Use and non-use of laboratory results on interstellar ices

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Astronomical setting
Desorption studies
Hydrogenation studies

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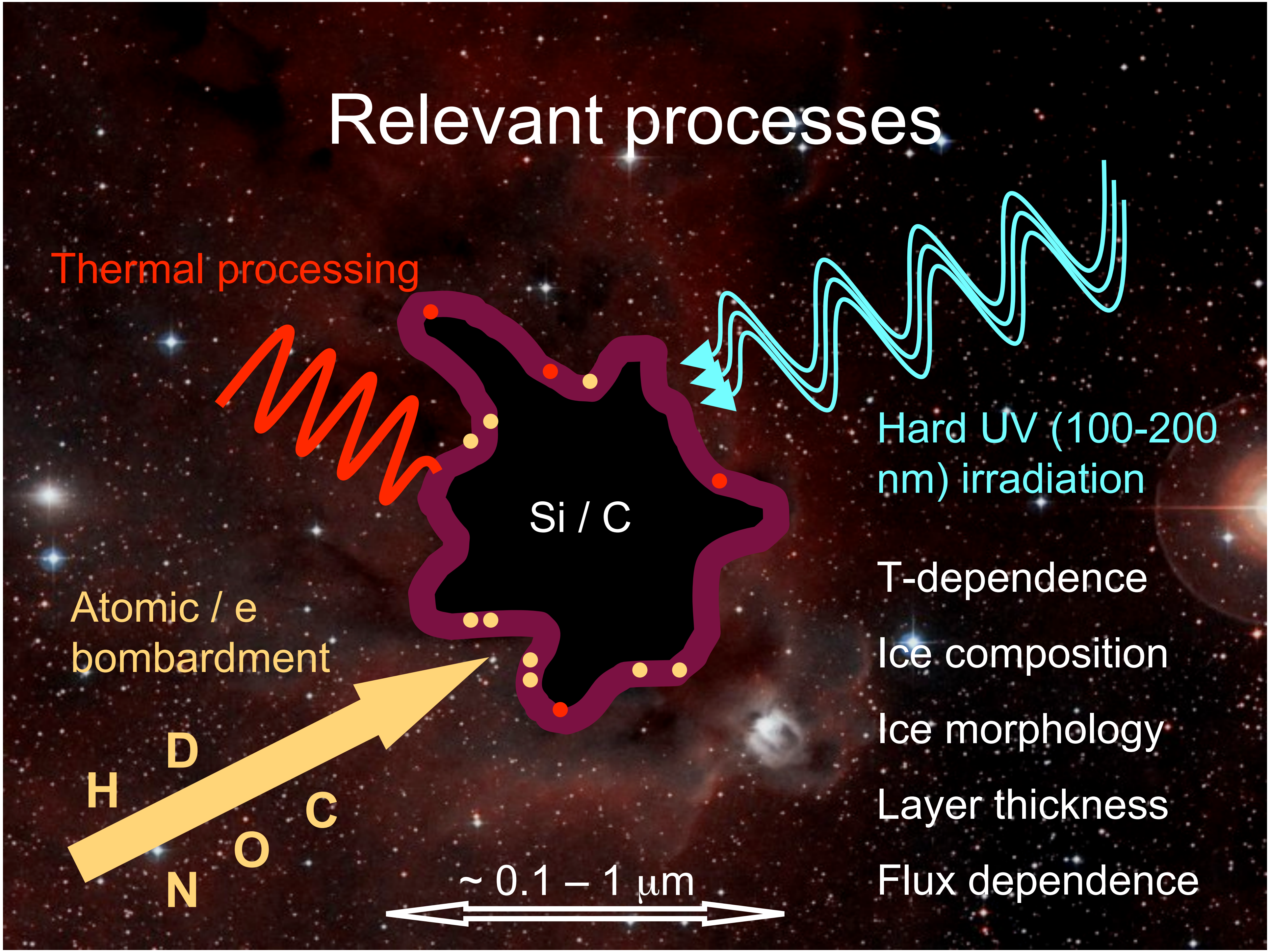
Astronomical setting

Öberg et al., A&A 462 (2007) 1187-1198

Bisschop et al., A&A 470 (2007) 749-759

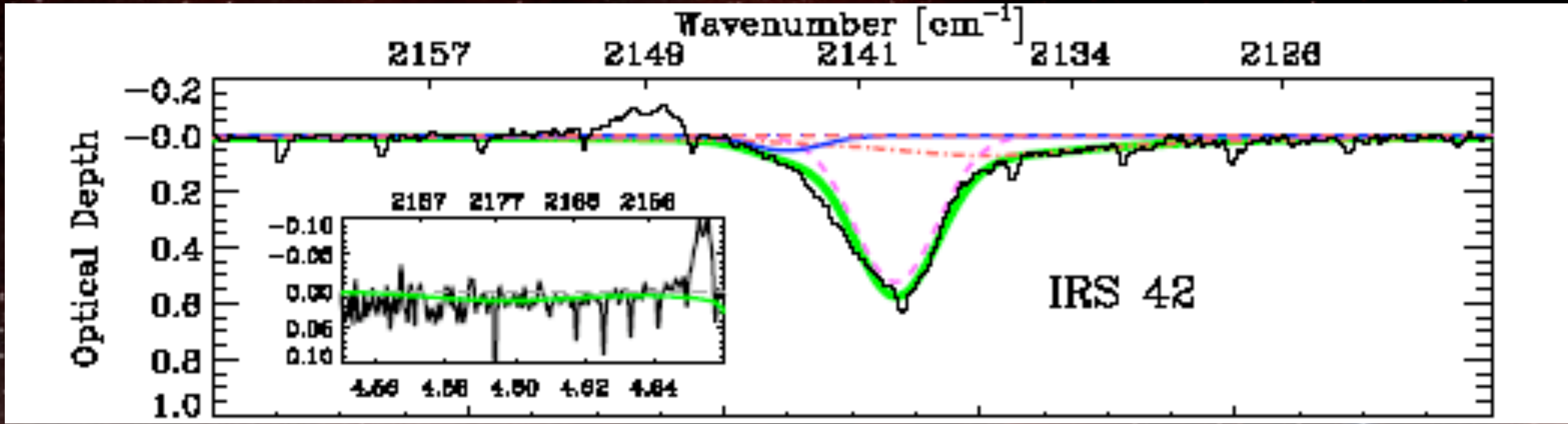
Bouwman et al., A&A 476 (2007) 995-1003


Relevant processes
Thermal processing
Hard UV (100-200 nm) irradiation
Si / C
Atomic / e bombardment
D
H
C
O
N
~ 0.1 – 1 μm
T-dependence
Ice composition
Ice morphology
Layer thickness
Flux dependence

Molecules discovered in space – d.d. januari 2008

2		3		4	5	6	7	8-9	10-13
H_2	PN	C_3	OCS	c-C_3H	C_5	C_5H	C_6H	CH_3C_3N	CH_3C_5N
AlF	SO	C_2H	NaCN	l-C_3H	C_4H	l-H_2C_4	CH_2CHCN	$HCOOCH_3$	$(CH_3)_2CO$
AlCl	SO^+	C_2O	SO_2	C_3N	C_4Si	C_2H_4	CH_3C_2H	CH_3COOH	$(CH_2OH)_2$
C_2	SiN	C_2S	c-SiC_2	C_3O	l-C_3H_2	CH_3CN	HC_5N	C_7H	CH_3CH_2CHO
CH	SiO	CH_2	CO_2	C_3S	c-C_3H_2	CH_3NC	$HCOCH_3$	H_2C_6	
CH^+	SiS	HCN	NH_2	C_2H_2	CH_2CN	CH_3OH	NH_2CH_3	CH_2OHCHO	HC_9N
CN	CS	HCO	H_3^+	HCCN	CH_4	CH_3SH	c-C_2H_4O		CH_3C_6H
CO	HF	HCO^+	SiCN	$HCNH^+$	HC_3N	HC_3NH^+	CH_2CHOH	CH_3CH_4	
CO^+	SH	HCS^+	SiNC	HNCO	HC_2NC	HC_2CHO	C_6H^-	CH_3CH_2CN	$(CH_3OC_2H_5)$
CP	CF^+	HOC^+	AlNC	HNCS	HCOOH	NH_2CHO		CH_3OCH_3	(C_6H_6)
SiC	FeO	H_2O		$HOCO^+$	H_2CHN	C_5N		CH_3CH_2OH	
HCl	SiH	H_2S		H_2CO	H_2C_2O	l-HC_4N		HC_7N	$HC_{11}N$
KCl	O_2	HNC		H_2CN	H_2NCN	C-H_2C_3O		C_8H	
NH		HNO		H_2CS	HNC_3	H_2CCNH		CH_3CONH_2	
NO		MgCN		H_3O^+	SiH_4			C_8H^-	
NS		MgNC		NH_3	H_2COH^+				
NaCl		N_2H^+		C-SiC_3	C_4H^-				
OH		N_2O		CH_3					

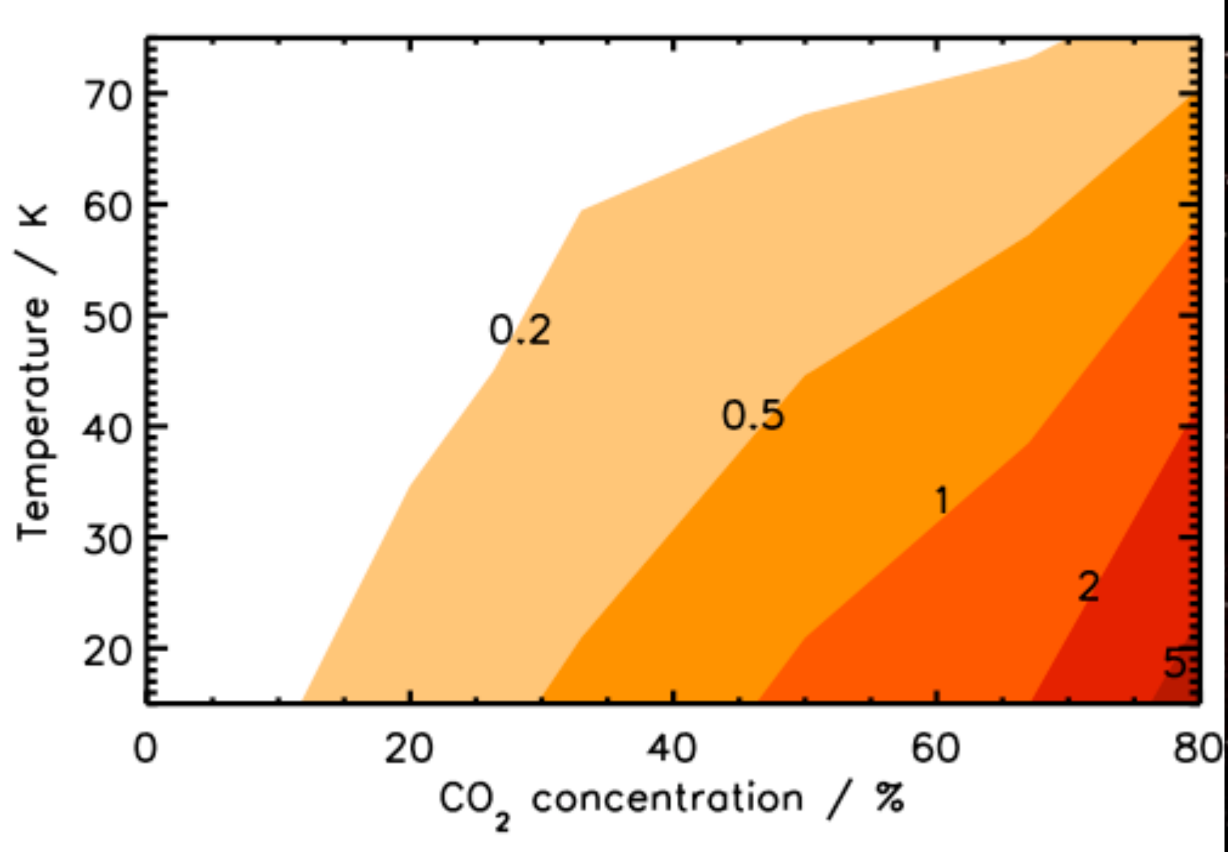
Relevant matter



Molecule	H_2O	CO	CO_2	CH_4	CH_3OH	H_2CO	OCS	NH_3	HCOOH	HCN
W33A	100	9	14	2	22	1.7-7	0.3	15	0.4-2	<3
Elias29	100	5.6	22	<1.6	<4	-	<0.1	<9.2	-	-

pure, mixed and layered - amorphous vs. crystalline

FTIR transmission spectroscopy of interstellar ices



► (%,T) correlation diagram: 3.6 μm band intensity ratio

Example: CO_2 dependence of fundamental integrated absorption strength on mixing ratio

