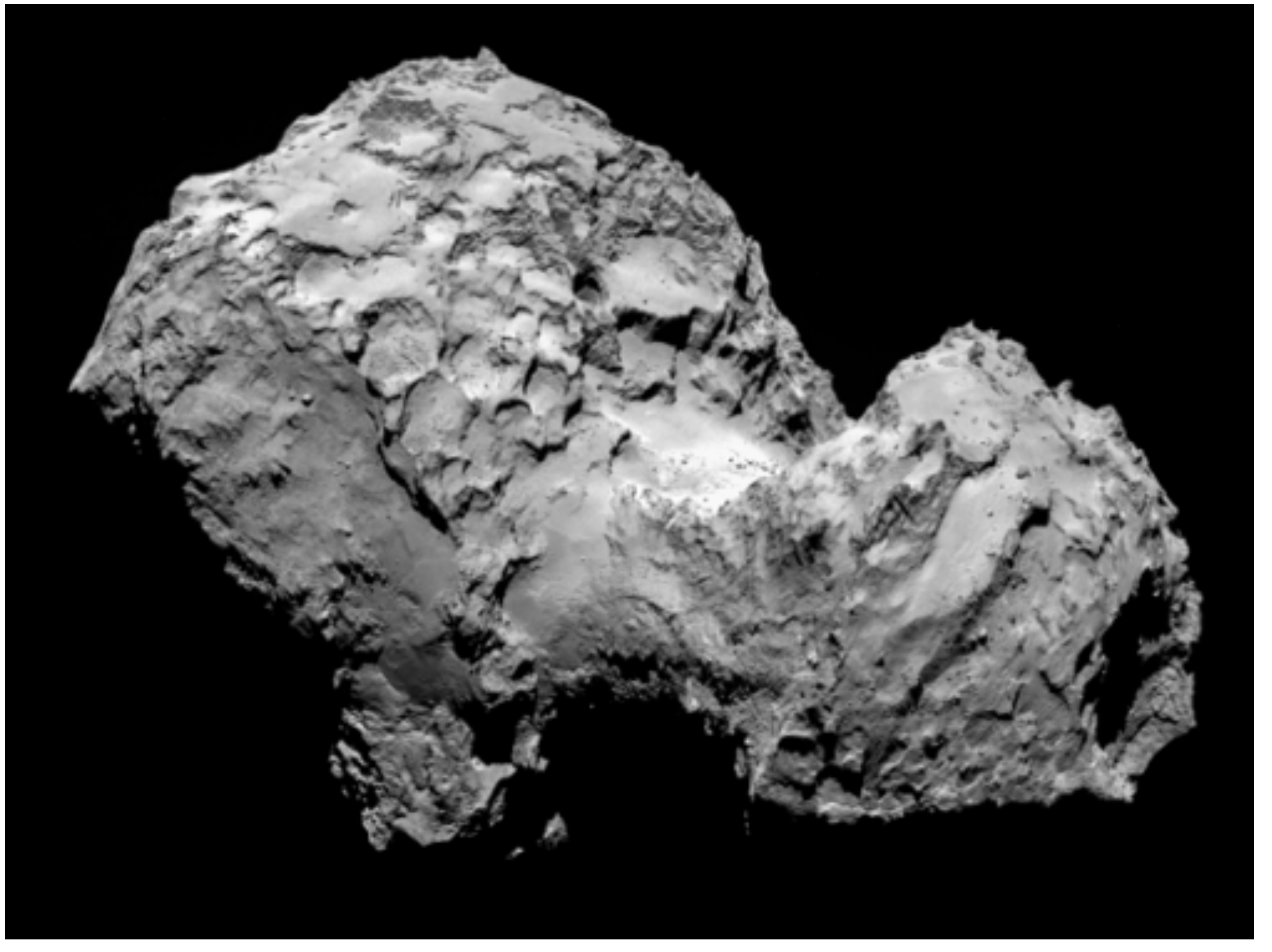
On the origin of molecular oxygen in comets



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Water in the Universe, 13/04/2016, ESTEC

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Importance of Molecular oxygen

Importance of Molecular Oxygen:

- **Dominant component of Earth's atmosphere** (21 % by volume)

- Byproduct of photo-synthesis → **Potential marker for biological activity**

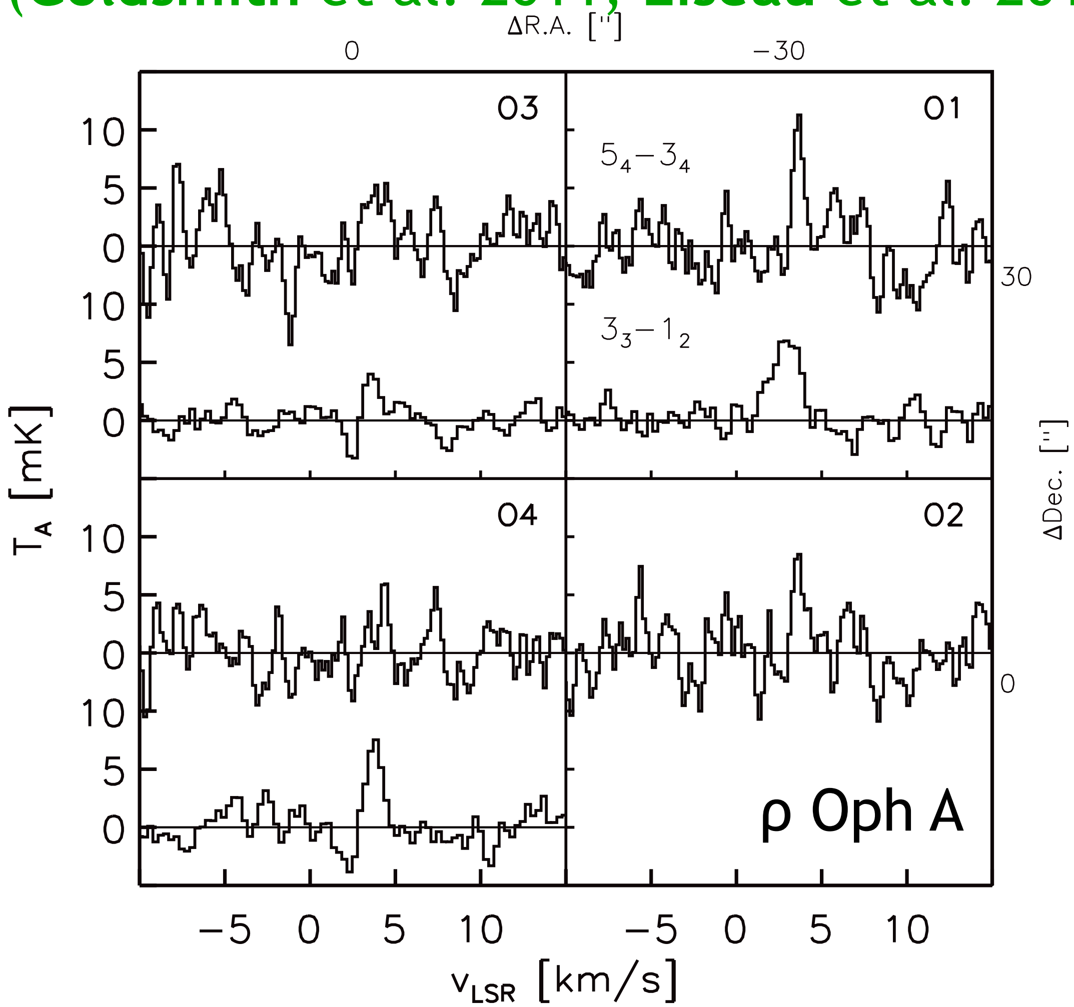
- O is the third most abundant element → **O_2 potentially abundant in the ISM**

