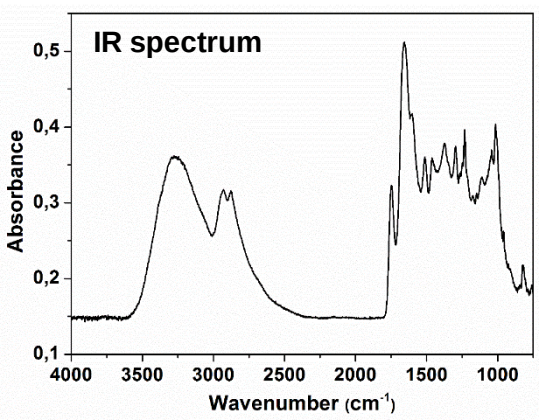

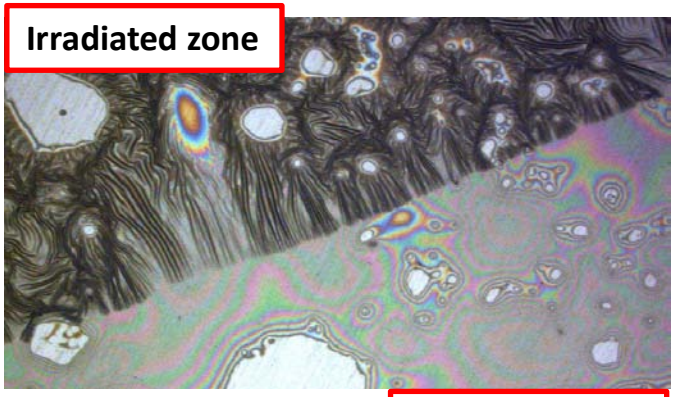

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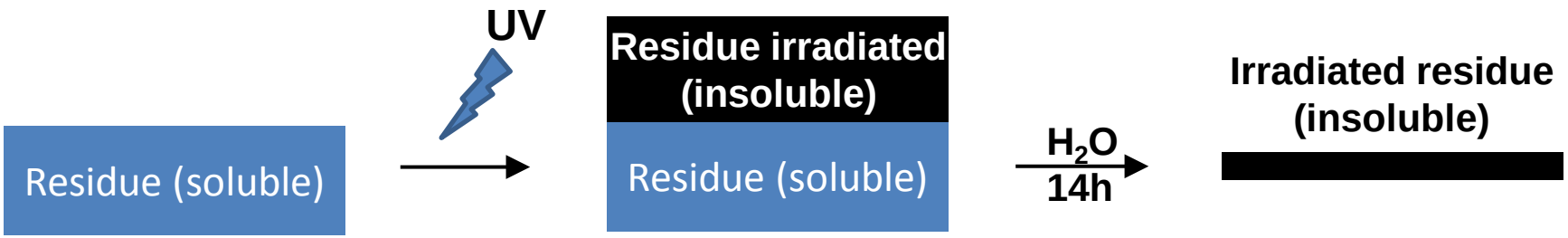

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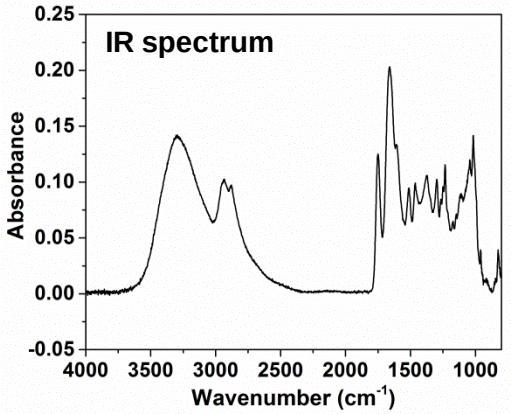

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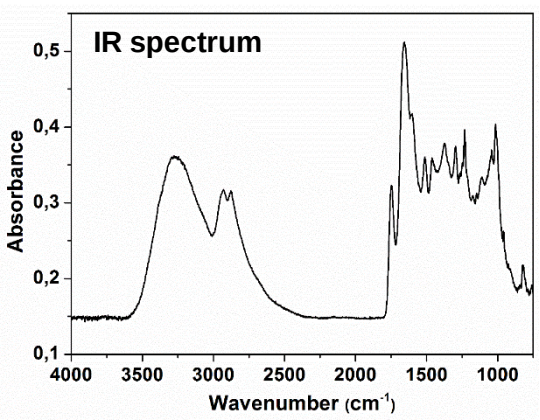