Desorption Processes

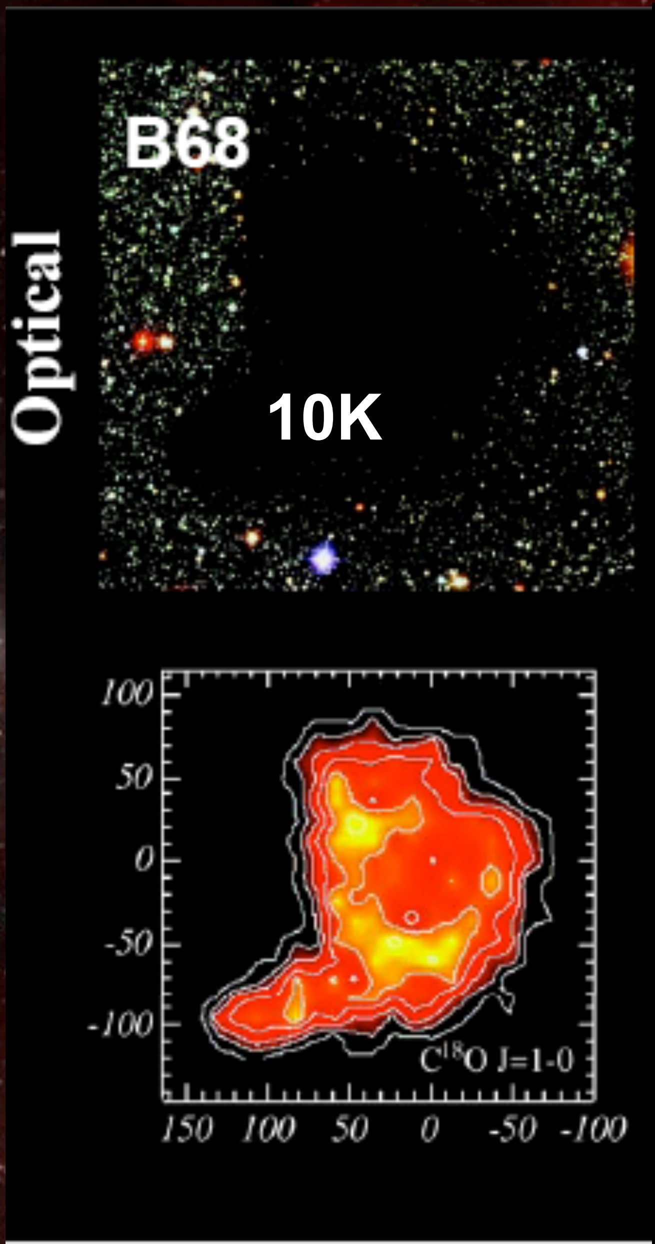
-Thermally induced

-Photon induced

Fuchs et al., Far. Disc. 133 (2006) 331

Acharyya et al., A&A 466 (2007) 1005-1012

Öberg et al., ApJ 662 (2007) L23-26



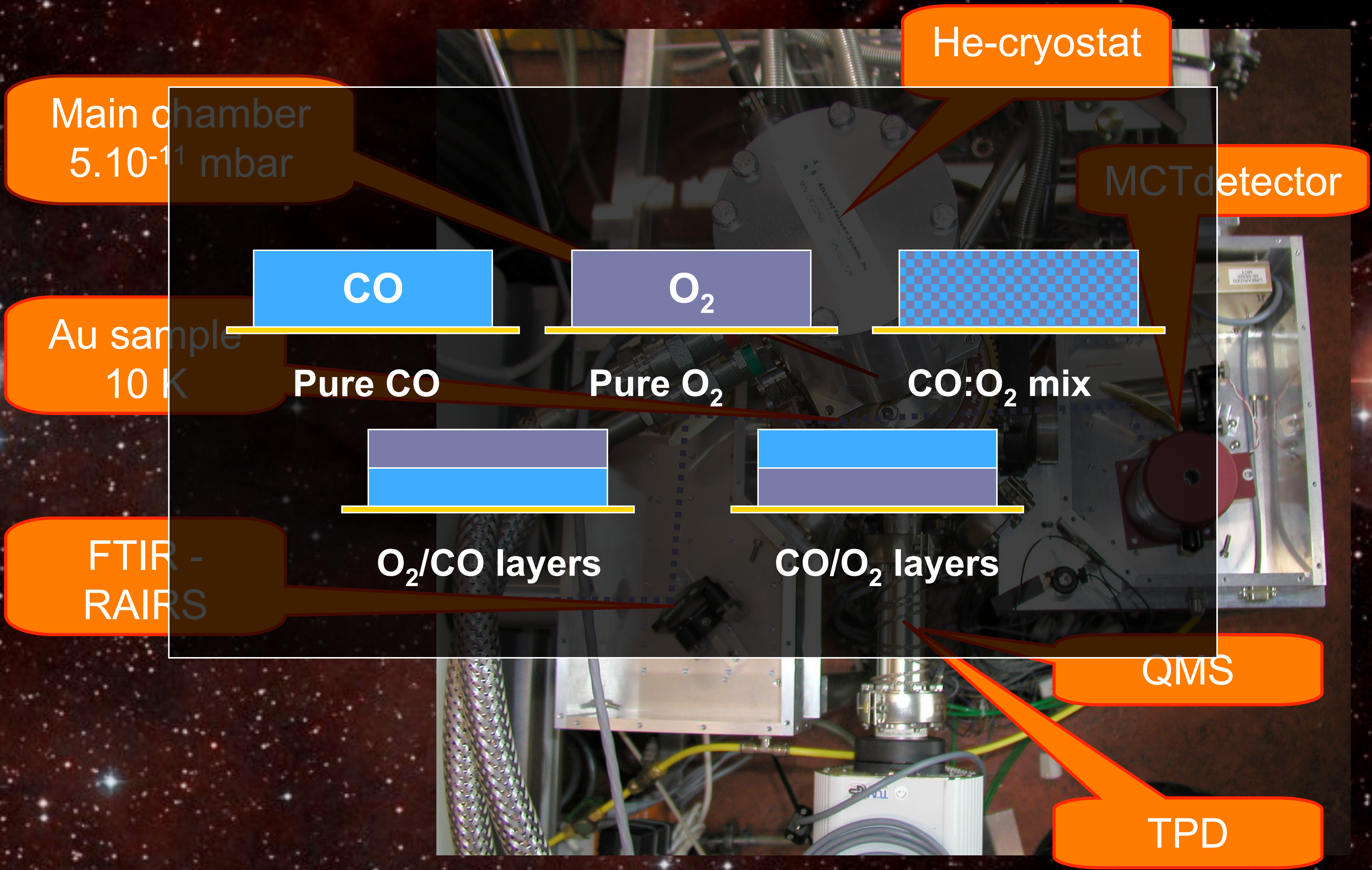
Optical picture

CO in gas phase at 10 K
→ non-thermal desorption mechanism

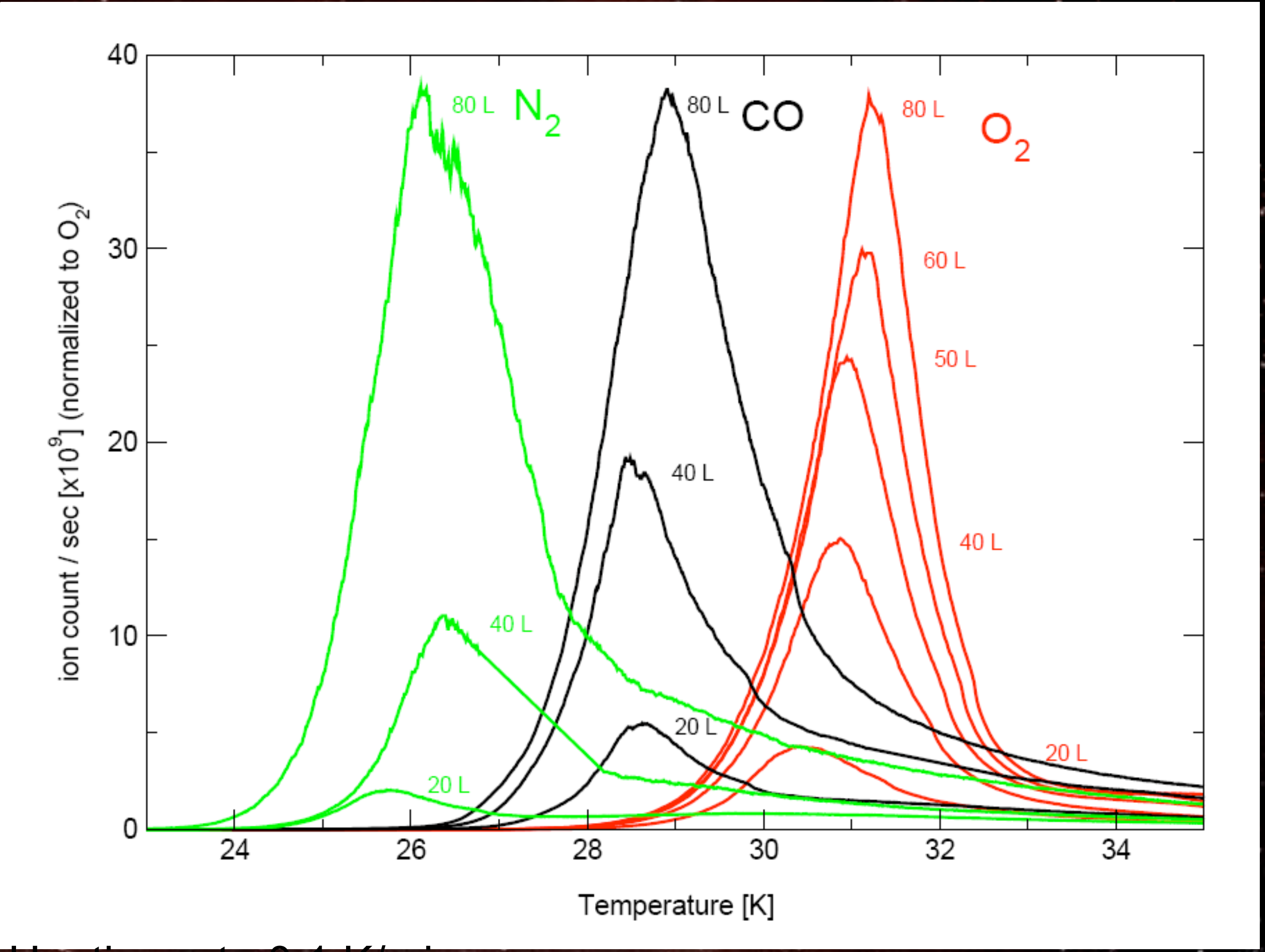
Photo-desorption: 10^{-5}-10^{-8} CO-molecules / UV photon
→ generally neglected in astrochemical models