- O_2 is a **key molecule** for the **water chemical network**

O_2: an elusive interstellar molecule

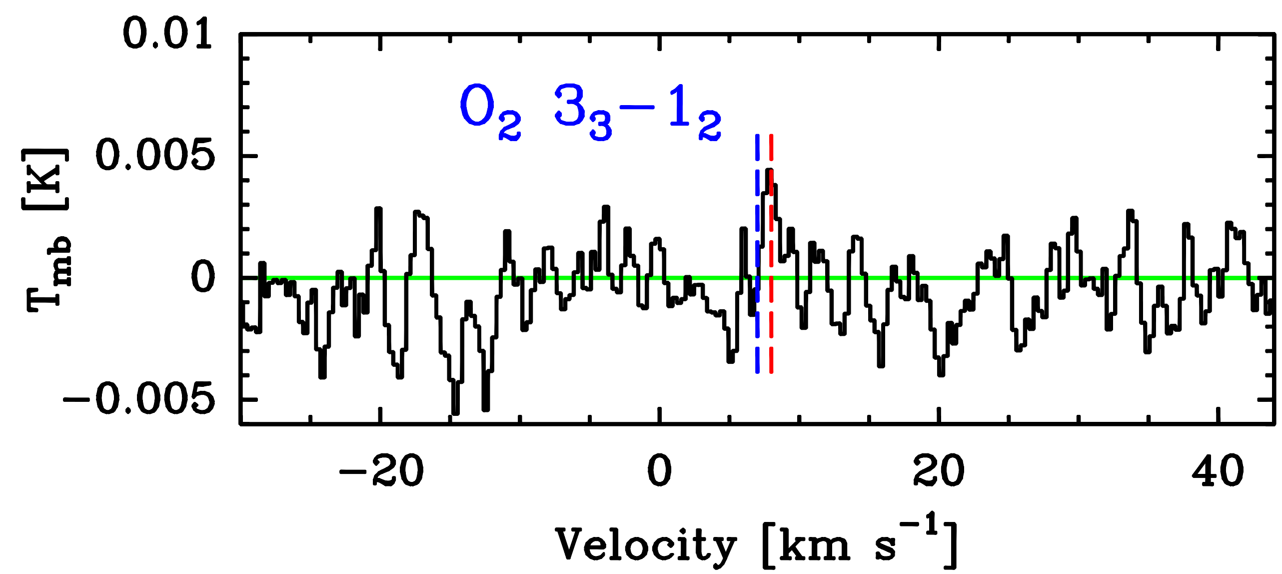
Zero electric dipole moment → difficult to detect O_2 in the cold ISM

Only two detections in dark clouds:
Orion and ρ Oph A
(**Goldsmith** et al. 2011; **Liseau** et al. 2012)



→ $X(O_2)_{obs} << X(O_2)_{mod}$

No detection toward protostars:
strong upper limit in NGC1333-IRAS4A
$X(O_2) < 6 \times 10^{-9}$ (**Yildiz** et al. 2013)



+ **No clear detection in comets** either through remote or *in-situ* observations

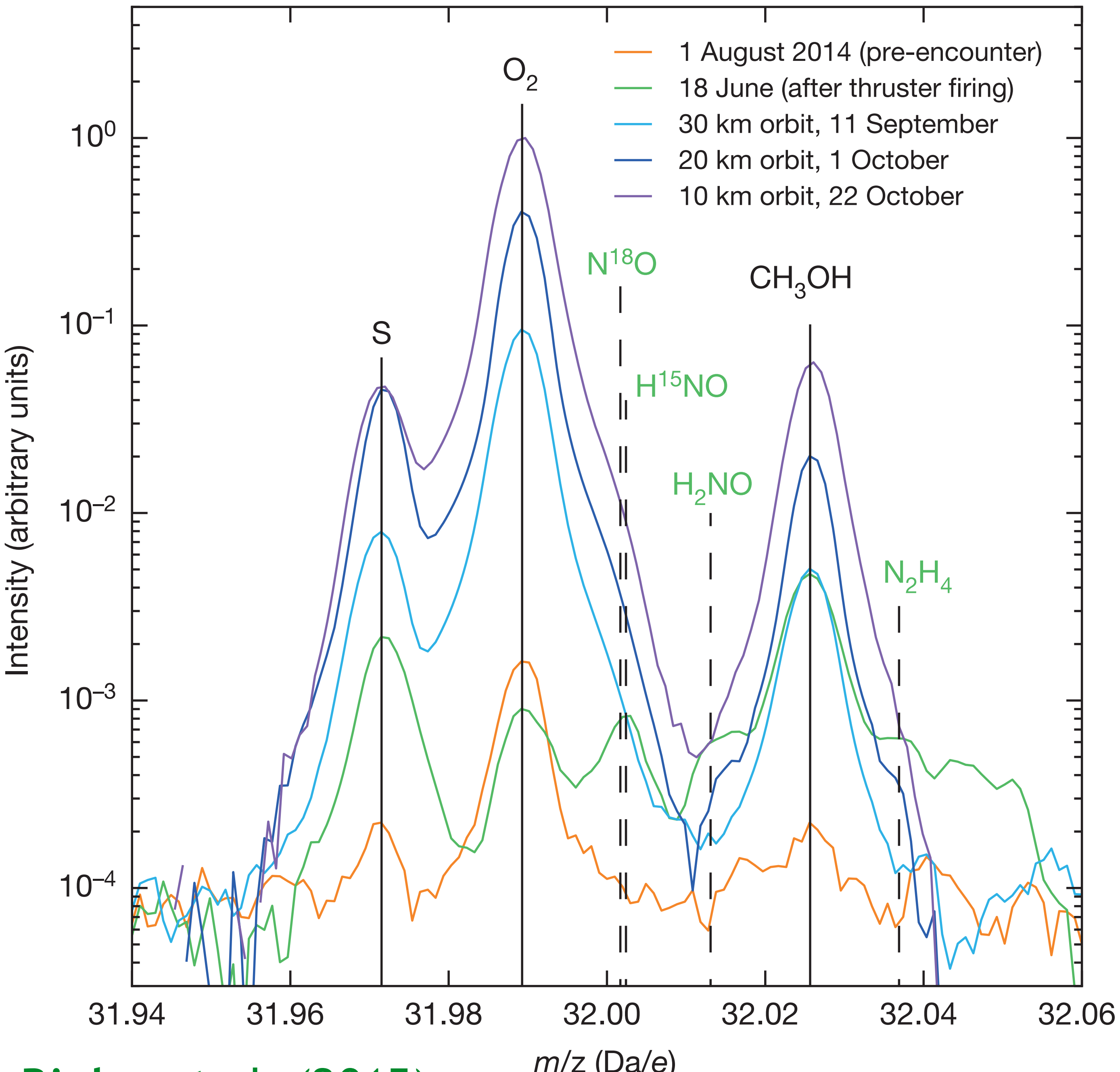
Detection of O_2 in the comet 67P

First detection of molecular oxygen in a comet by Rosetta:

- **High resolution** of the **ROSINA-DFMS** distinction of O_2 from other species of same mass 32

- **$X(O_2) / X(H_2O) = 3.8 \pm 0.9$ %**
→ forth most abundant molecule

+ **Re-analysis** of the **Giotto** data toward **1P/Halley** results in a **similar abundance** of 3.7 % / H_2O !
(**Rubin** et al. 2015)

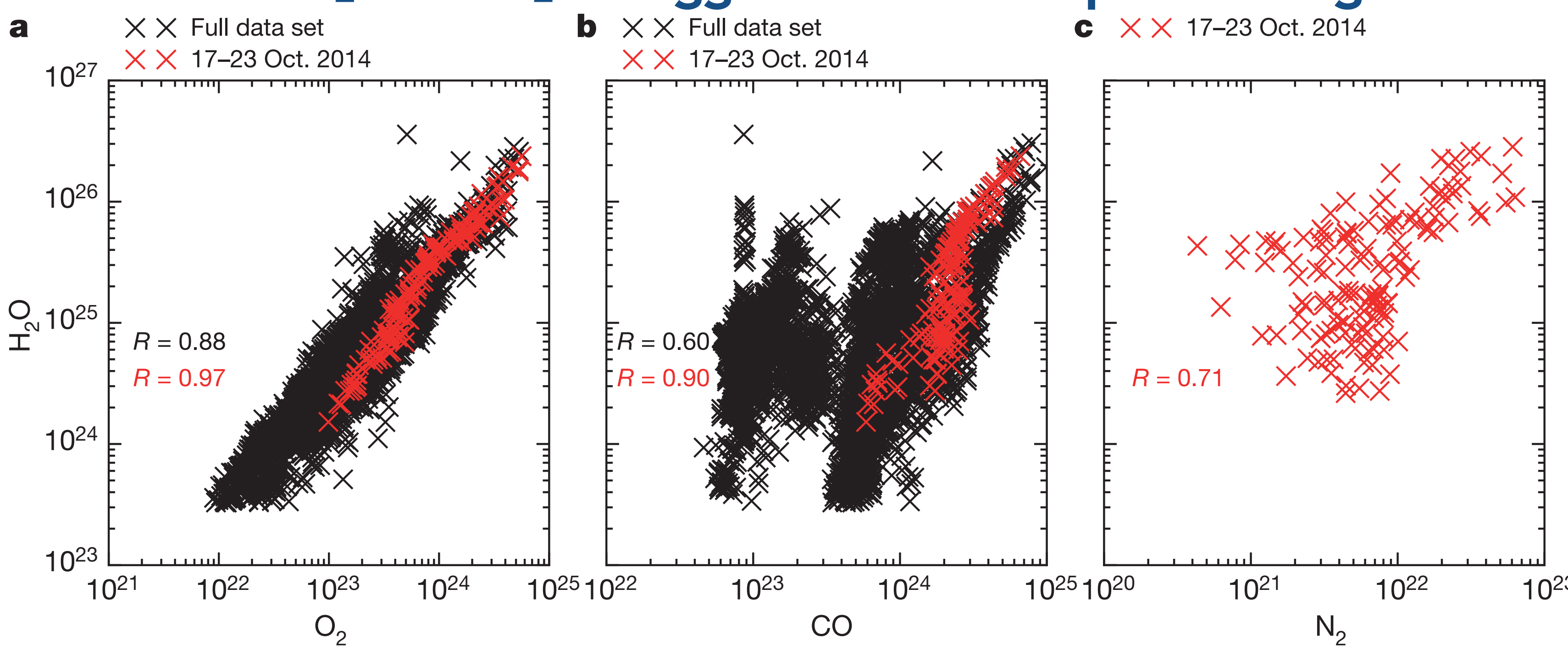


Bieler et al. (2015)

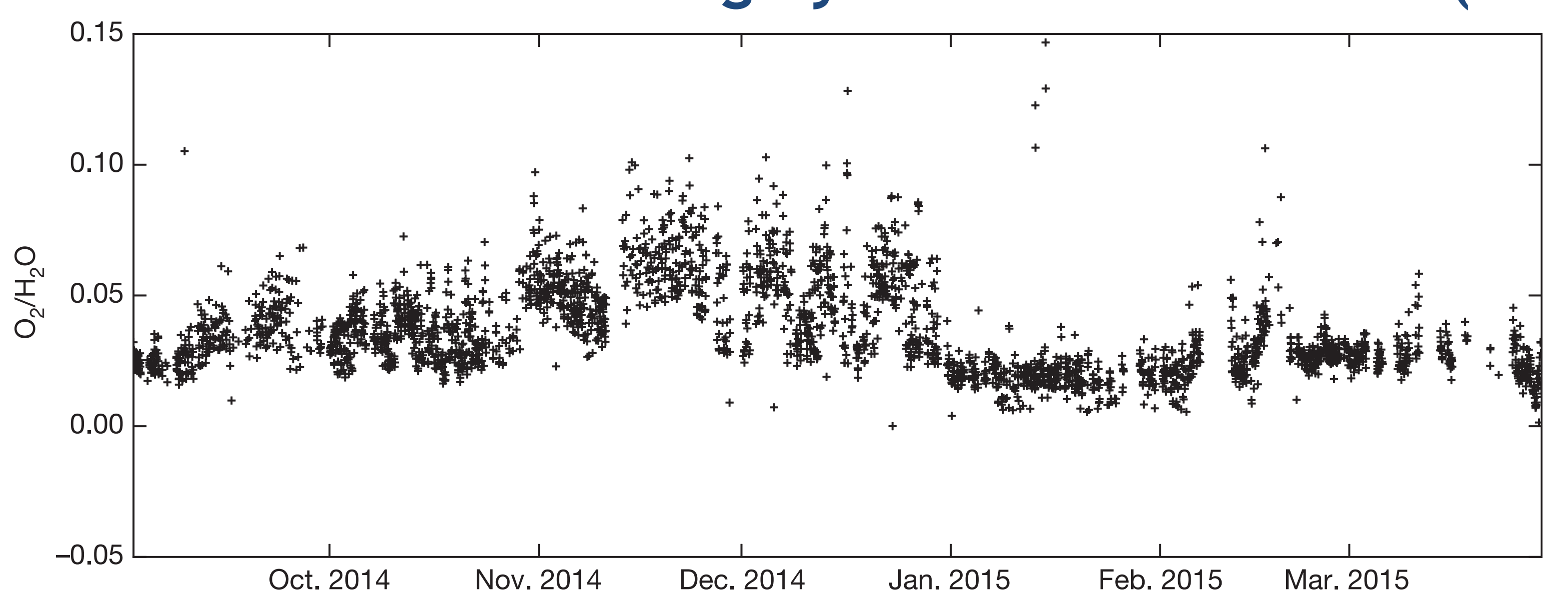
Abundant O_2 trapped into water ice matrix

