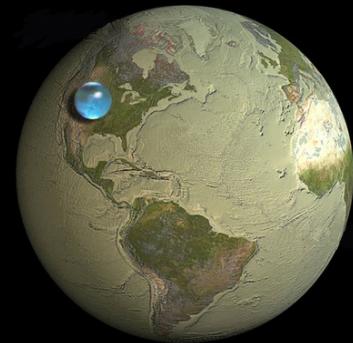


Interstellar Water Ice Formation: A laboratory perspective

Sergio Ioppolo

Department of Physical Sciences, The Open University, Walton Hall, Milton Keynes MK7 6AA, UK

Water in space



- Fundamental for life on Earth

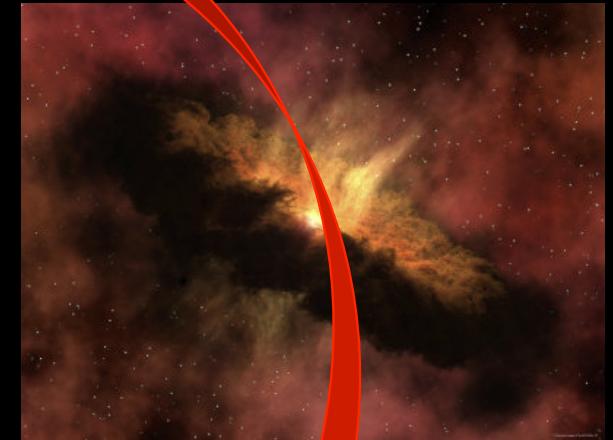
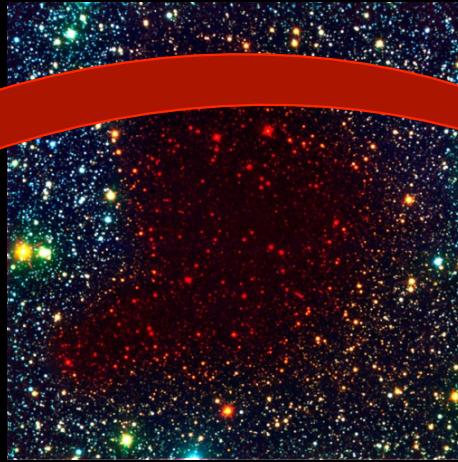
**What is its origin and
how was it delivered to the Earth?**