Submm spectrum CO

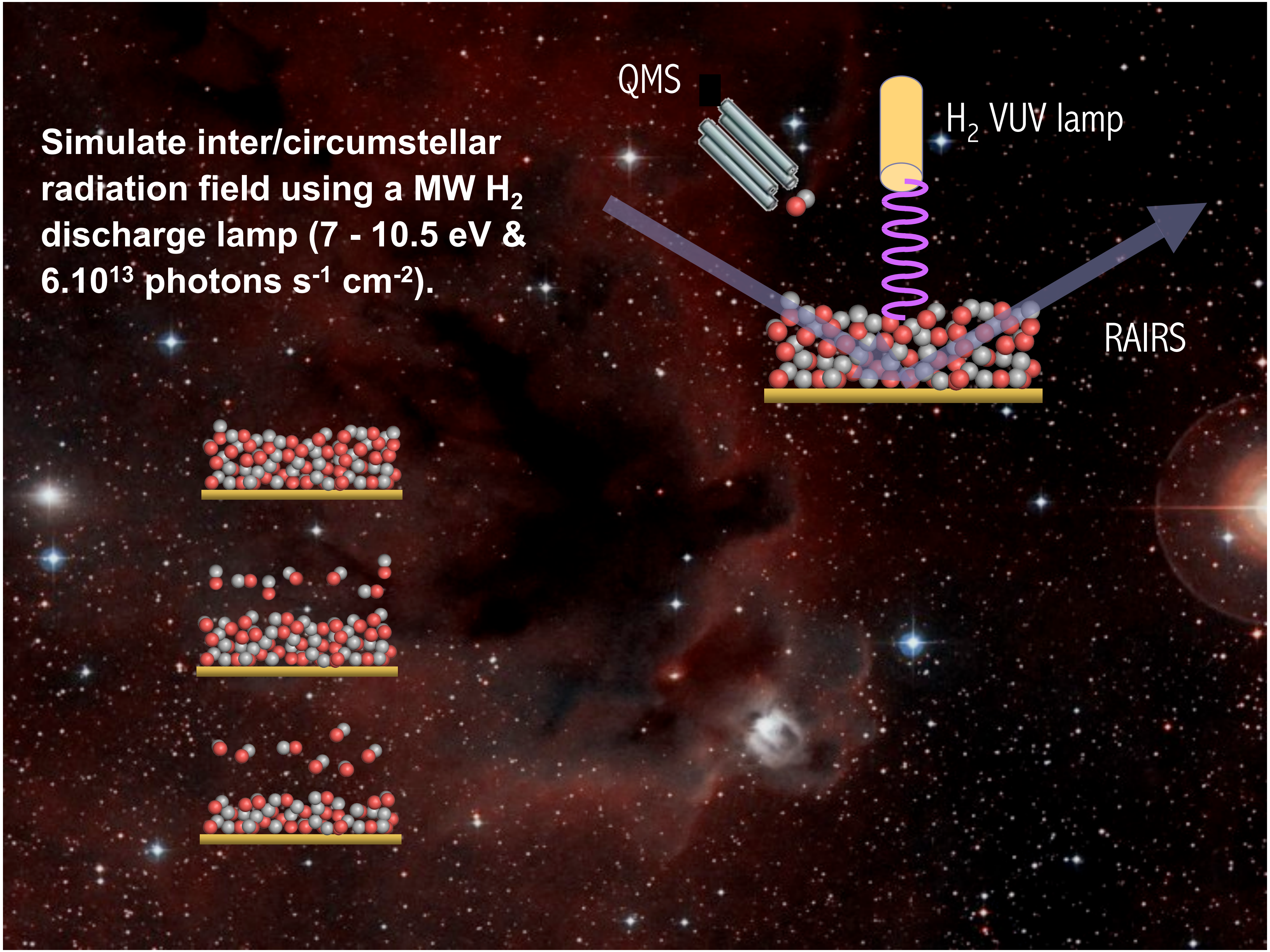
UHV setup - CRYOPAD



Thermal desorption of ice

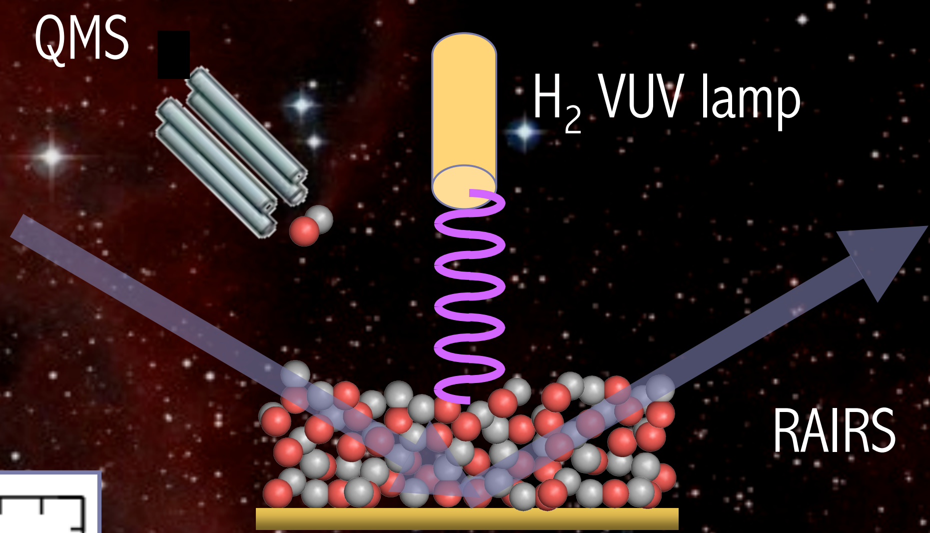


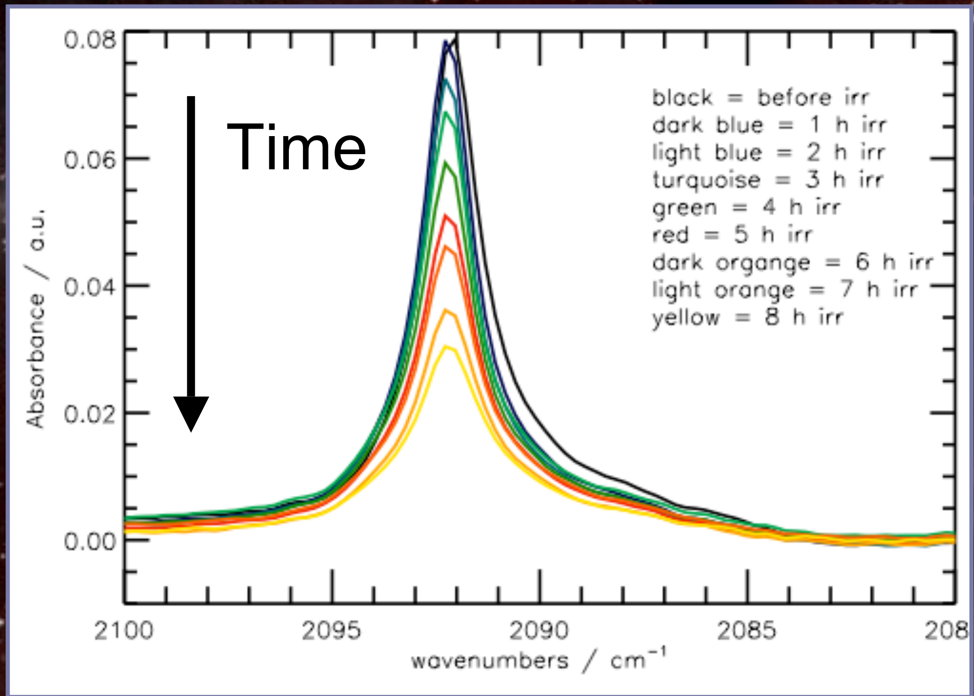
Heating rate 0.1 K/min



Simulate inter/circumstellar radiation field using a MW H_2 discharge lamp (7 - 10.5 eV & 6.10^{13} photons s^{-1} cm^{-2}).
QMS
H_2 VUV lamp
RAIRS

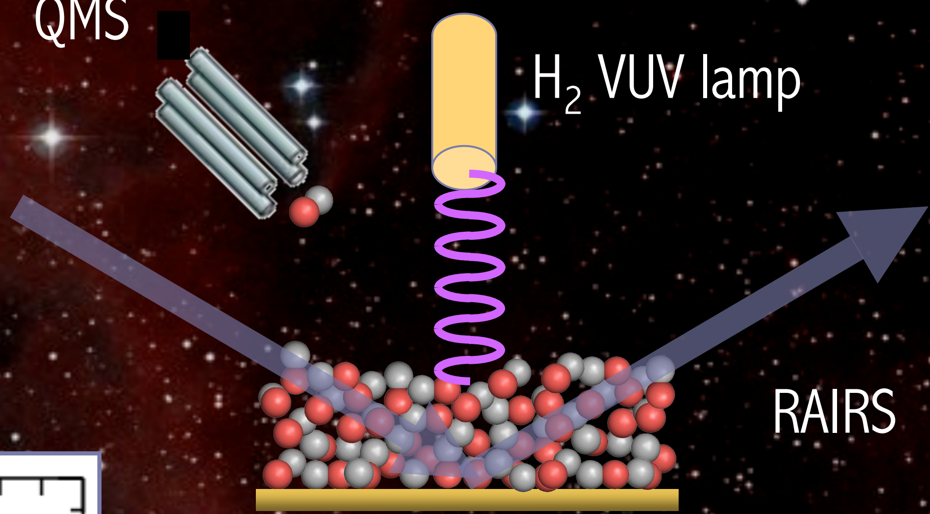
Simulate inter/circumstellar radiation field using a MW H_2 discharge lamp (7 - 10.5 eV & 6.10^{13} photons s^{-1} cm^{-2}).

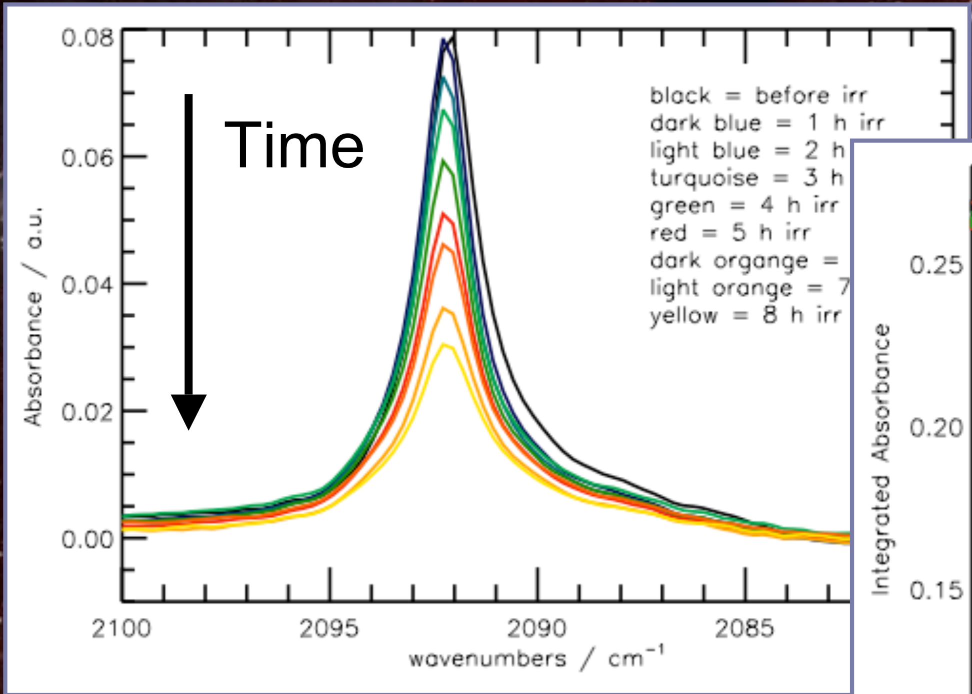




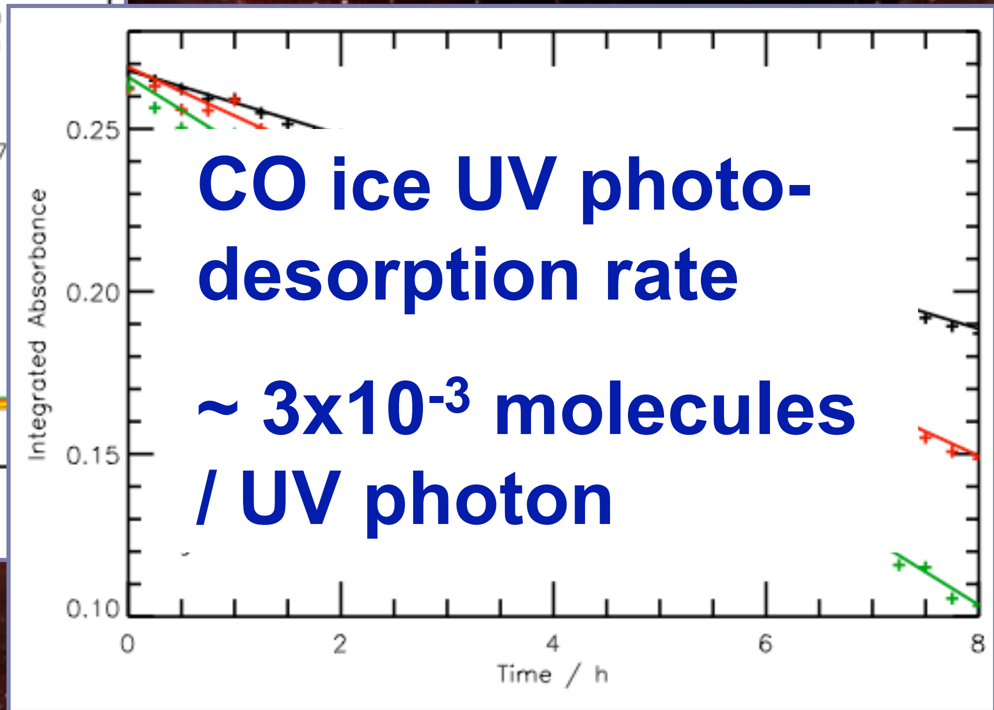
RAIR Spectra

CO photodesorption rate scales with the flux of the MW H_2 discharge lamp, i.e. no local heating.