O_2 is trapped into a likely pristine water ice matrix

Strong correlation of O_2 and H_2O suggests similar spatial origin and mechanisms



The O_2/H_2O abundance ratio remains roughly constant over time (3.8 ± 0.9 % / H_2O)



Bieler et al. (2015)

→ O_2 was likely already present in the ice mantle prior to comet formation

Interstellar chemistry of O_2

O_2 is involved in the **chemical network** forming interstellar (icy) **water**

O_2 formation and survival in interstellar ices depend on:

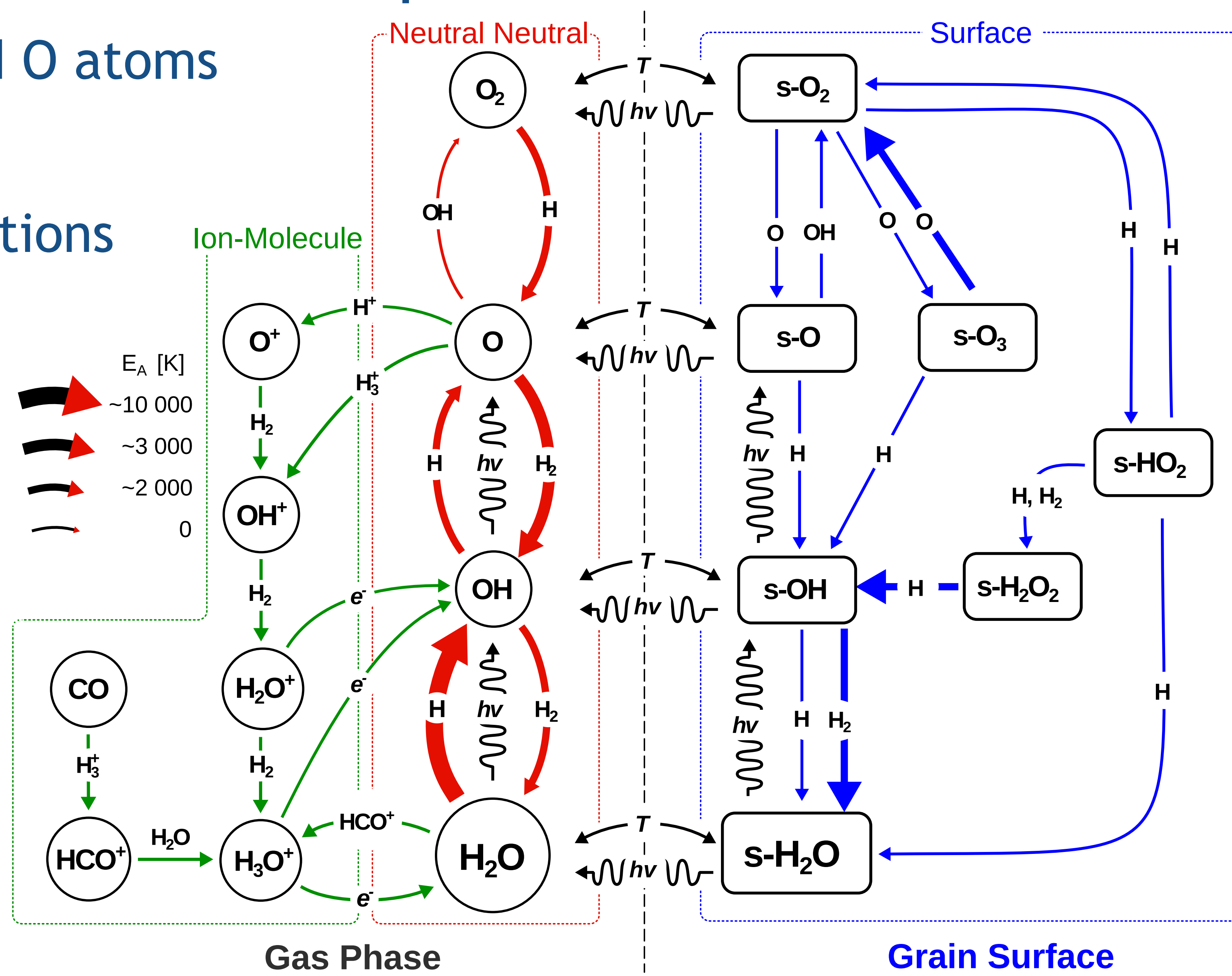
1) Gas phase abundance of H and O atoms

2) Mobility of O atoms

3) Activation barriers of key reactions

→ O_2 production should be accompanied by **O_3, HO_2 and H_2O_2** but ROSINA measured low abundances in 67P:

- $X(HO_2) \sim X(H_2O_2) = 6\ 10^{-4}\ /\ O_2$
- $X(O_3) < 3\ 10^{-5}\ /\ O_2$



Credit: M. Persson

Objectives of this work

Give an explanation of the observations of 67P/C-G by Rosetta/ROSINA:

1) **Primordial formation of O_2** prior to comet formation
2) **High abundance** of 3.8 % of **O_2** relative to water but **low abundance** of the chemically related species **HO_2, H_2O_2, and O_3** (lower than 6 x 10^{-4} / O_2)
3) **Strong correlation** between **O_2 and H_2O** signals but **weak correlation** between **N_2, CO and H_2O** signals

Exploration of three different scenarios:

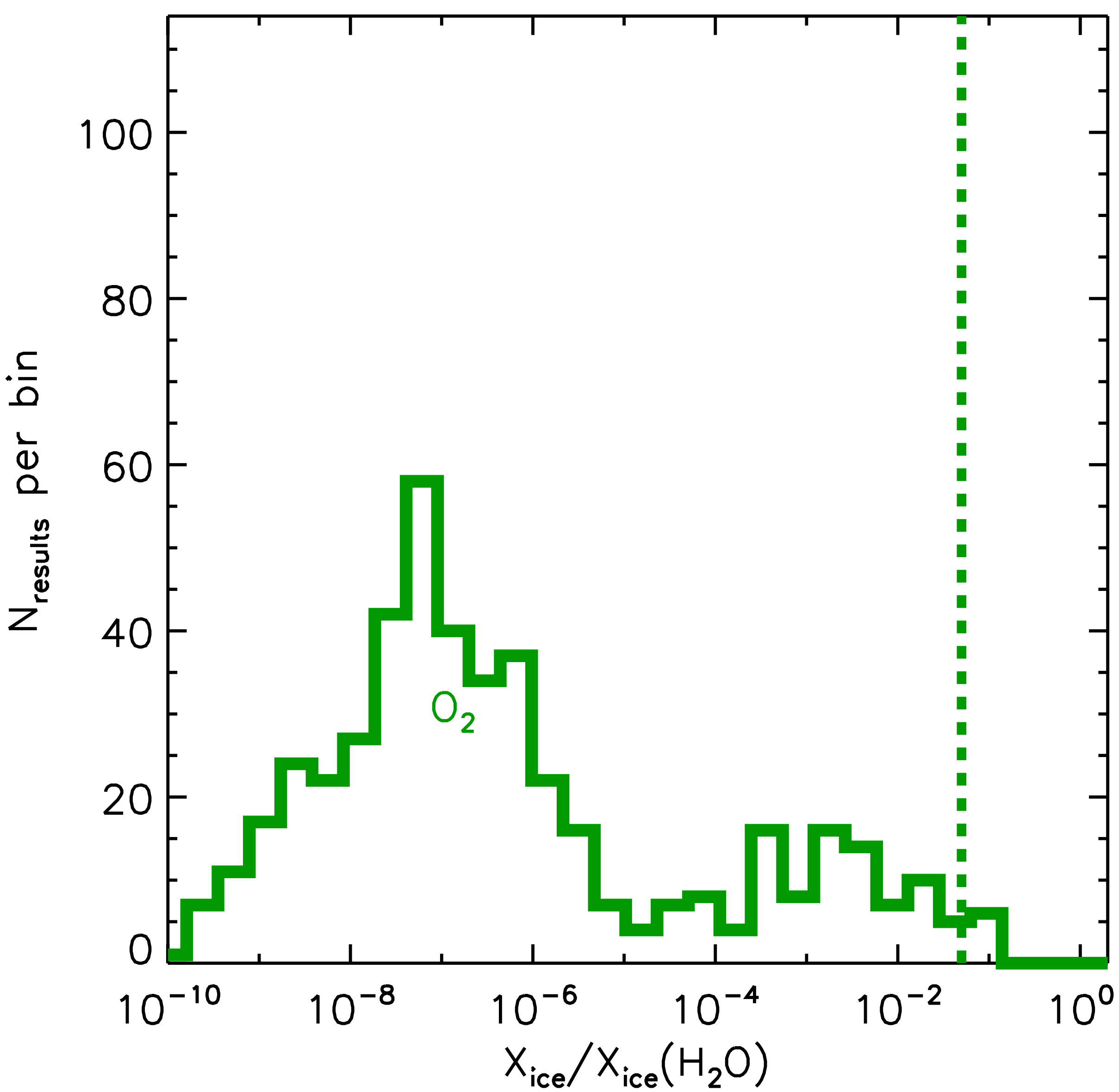
1) O_2 formation and survival in **molecular clouds**
2) O_2 formation and survival during **protoplanetary disk formation**
3) O_2 formation and survival within **protoplanetary disks**

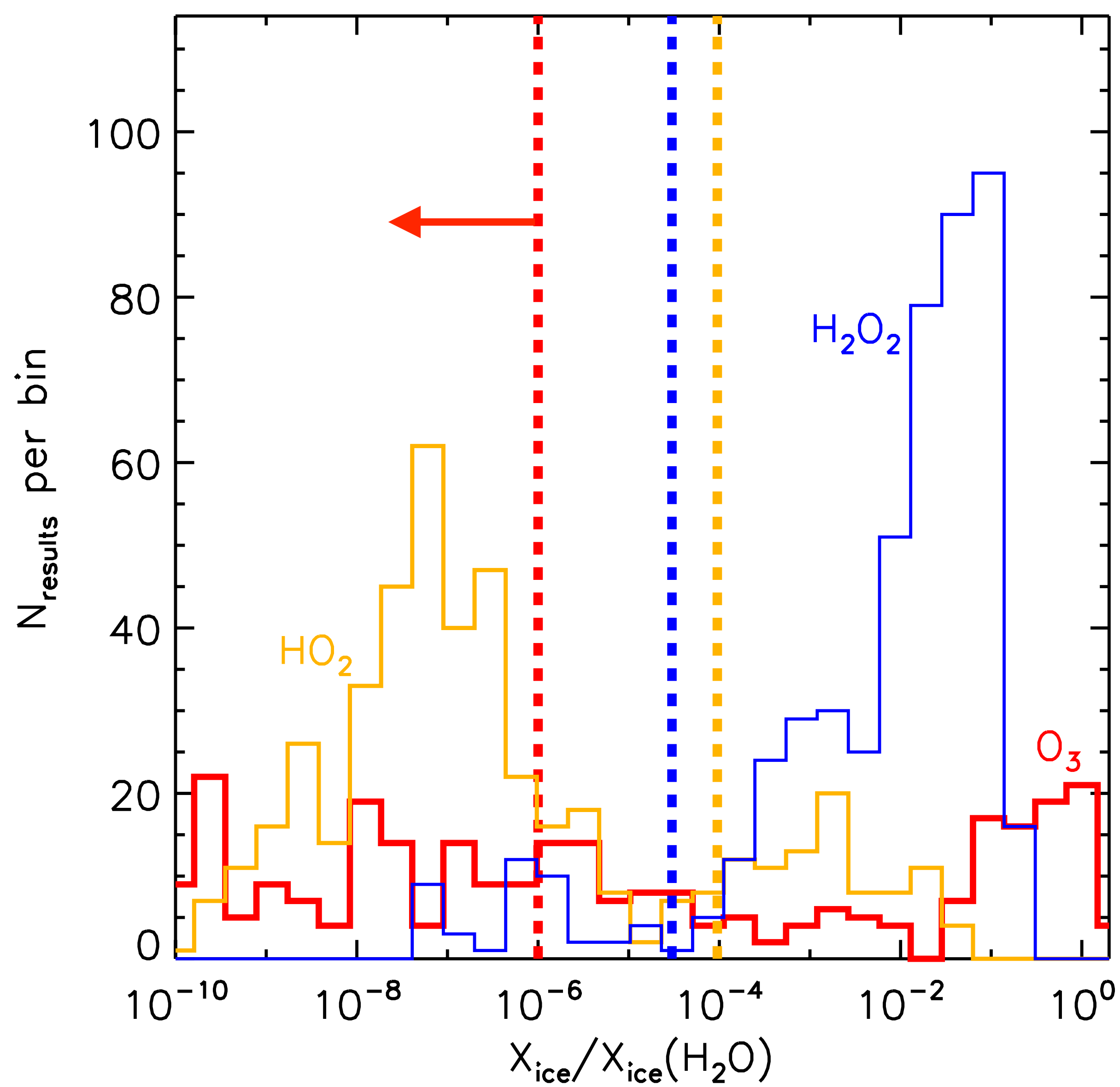
→ Two multi-phase (bulk, surface, gas) astrochemical models are used to study the cold and warm gas-grain chemistries
(**Taquet** et al. 2014, **Furuya** et al. 2015)

O_2 formation in dark clouds ?