**GAS PHASE
REACTIONS**

No efficient cold gas-phase routes

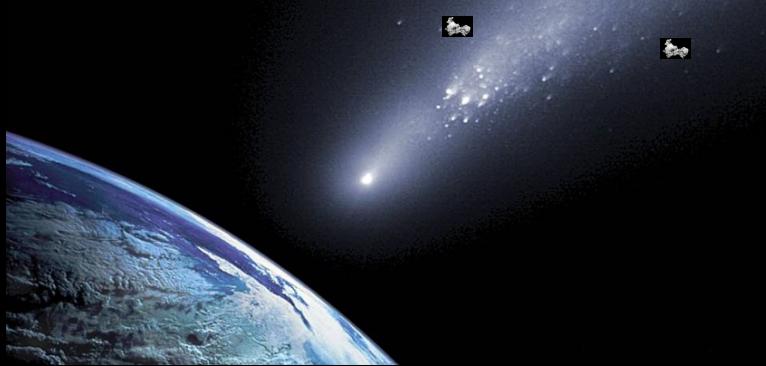
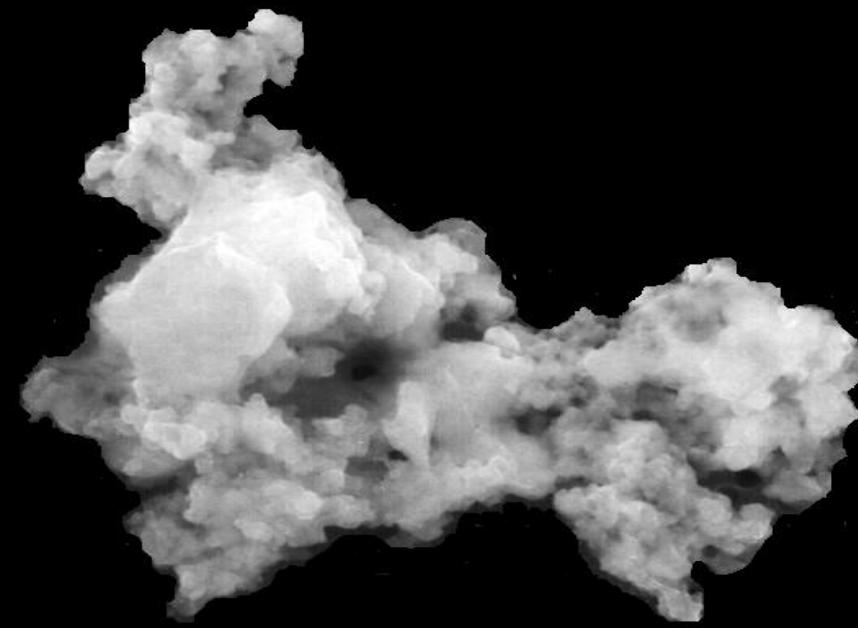
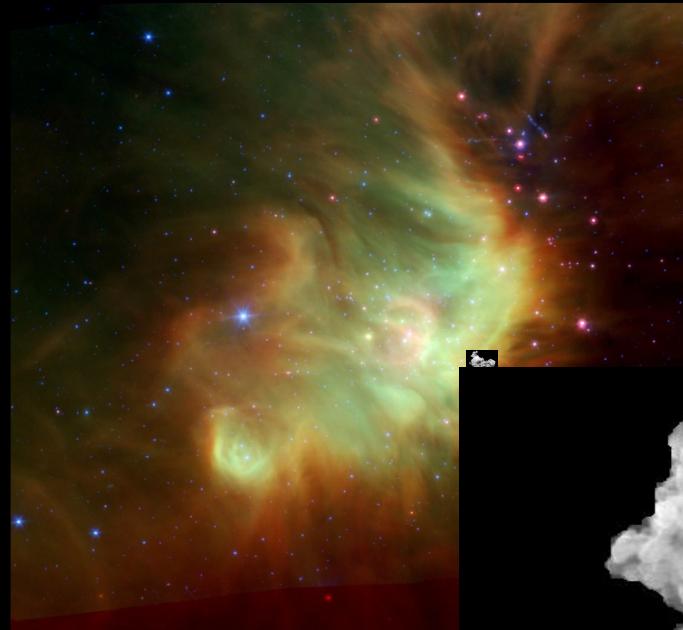
**SOLID PHASE
REACTIONS**