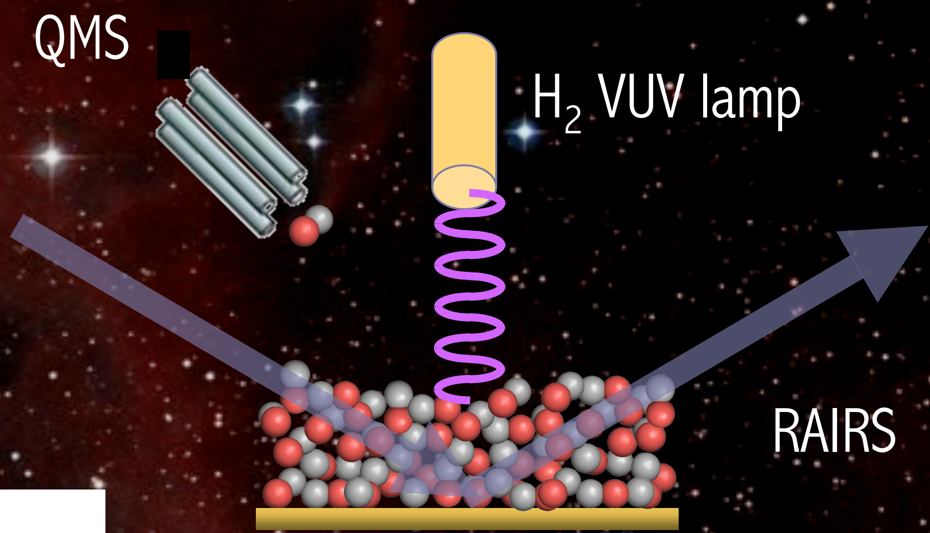
RAIR Spectra

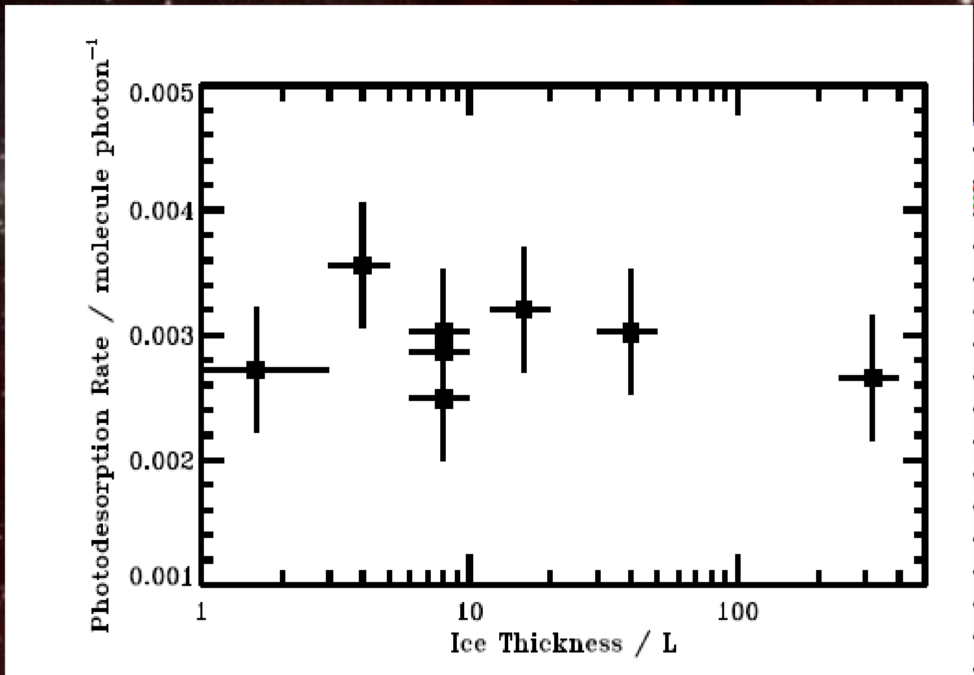


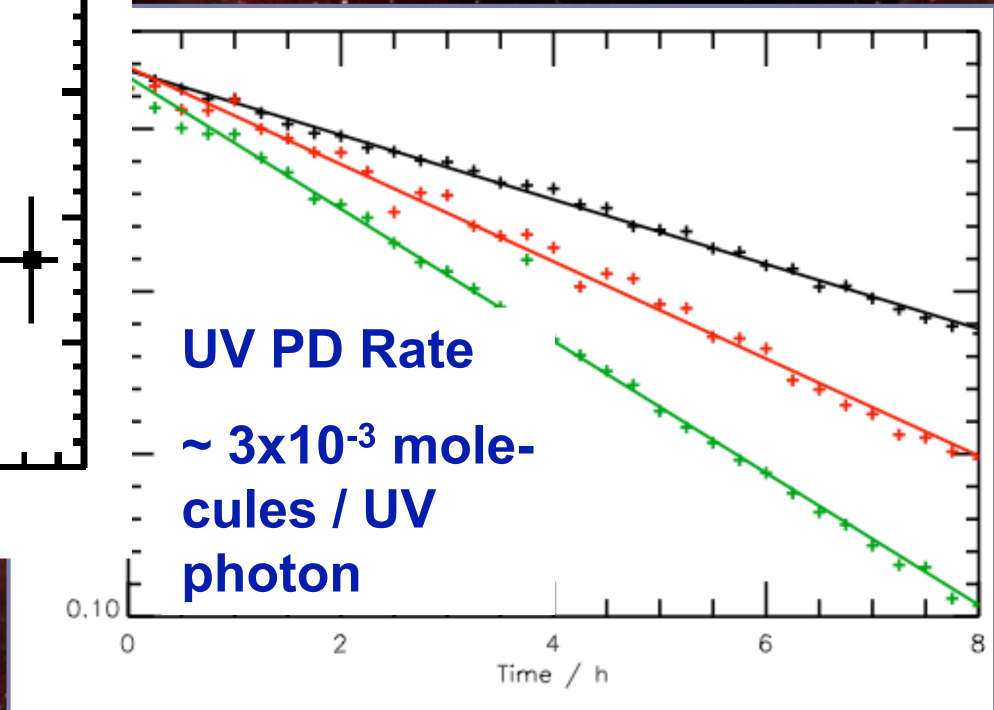
CO ice UV photo-desorption rate

~ $3x10^{-3}$ molecules / UV photon

The final value for the photo desorption rate is not sensitive to layer thickness, i.e. not substrate mediated.







RAIR Spectra

Öberg et al. ApJL 2007

Experimental checks !

- **Not a thermal effect**
  Immediate onset TPD signal upon irradiation.

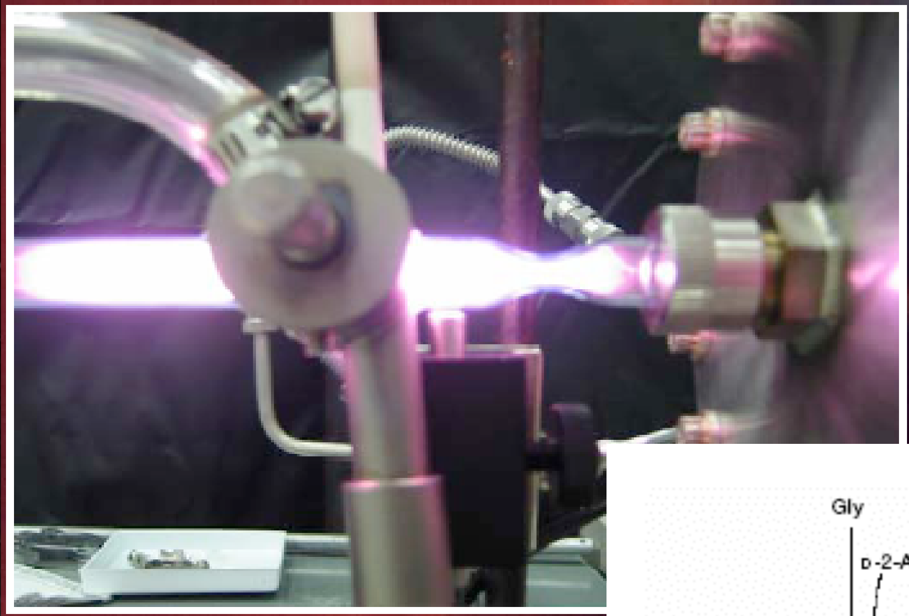
- **No photo-processing**
  After 8 hrs of irradiation < 0.2 % CO_2

- **Not a substrate effect**

  Bilayered experiments ($C^{18}O/C^{16}O$) with several top layer thicknesses show that process is restricted to top layers.

  Independent of ice thickness until sub monolayer situation.

  CO photodesorps, N_2 does not ($< 2.10^{-4}$).



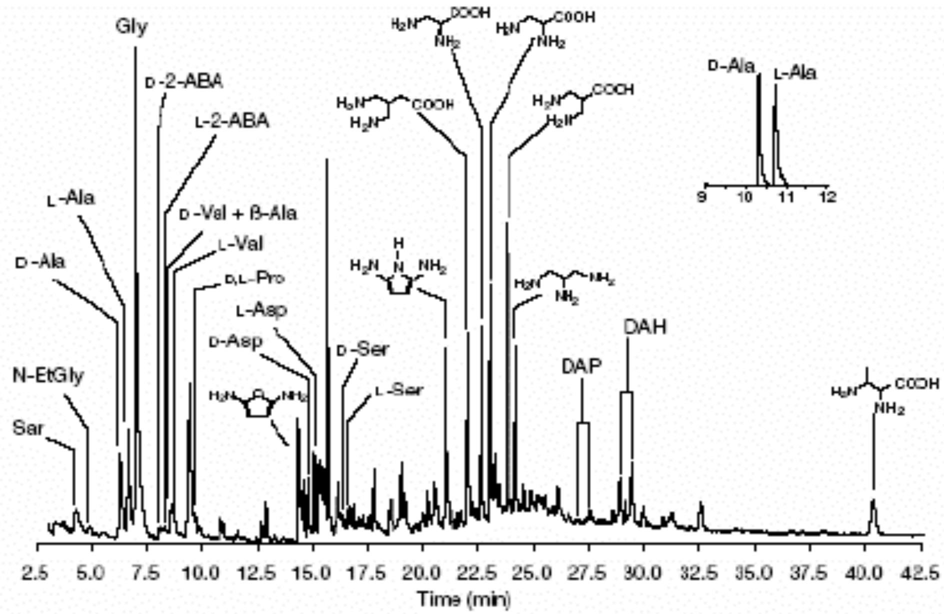


Fig. 2. Gas chromatogram showing a rich variety of amino acids and other compounds generated from a photo-processed ISM ice, containing H_2O, CH_3OH, NH_3, CO and CO_2. (Taken from G.M.M. Caro et al, Nature 416 (2002) 403.)

Gas chromatogram 'Yellow stuff', Nature 416 (2002) 403

Likely photodesorption mechanism

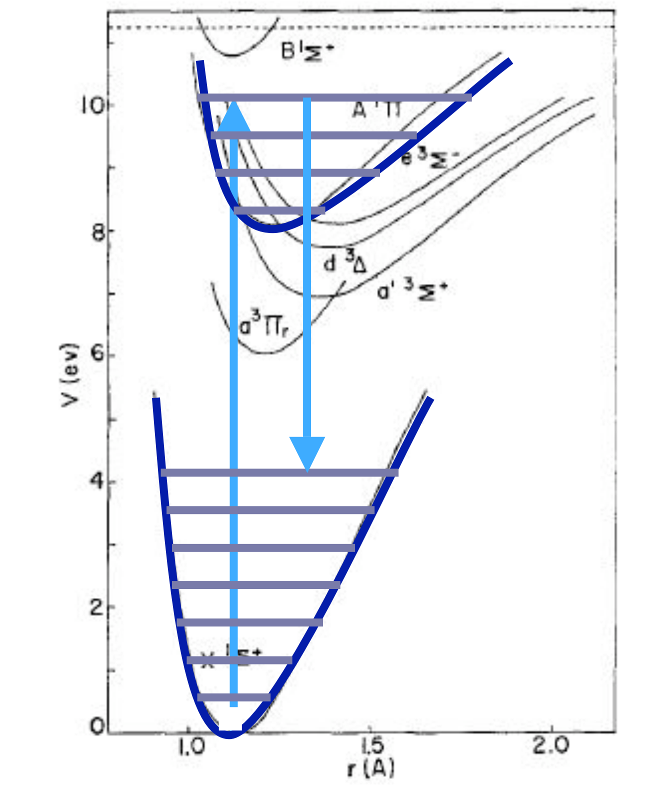
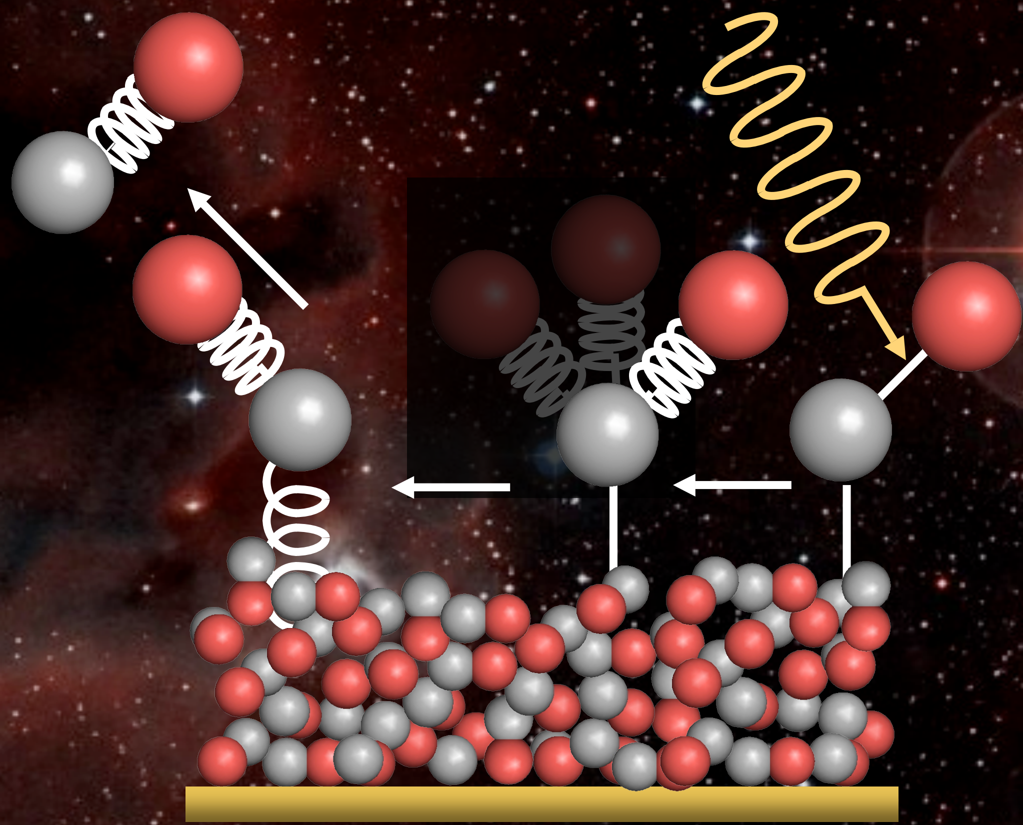
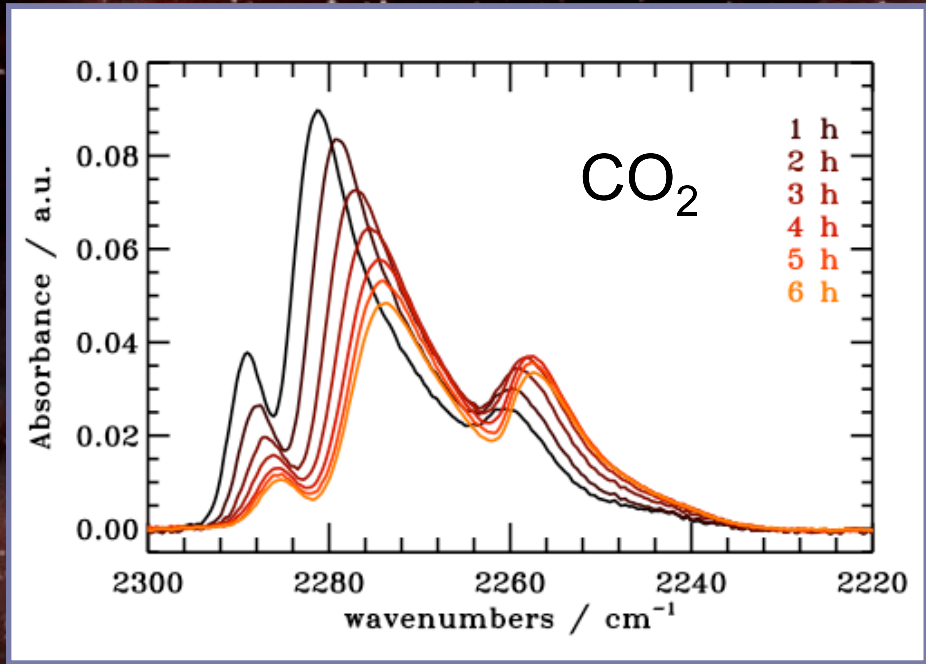