Multi-phase gas-grain model applied to a parameter approach via a grid of models:

Parameter	Range of explored values
	Physical conditions explored in the model grids
Total density (cm^{-3})	$10^3 - 10^4 - 10^5 - 10^6$
Temperature (K)	10 - 15 - 20 -25 - 30
ζ (s^{-1})	10^{-18} - 3×10^{-18} - 10^{-17} - 3×10^{-17} - 10^{-16}
A_V (mag)	2 -4 - 6 - 8 - 10





→ Abundances in interstellar ices highly depend on physical conditions

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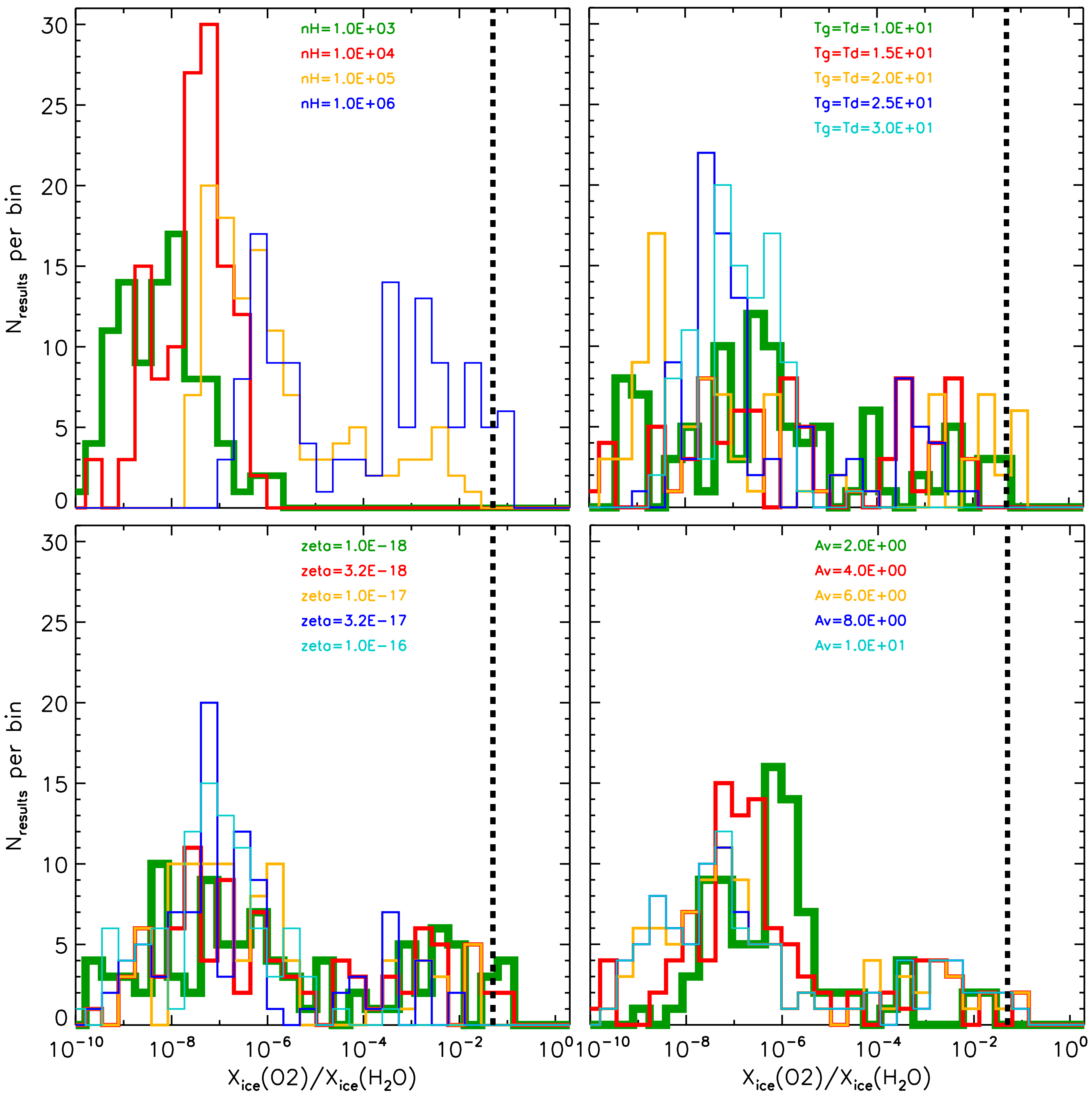


→ **O_2 abundance derived in 67P can be reproduced with dense ($n_H = 10^6$ cm^{-3}) and lukewarm (T = 20 K) conditions**