Formation on dust grains



Cycle of Dust





Interstellar ice chemistry

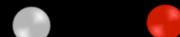
Carbonaceous/Silicate Grains

DESORPTION



ADSORPTION

DIFFUSION



REACTION



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



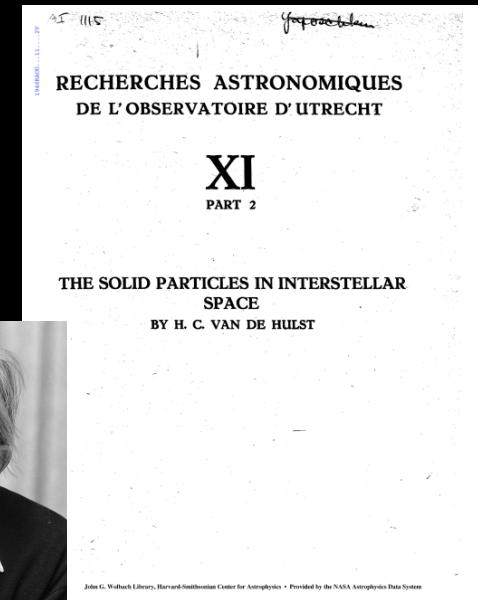
Interstellar ice chemistry

Carbonaceous/Silicate Grains



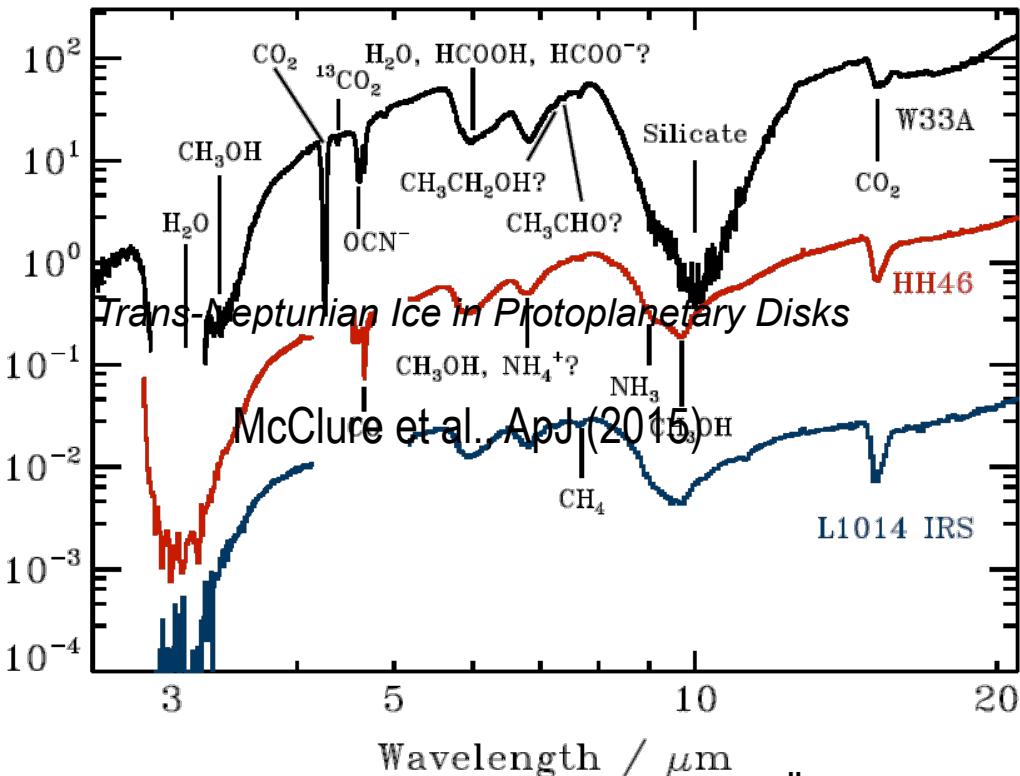
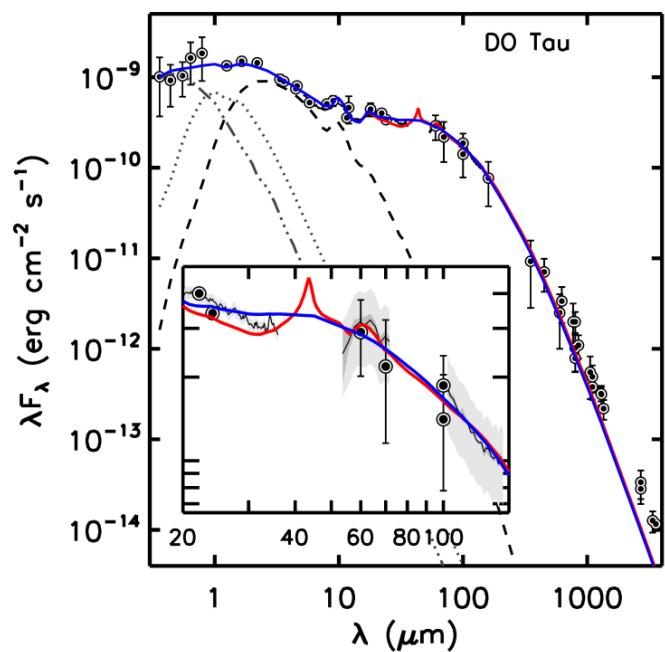
$$T = 10\text{-}20 \text{ K}$$
$$n > 10^2 \text{ cm}^{-3}$$

$< 1 \mu\text{m}$



van de Hulst, RAOU (1946)