FIG. 1. Potential curves for the different electronic states of CO.



Consequences for the models

- **Photodesorption rate orders of magnitudes higher than assumed so far in astrochemical models → explains gas phase CO at temperatures below accretion temperature.**
- **With this excitation mechanism other ice species should photodesorb as well.**
- **And in addition CO co-photodesorption may become possible.**

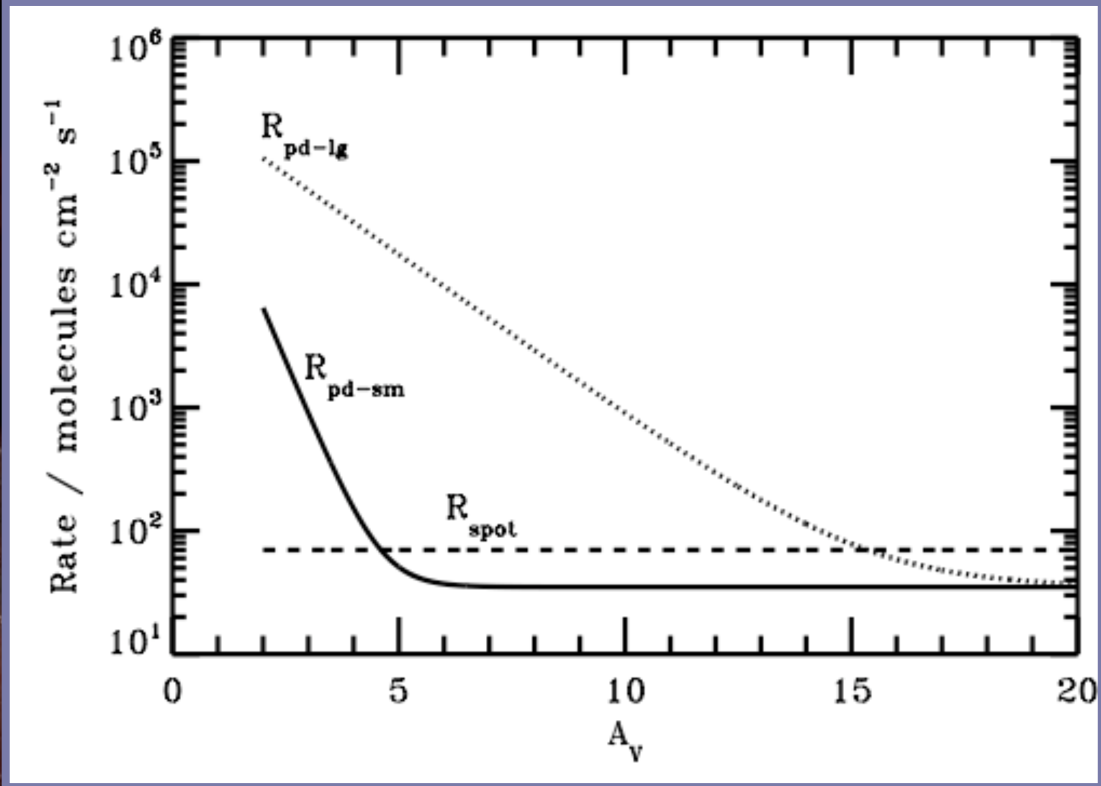


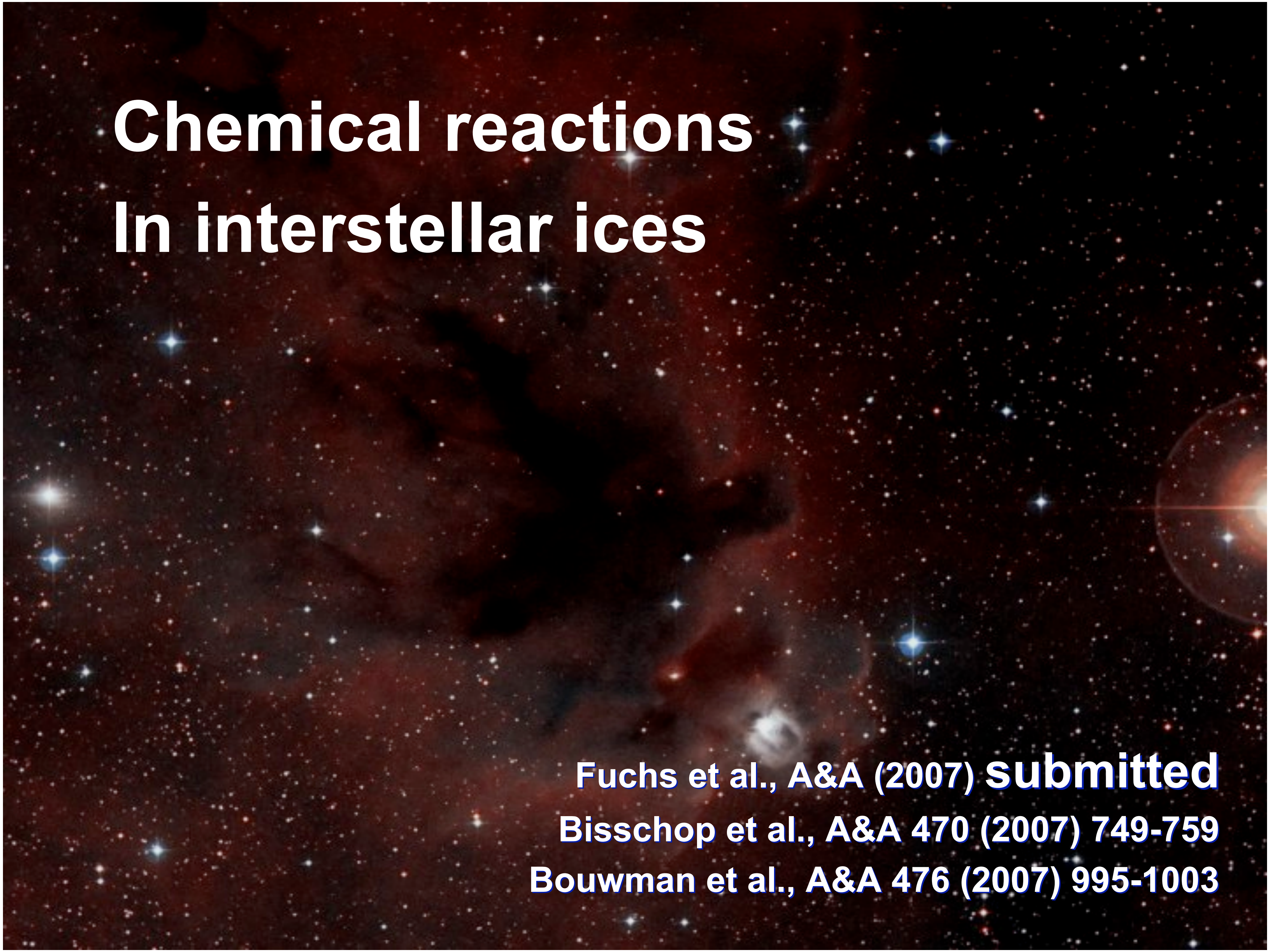
$$R_{E-UV-PD} = I_{ISRF-VUV} e^{-\gamma A_V} Y_{PD} \approx 3\times10^5 e^{-\gamma A_V}$$
$$R_{CR-UV-PD} = I_{CR-VUV} Y_{PD} \approx 30$$
$$R_{CR-spot-heating} \propto I_{CR-VUV} \approx 70$$