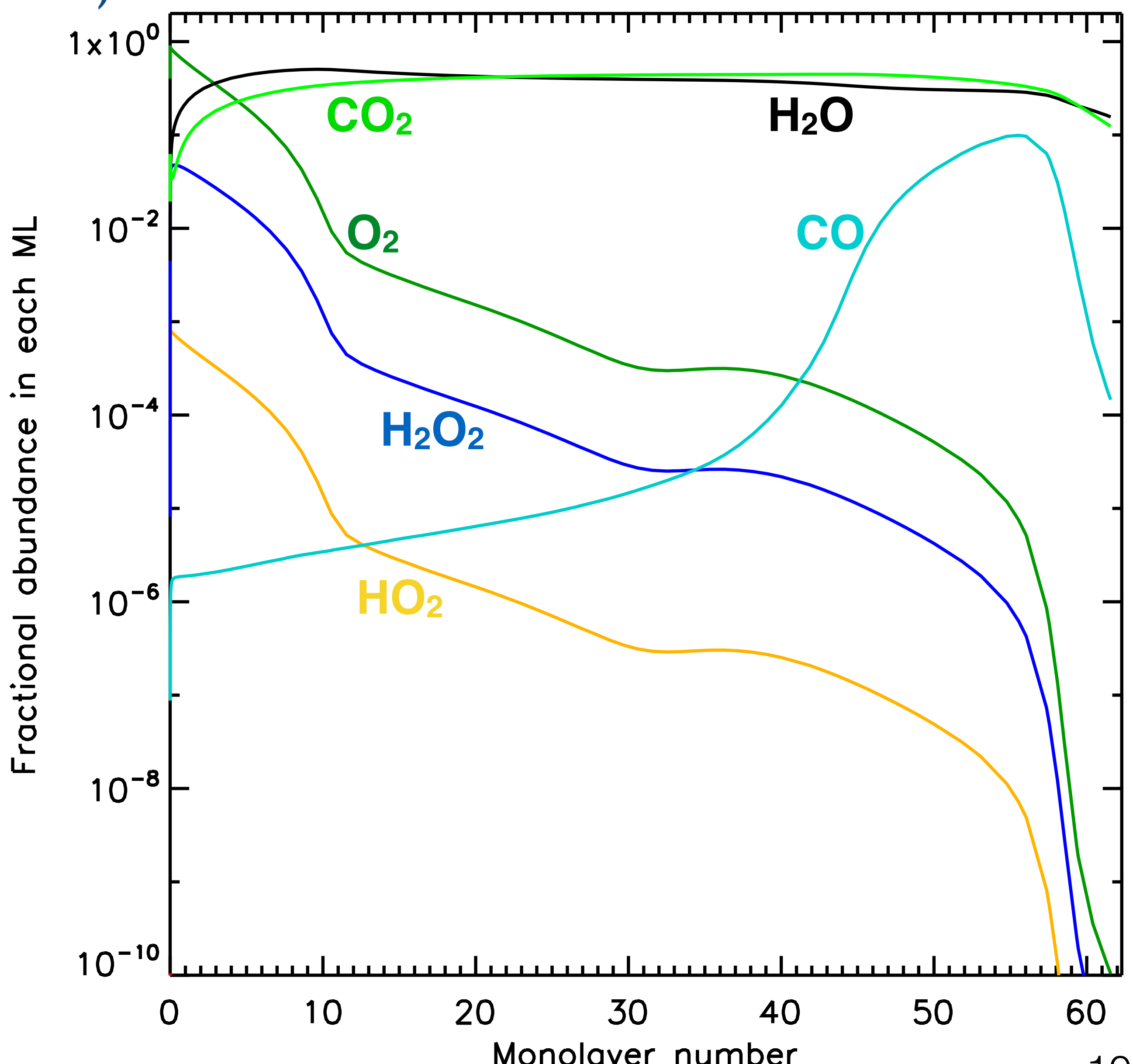
Chemical properties in ices

Physical conditions **needed to reproduce the O_2 abundance seen in 67P are** **consistent** **with those of** **ρ Oph A** **($n_H = 10^6$ cm^{-3}; T_{dust} = 21 K):**

- Low **$X(O_3)$ and $X(HO_2)$** in 67P **reproduced** with **$E_a(O_2+O)$ ~ $E_a(O_2+H)$ ~ 300 K**
→ consistent with Monte-Carlo models by Lamberts et al. (2013)
(but H_2O_2 still overproduced by a factor of 10)

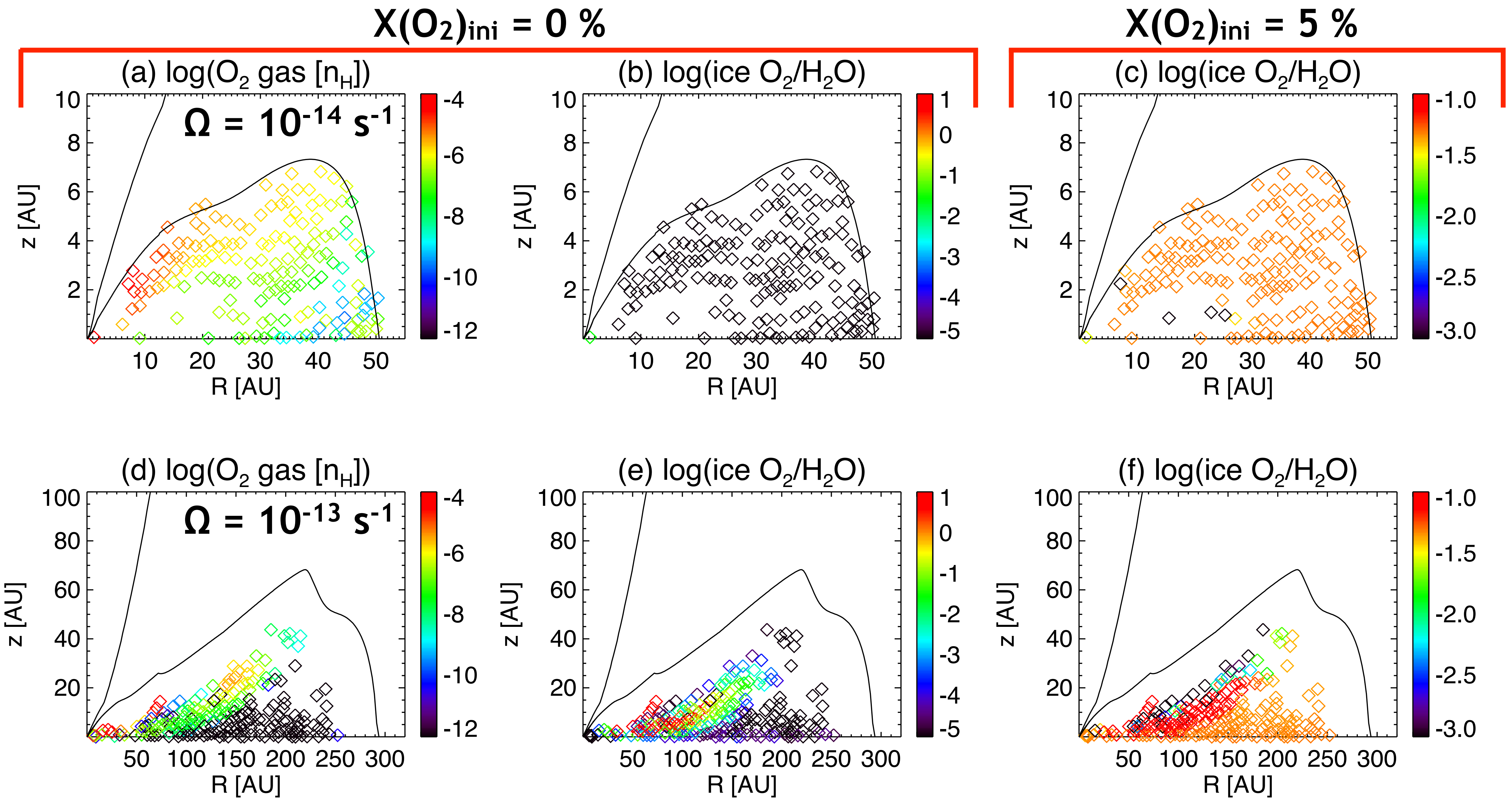
- **O_2 is trapped into the inner part** of the ices, unlike **CO** (and N_2) which are mostly **present at the surface**

→ Explanation of the correlation between O_2 and H_2O signals seen in 67P, and anticorrelation for CO and N_2



O_2 formation during the disk formation ?