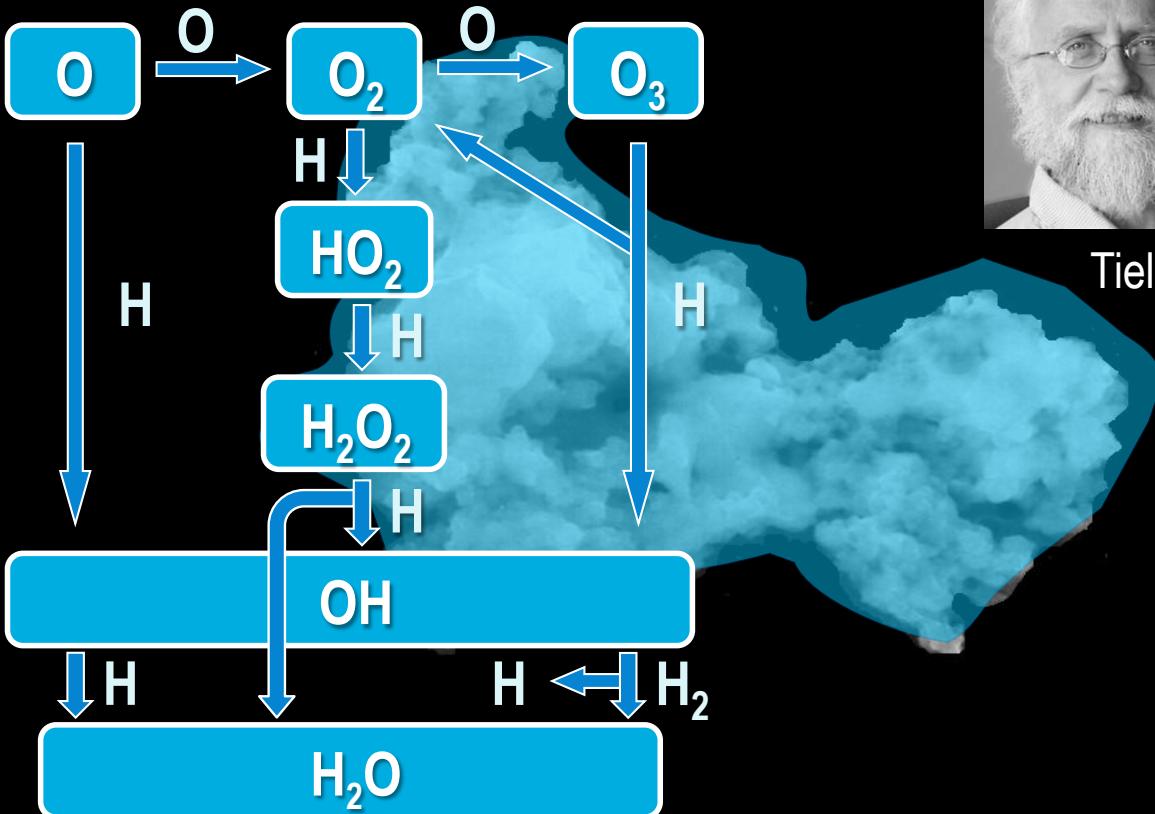
Ice Observations



Öberg (2009)

ICE FEATURE	LOW MASS	HIGH MASS	BACKGROUND
H ₂ O	100	100	100
CO	29	13	31
CO ₂	29	13	38
CH ₃ OH	3	4	4
NH ₃	5	5	
CH ₄	5	2	
XCN	0.3	0.6	

Interstellar water ice



Tielens & Hagen, A&A (1982)

E&PSL, 114, 245–260 (1982)
Astron. Astrophys. 114, 245–260 (1982)
A. G. G. M. Tielens* and W. Hagen**
Laboratory Astrophysics Group, Rijksuniversiteit, 2300 RA Leiden, The Netherlands
Received February 1, accepted May 19, 1982

Model Calculations of the Molecular Composition of Interstellar Grain Mantles
A. G. G. M. Tielens* and W. Hagen**
Laboratory Astrophysics Group, Rijksuniversiteit, 2300 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 model. The chemical composition of the gas phase and the surface reactions. The equilibrium abundances of the molecules in the gas are calculated using gas-phase reaction theory for H₂, forming the basis for calculating grain-mantle compositions determined on the basis of the relative accretion rates of the gas-phase species.

The results show that in most circumstances grain mantles consist mainly of oxygen, with CO, CO₂, H₂O₂, H₂O, NH₃, and N₂H₃. The relative concentrations of these species depend strongly on the physical conditions in the gas. The formation of H₂O₂ and H₂O is explained by the fact that these molecules proceed through hydrogen abstraction from molecules like H₂O₂, H₂O, and NH₃. The H₂O₂ and H₂O molecules themselves act as enhanced binding sites for H atoms.

The models predict that the most concentrated grain mantles are distributed with an emphasis on the observed 250 μm^{-1} – 450 μm^{-1} and 320 μm^{-1} “ice” band. It is suggested that the low frequency wing of the features observed in interstellar emission is due to absorption by H₂O₂, H₂O, and NH₃ hydrogen-bonded

oligomers.