molecules cm^{-2} s^{-1}

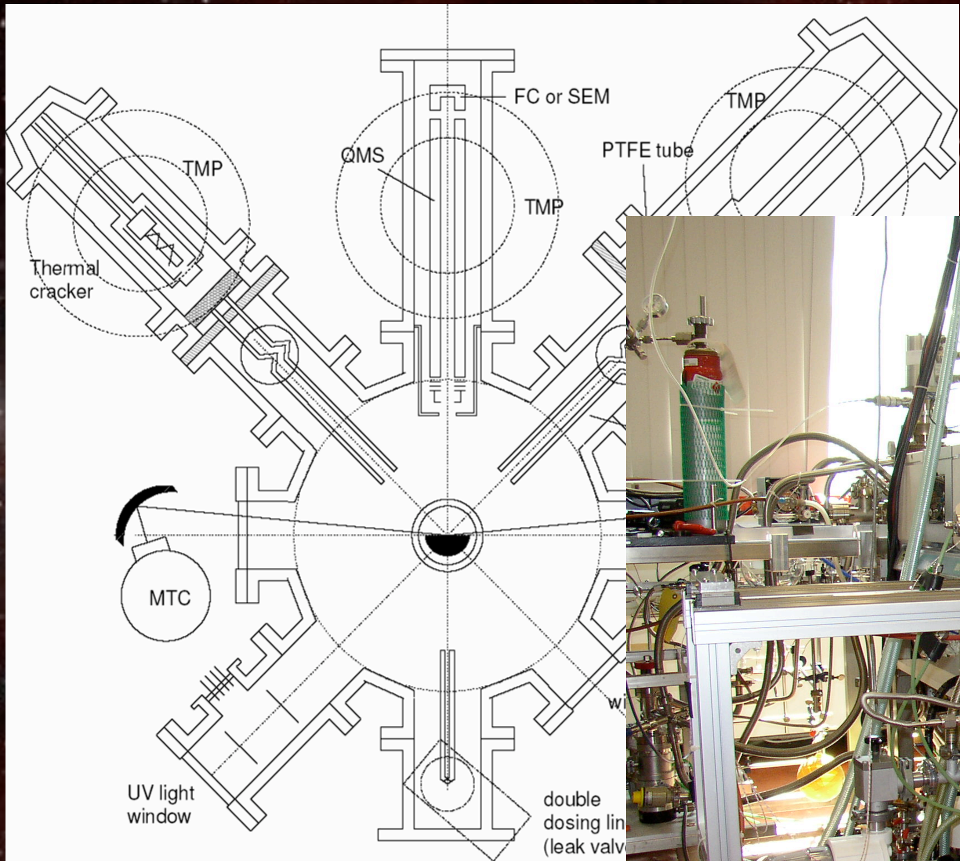
Dark cloud

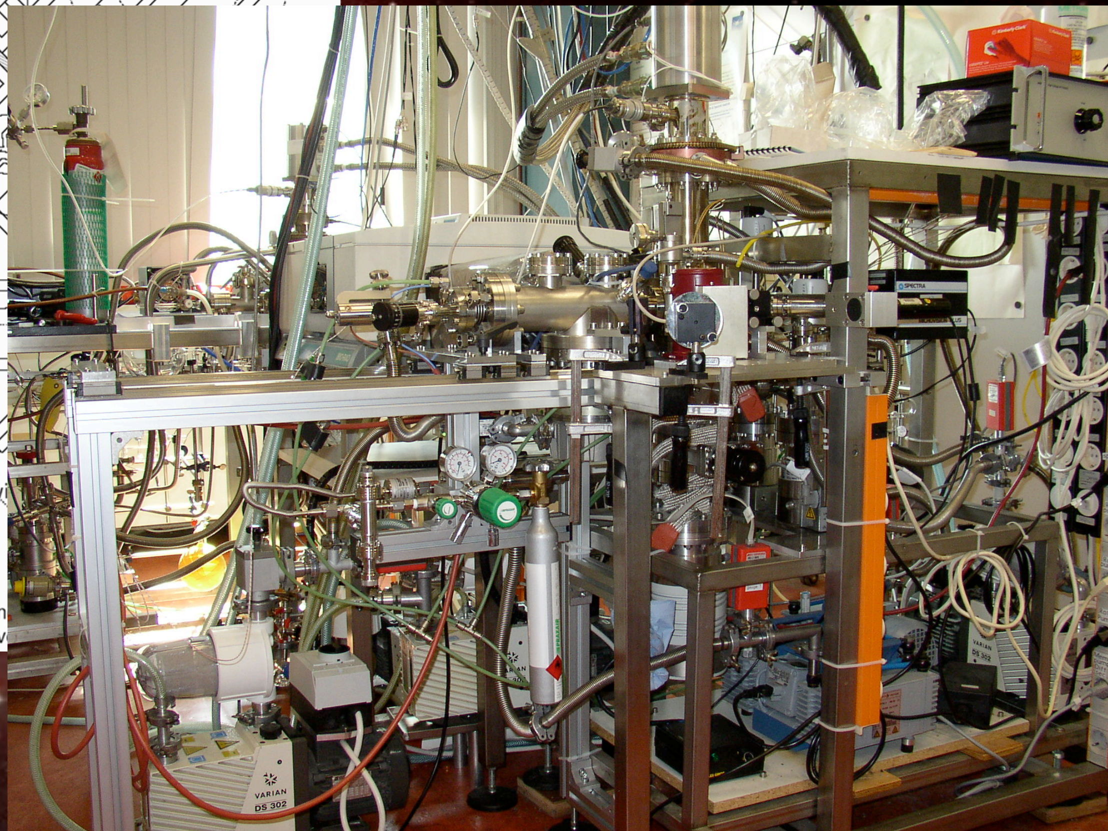
Comparison photodesorption and spot heating for small and larger grains

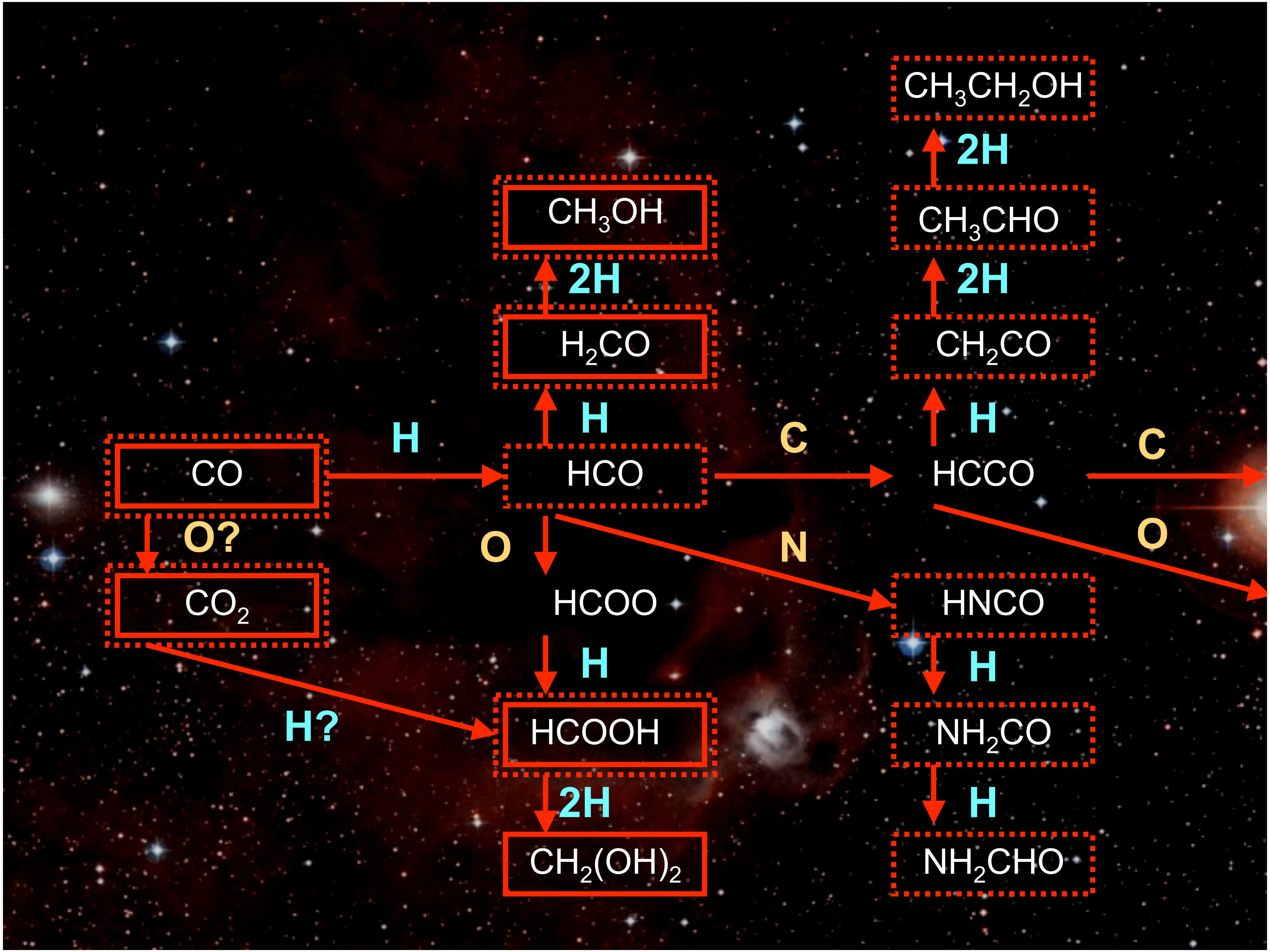



Chemical reactions
In interstellar ices
Fuchs et al., A&A (2007) submitted
Bisschop et al., A&A 470 (2007) 749-759
Bouwman et al., A&A 476 (2007) 995-1003

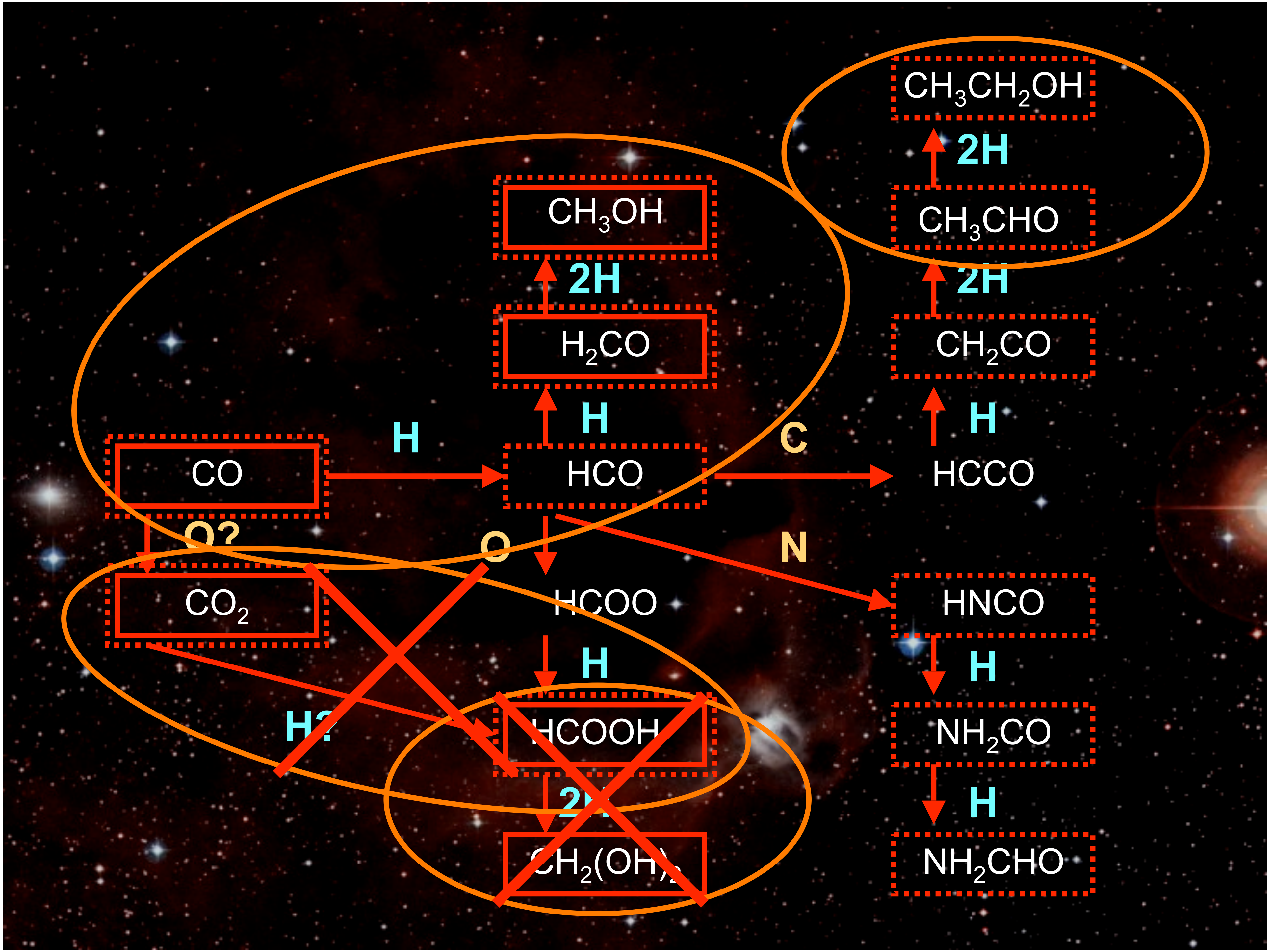
UHV setup - SURFRESIDE





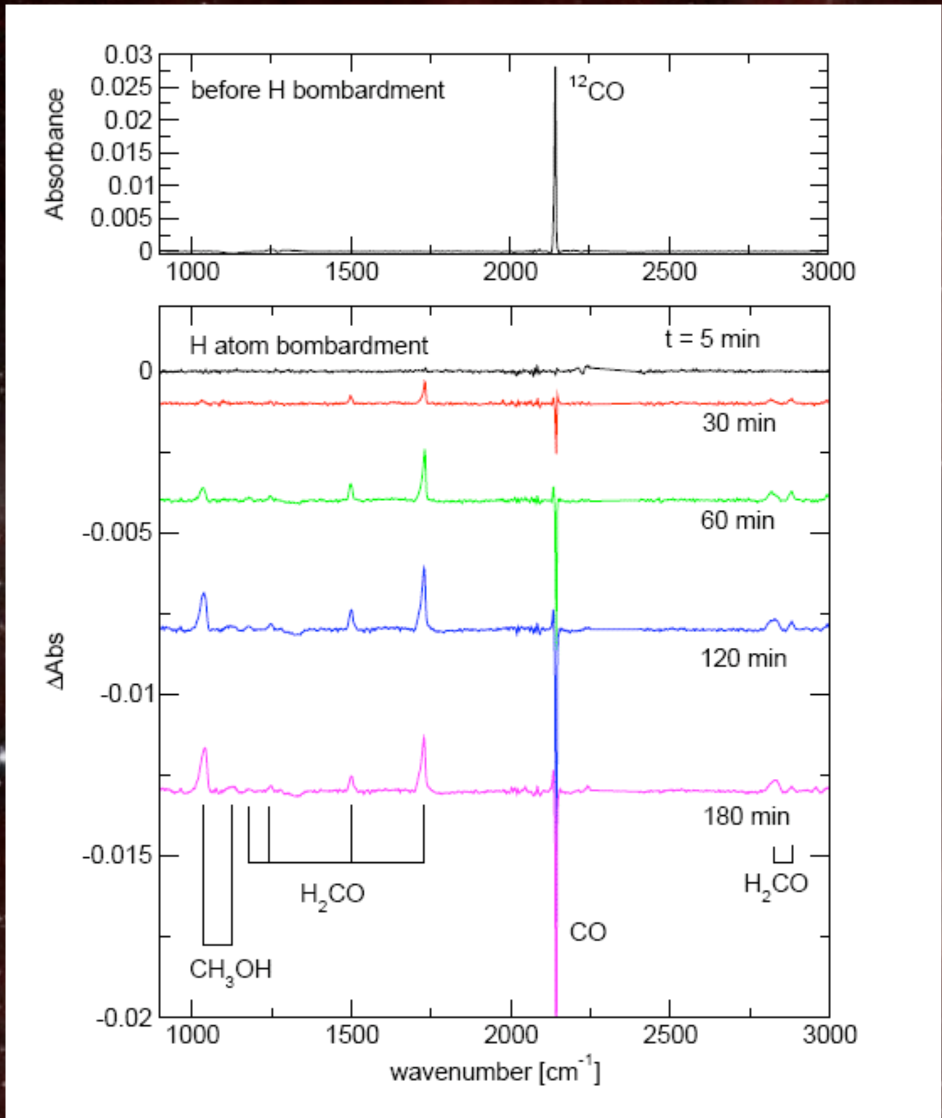


CH3CH2OH
2H
CH3CHO
2H
CH2CO
H
CH3OH
2H
H2CO
H
CO
H
HCO
C
HCCO
C
O?
O
N
O
CO2
HCOO
HNCO
H
H
H?
HCOOH
NH2CO
2H
H
CH2(OH)2
NH2CHO