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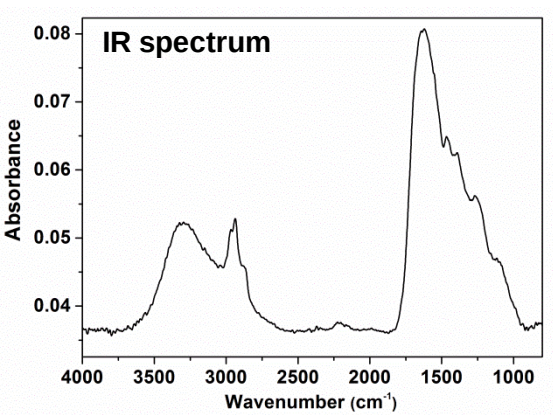
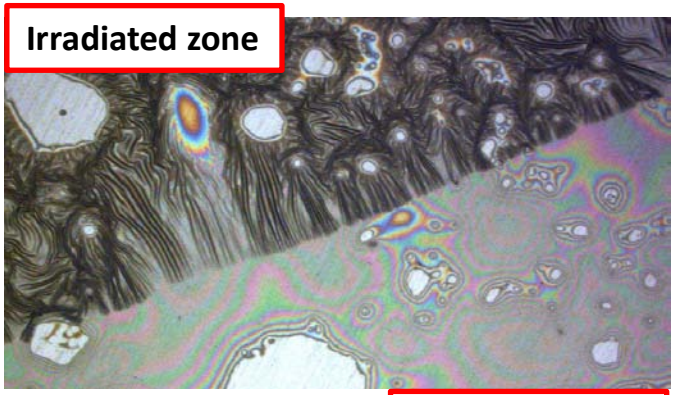
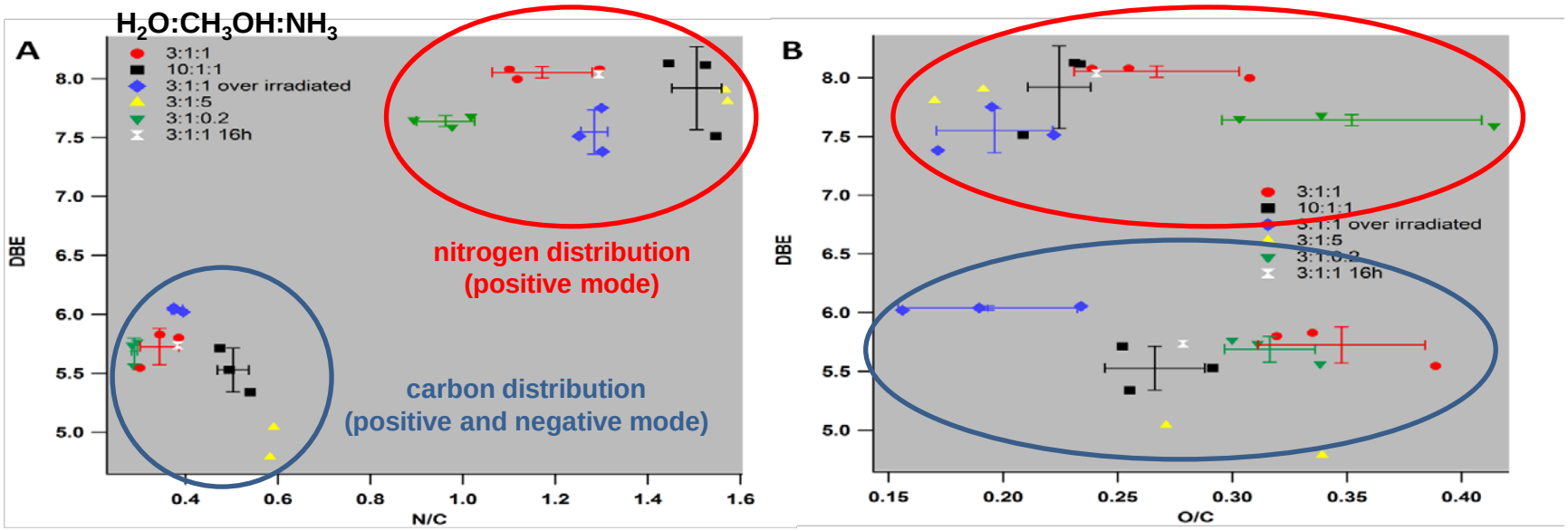




de Marcellus et al., MNRAS, 2017, 464, 114

Impact of the ice composition on residue composition



DBE vs N/C **DBE vs O/C**

① Fraction of NH_3 increases in the ice = more nitrogen in residues

② Fraction of H_2O increases in the ice = more nitrogen and oxygen depletion in residues

③ Over irradiation of residue at 300K = oxygen depletions in the soluble part of residues

radical and thermal reactivities

Development of an evolution mapping of residue depending on their modes of formation and alteration

Fresneau et al., ApJ, 2017, 837, 168

Follow the evolution of organic matter using laboratory experiments from volatile organics to organic residues

GC-MS analyses

- We could **quantify** « the consequences » of this solid phase chemistry in the **gaseous phase.**

Gas Phase

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20 K – 150 K

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