Keywords: dust – infrared – interstellar matter – molecular clouds

Introduction
The first detection of interstellar emission provided definite evidence for the presence of interstellar dust (Trumpler, 1930), and the composition of the grains has been the subject of much discussion. Among the proposed grain materials are a “dirty ice” mixture of various ices (Tielens et al., 1978; Tielens and Hagen, 1982; Hoyle and Wickramasinghe, 1982; Kamijo, 1983). The dust may also consist of a solid solution of a number of different H₂O ice with embedded impurities containing other elements all proportionate to their elemental abundances (van de Hulst, 1949).

ad offere requeste: Dr. A. G. G. M. Tielens
Present address: Space Research Center, M.S.
245-6, Moffett Field, CA 94035, USA
Present address: Koninklijke/Shell Laboratorium,
Amsterdam, The Netherlands

Infrared spectroscopy is an important tool for the study of interstellar dust particles. Finely dust particles emit most of their energy in the infrared, and the infrared spectra of interstellar grains, which have become available during the last decade, contain direct information on the molecular composition of grains.

Indirect observations of interstellar grains are the solid particles found in the surface of late-type stars (Gilliland et al., 1968).

The infrared spectrum of the star *tau* Ceti is very similar to that expected from a cool stellar photosphere at the temperature indicated by the optical spectra (Merrill et al., 1976).

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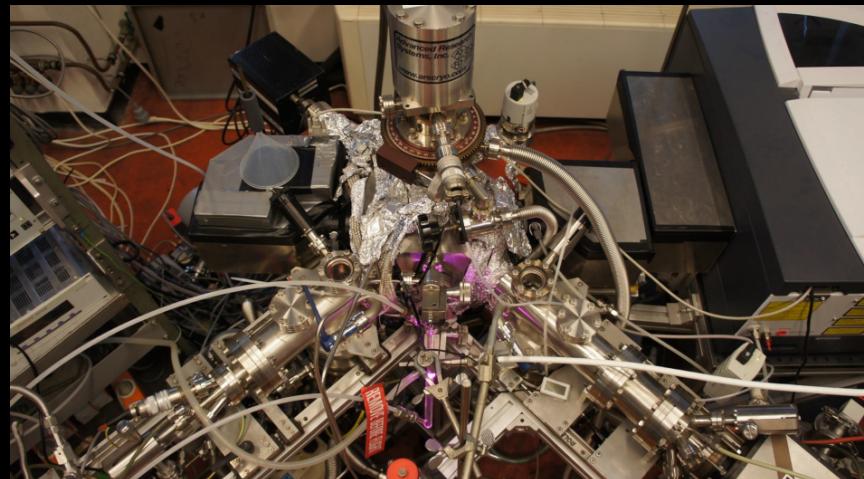
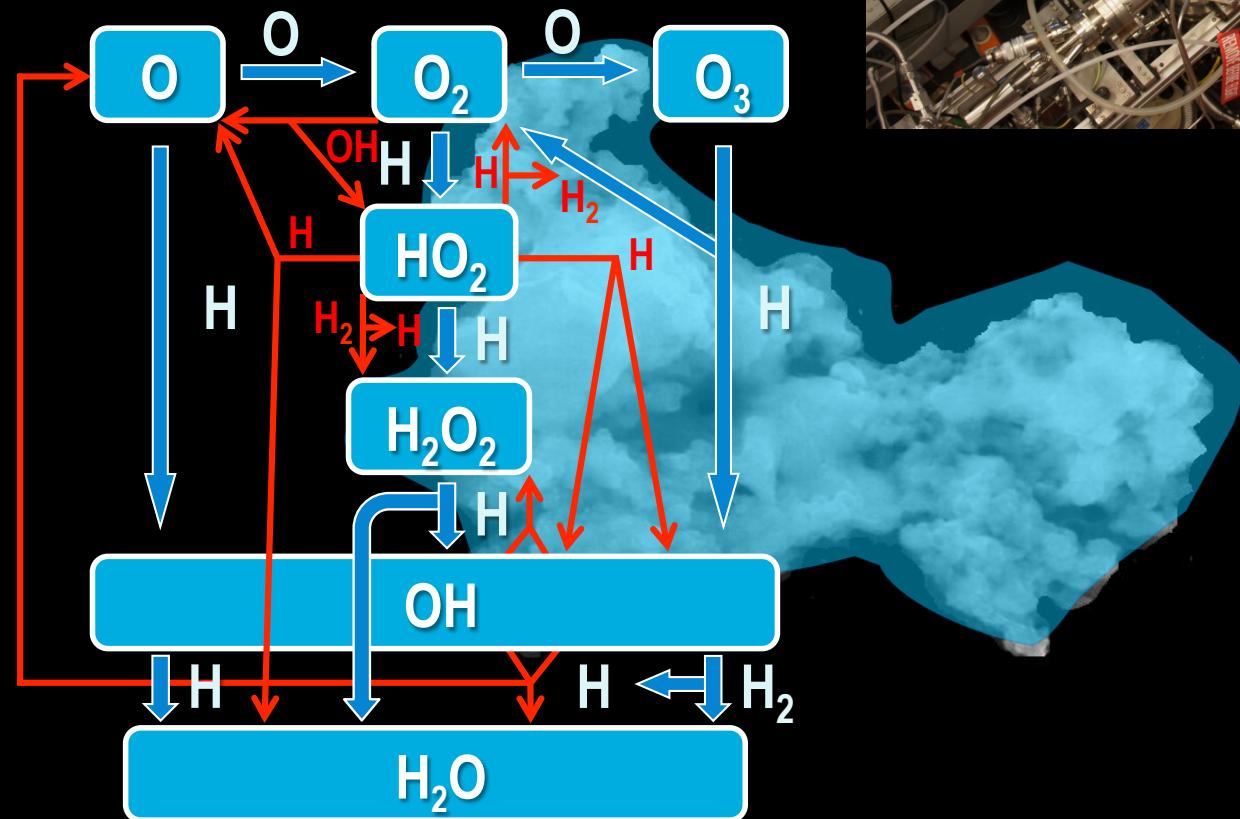
The infrared spectrum of the star *tau* Ceti is very similar to that expected from a cool stellar photosphere at the temperature indicated by the optical spectra (Merrill et al., 1976).