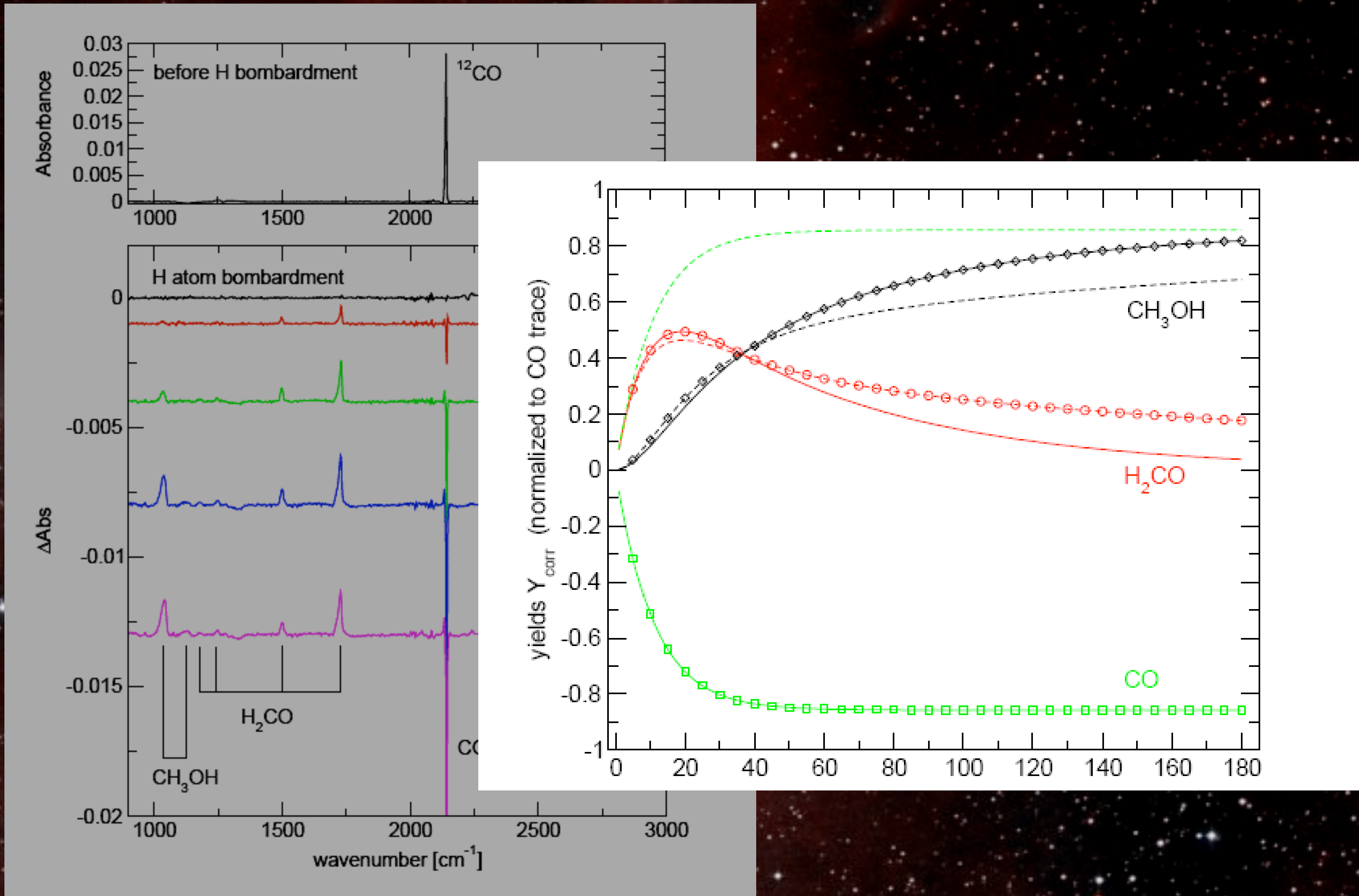


CH3CH2OH
2H
CH3CHO
2H
CH2CO
H
HCCO
CH3OH
2H
H2CO
H
HCO
H
CO
C
O?
O
N
CO2
HCOO
HNCO
H
H
H?
HCOOH
NH2CO
2H
H
CH2(OH)2
NH2CHO

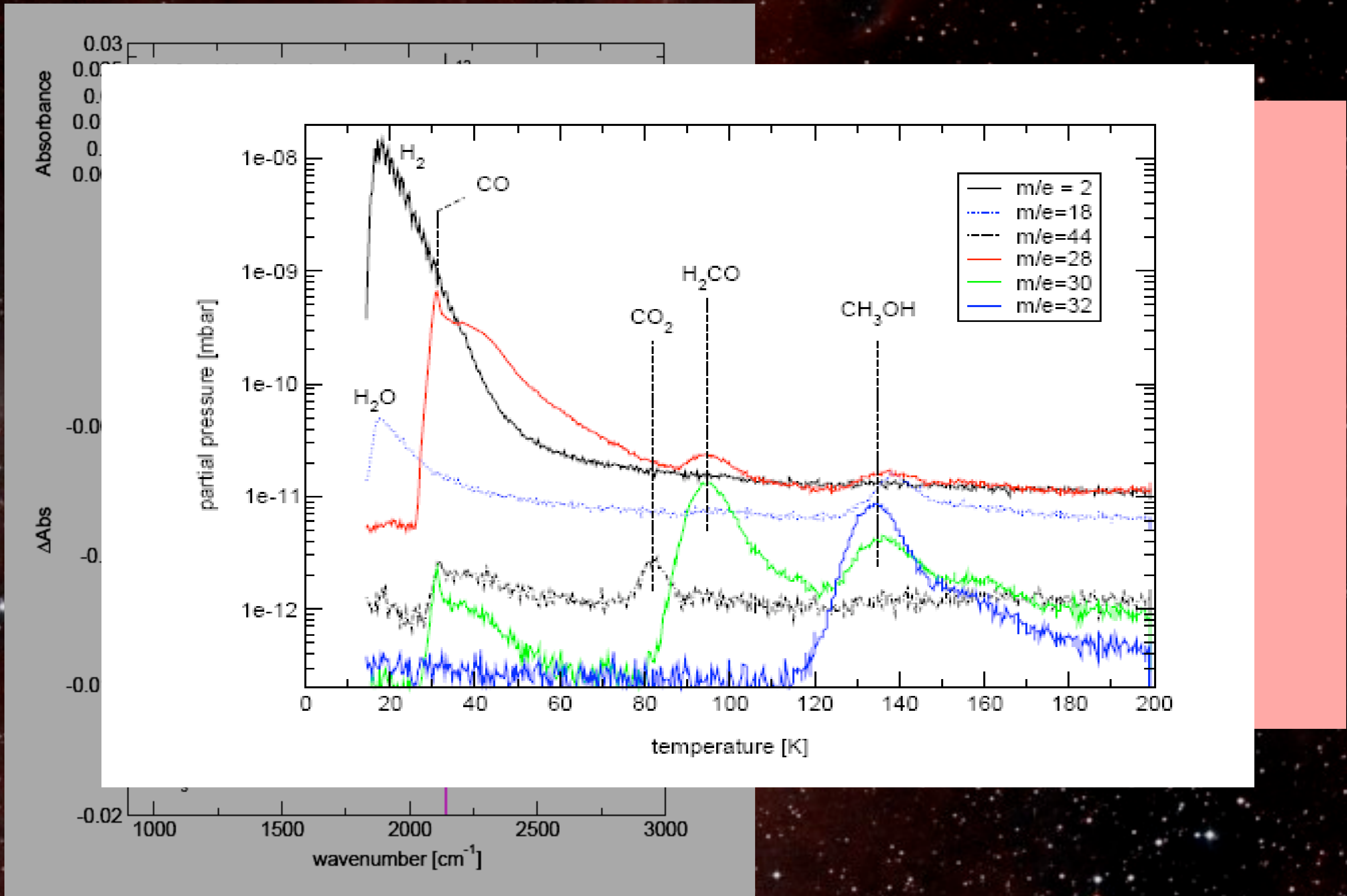
$$CO \xrightarrow[i=0]{k_0} HCO \xrightarrow[i=1]{k_1} H_2CO \xrightarrow[i=2]{k_2} CH_3O \xrightarrow[i=3]{k_3} CH_3OH$$



$$CO \xrightarrow[i=0]{k_0} HCO \xrightarrow[i=1]{k_1} H_2CO \xrightarrow[i=2]{k_2} CH_3O \xrightarrow[i=3]{k_3} CH_3OH$$

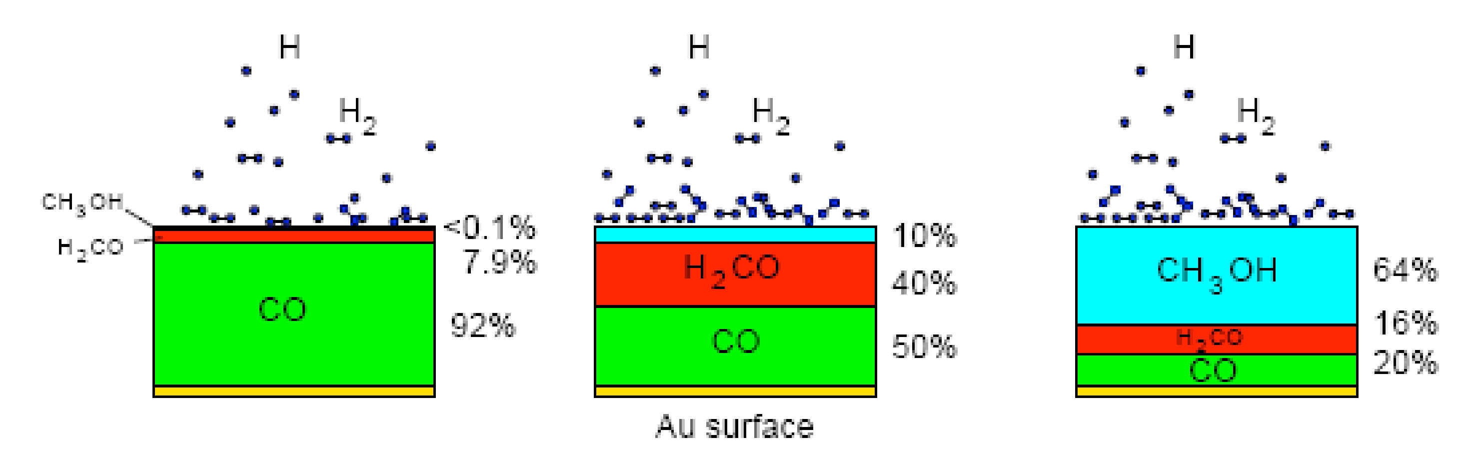


$$\mathrm{CO} \xrightarrow[i=0]{k_0} \mathrm{HCO} \xrightarrow[i=1]{k_1} \mathrm{H_2CO} \xrightarrow[i=2]{k_2} \mathrm{CH_3O} \xrightarrow[i=3]{k_3} \mathrm{CH_3OH}$$



Qualitative conclusions

- Independent experiments performed for 12-20 K, 5.5-70 ML, H-flux between 10^{12} - 10^{14} H-atoms cm^{-2} s^{-1}.
- Optimum reaction rates between T = 13 – 15 K.
- Results put an end to Watanabe-Hiraoke discussion
- For ices thicker than 10 ML no relevant thickness dependence is observed.