Multi-phase astrochemical model applied to a 2D semi-analytical model of core contraction (Visser et al. 2009)

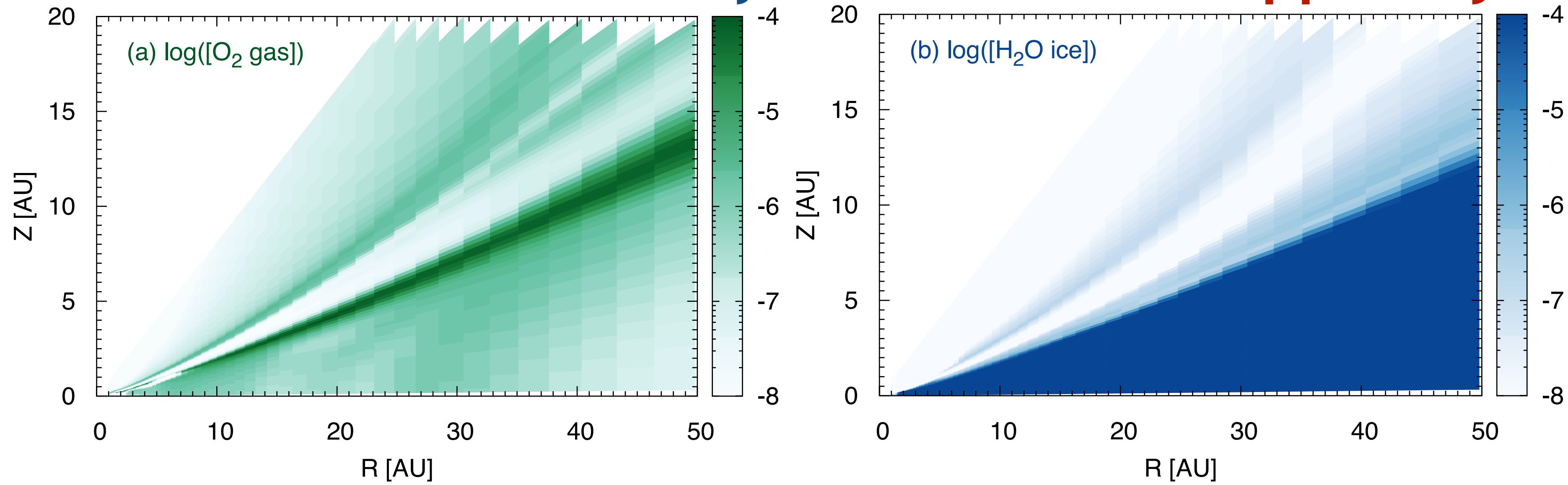


- Efficient formation of O_2 vapour, but no production of O_2 ice into water matrix
- O_2 ice formed in ISM can survive during its journey to the disk

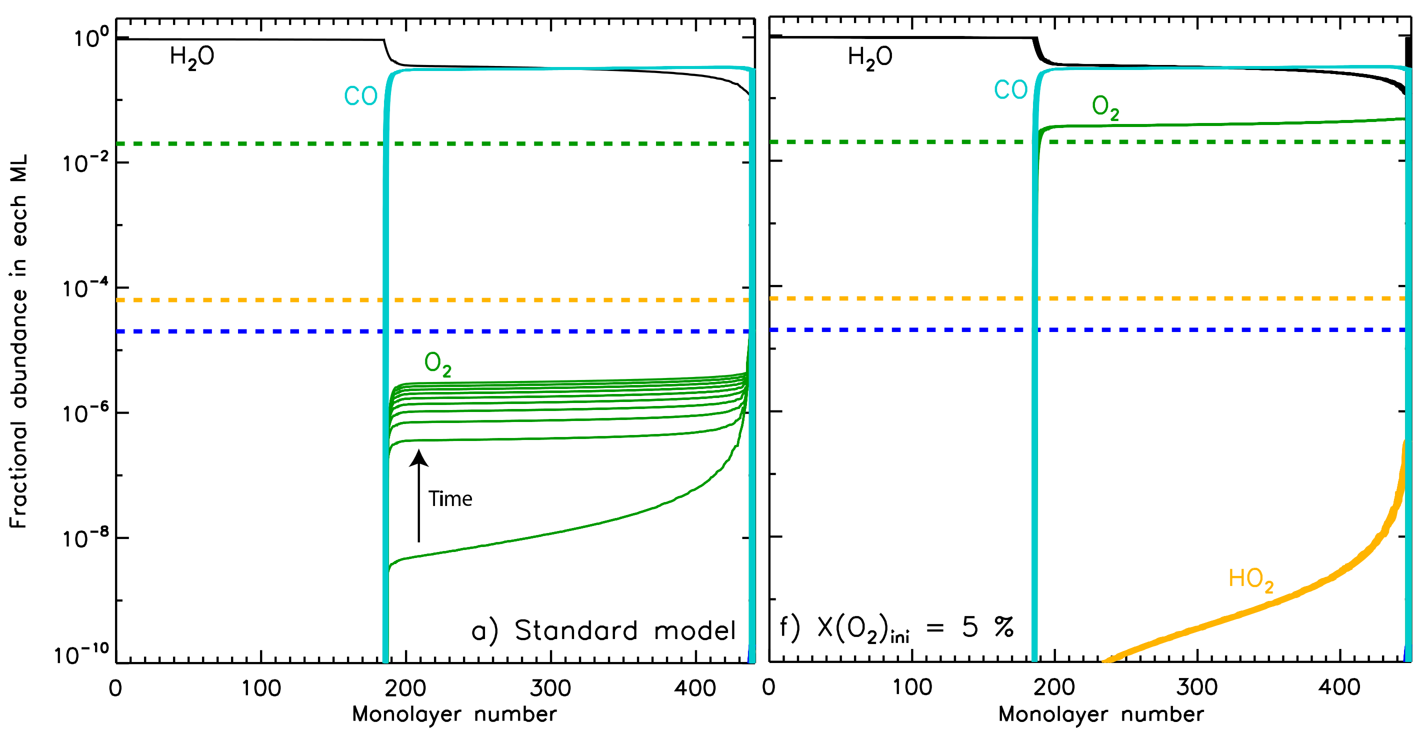
O_2 formation in protoplanetary disks ?

Can O_2 be formed and trapped into water ice in the solar nebula ?

→ **Gas phase** formation of O_2 is only efficient in the **upper layers** of the disk



Can O_2 be formed during luminosity outbursts and trapped with water during the cooling ?



- **Luminosity outbursts** are **too short** to produce O_2 in quantities observed in comets

- **CO and O_2** are **trapped together** during the cooling
→ cannot explain the correlation of O_2 and non-correlation of CO/N_2 with water

Conclusions

High abundance of O_2 trapped into water ice observed in 67P by Rosetta/ROSINA can be explained by:

- an efficient formation in **dense** and **lukewarm** molecular **clouds**

- a **survival** of the **O_2-H_2O ice mixture** in the solar nebula

→ consistent with some properties of our Solar System, suggesting that it was **born in a dense cluster of stars** (see Adams 2010)

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Thank you !