- But how about the numbers …

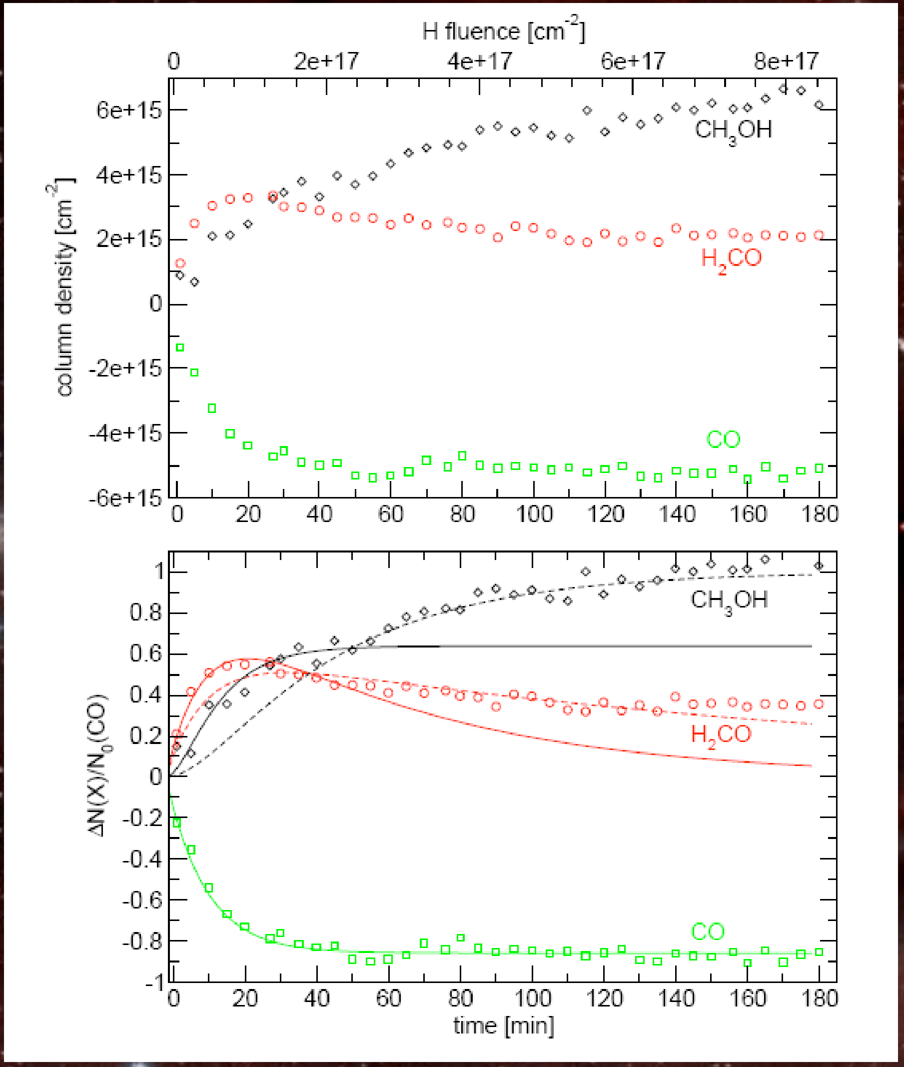
$$\mathrm{CO} \xrightarrow[\mathrm{i=0}]{k_0} \mathrm{HCO} \xrightarrow[\mathrm{i=1}]{k_1} \mathrm{H_2CO} \xrightarrow[\mathrm{i=2}]{k_2} \mathrm{CH_3O} \xrightarrow[\mathrm{i=3}]{k_3} \mathrm{CH_3OH}$$

$$\mathrm{CO} \xrightarrow[\mathrm{i=0}]{k_0} \mathrm{H_2CO} \xrightarrow[\mathrm{i=2}]{k_2} \mathrm{CH_3OH}$$

$$\beta_i = 60\, k_i\, N_{\mathrm{H}} \quad \text{in } [\mathrm{min}^{-1}]$$

$$\frac{N_{\mathrm{H_2CO}}(t)}{N_{\mathrm{CO}}(0)} = \alpha_2 \left(\frac{\beta_0}{\beta_2 - \beta_0}\right) (\exp[-\beta_0 t] - \exp[-\beta_2 t])$$

$$\frac{N_{\mathrm{CH_3OH}}(t)}{N_{\mathrm{CO}}(0)} = \tilde{\alpha}_2 \left(\frac{\beta_0 \beta_2}{\beta_2 - \beta_0}\right) \left(\frac{1 - \exp[-\beta_0 t]}{\beta_0} - \frac{1 - \exp[-\beta_2 t]}{\beta_2}\right) \tag{12}$$



CO ice 5 ML, 15 K, ~ 8.10^{13} H-atoms cm^{-2} s^{-1}

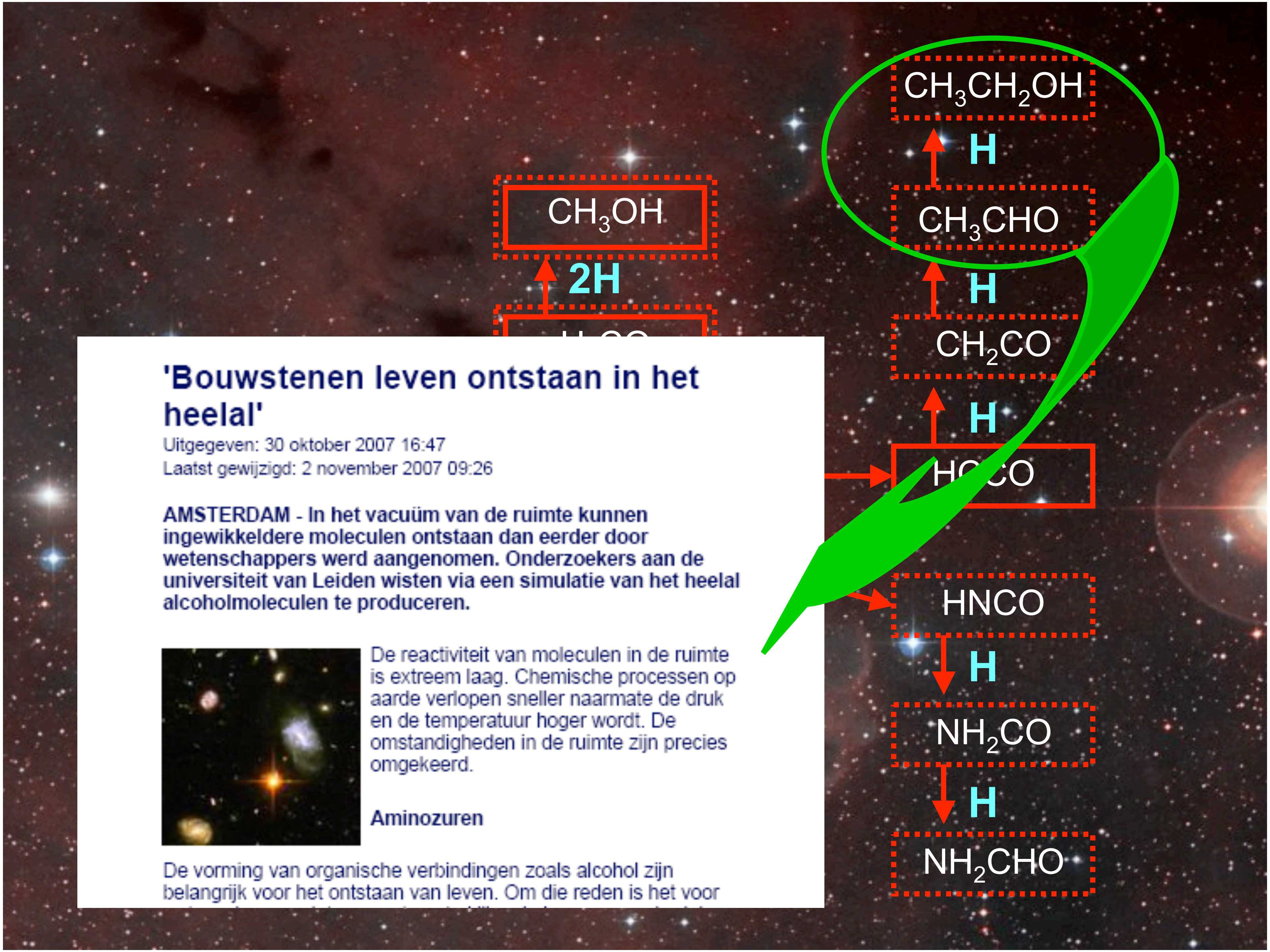
RAIRS data converted in time dependent column densities

Two time domains: 40 min and 180 min.

Short time domain: β_0=0.1min^{-1} β_2=0.02 min^{-1}

Problems to take into account

- How about the surface: exact layer thickness / density and layer homogeneity ?
- Transforming RAIRS spectra into surface parameters is not that trivial.
- How well specified is the H-atom flux ? How about H-atom recombination and hydrogen poisoning ?
- How layer specific are reactions ?
- How about the temperature of the H-atom beam ? Is this relevant below 300 K ?
- Are laboratory data in this useful for astronomical conditions ? Saturation, multi-atom processes, heating?
- Very accurate controls necessary as well as simulations.



'Bouwstenen leven ontstaan in het heelal'

Uitgegeven: 30 oktober 2007 16:47
Laatst gewijzigd: 2 november 2007 09:26

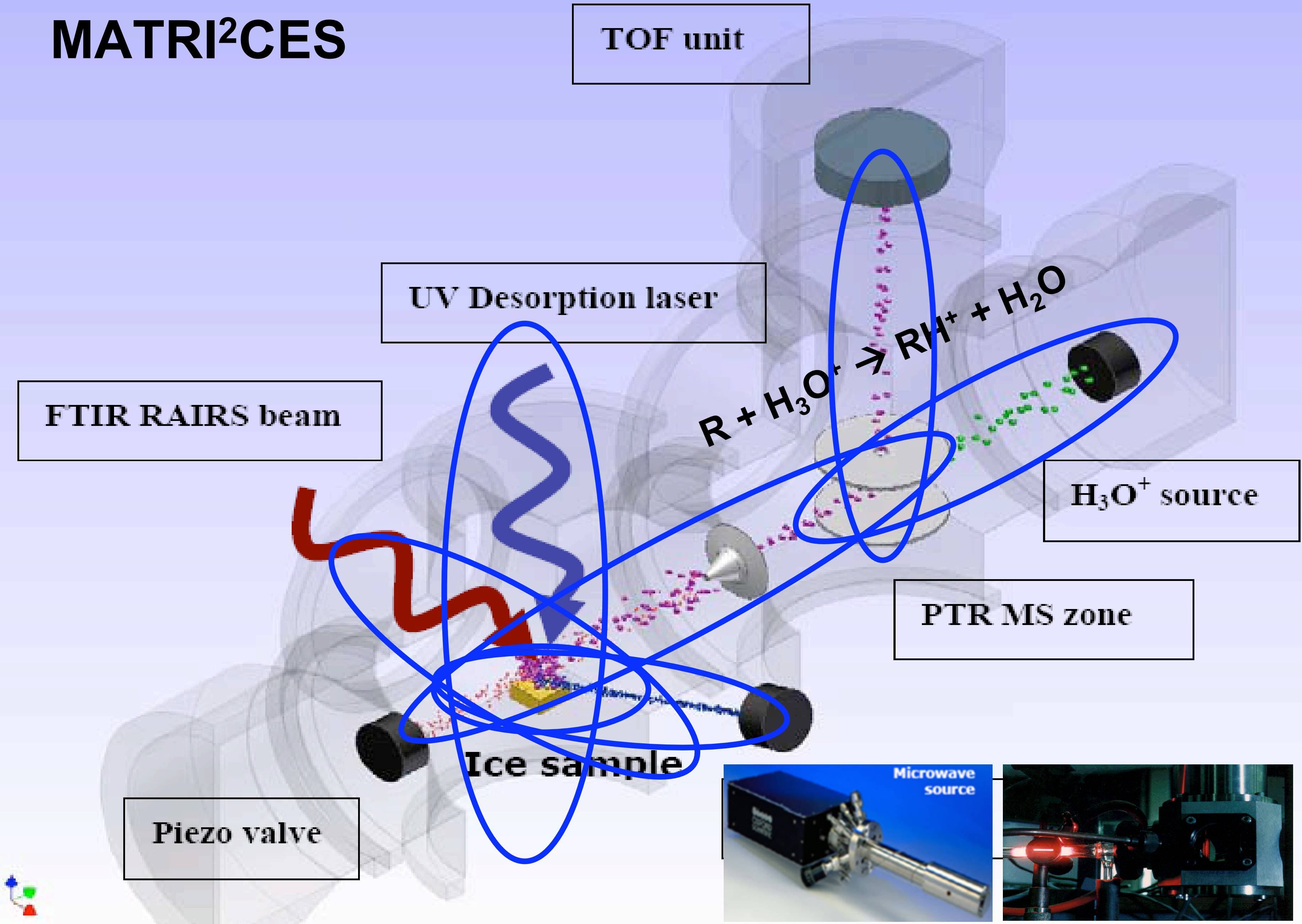
AMSTERDAM - In het vacuüm van de ruimte kunnen ingewikkeldere moleculen ontstaan dan eerder door wetenschappers werd aangenomen. Onderzoekers aan de universiteit van Leiden wisten via een simulatie van het heelal alcoholmoleculen te produceren.

De reactiviteit van moleculen in de ruimte is extreem laag. Chemische processen op aarde verlopen sneller naarmate de druk en de temperatuur hoger wordt. De omstandigheden in de ruimte zijn precies omgekeerd.

Aminozuren

De vorming van organische verbindingen zoals alcohol zijn belangrijk voor het ontstaan van leven. Om die reden is het voor

MATRI²CES



TOF unit
UV Desorption laser
FTIR RAIRS beam
$R + H_3O^+ \rightarrow RH^+ + H_2O$
H_3O^+ source
PTR MS zone
Ice sample
Piezo valve
Microwave source

Starring

Ewine van Dishoeck

& astrochemistry group

Guido Fuchs

Herma Cuppen

Claire Romanzin

Suzanne Bisschop

Karin Öberg

Sergio Ioppolo

Kinsuk Acharyya

Zainab Awad

Jordy Bouwman

Nadine Wehres

Harald Verbraak

Wiebke Ludwig

NOVA

Sterrewacht Leiden

FOM

Laser Centre

vrije Universiteit amsterdam