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Interstellar water ice



Interstellar water ice

Formation of hydrogen peroxide and water from the reaction of cold hydrogen atoms with solid oxygen at 10 K
N. Miyachi¹, H. Hidaka, T. Chigai, A. Nagakura, N. Watanabe, A. Kouchi
Institute of Space and Astronautical Science, Japan Aerospace Exploration Agency, 3-1-1, Yoshinodai, Sagamihara 252-5610, Japan

ARTICLE INFO
Article history:
Received 11 January 2008
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ABSTRACT
The reactions of cold D atoms with solid O₂ molecules were investigated at 10 K. The formation of H₂O₂ and H₂O has been confirmed by *in situ* infrared spectroscopy. We found that the reaction proceeds very efficiently and the yield of H₂O₂ is higher than that of H₂O. The formation mechanism of H₂O₂ is discussed based on the formation of water molecules under conditions mimicking those found in cold interstellar molecular clouds. Based on the experimental results, we discuss the reaction mechanism and astrophysical implications.

which has an activation energy of 5.16 located in the gas phase [7]. For the third process, Telionis and Hagen [8] proposed alternative reaction schemes:

$$\begin{aligned} \text{O} + \text{H}_2 &\rightarrow \text{OH} + \text{O}, & (4) \\ \text{O}_2 + \text{H} &\rightarrow \text{HO}_2 + \text{O}, & (5) \\ \text{HO}_2 + \text{H} &\rightarrow \text{H}_2\text{O}_2 + \text{O}, & (6) \\ \text{H}_2 + \text{O}_2 &\rightarrow \text{H}_2\text{O} + \text{OH}. & (7) \end{aligned}$$

Reaction (5) has essentially no barrier; theoretically estimated activation energies lie between 0.1 and 0.4 kcal/mol [9]. Reaction (7) has a barrier of 1.2 kcal/mol [10]. Activation energies of the other processes referred here are values in the gas phase. There has been no data on the activation energy of the reaction of H atoms with solid O₂. There are two main sources of water molecules in the gas phase: (1) H₂O₂ and (2) H₂O. These are formed via the reaction of O atoms with H atoms. There has been no data on the reaction of O atoms with H atoms either. It has been clarified that the formation of water molecules in the gas phase is due to the reaction of O atoms with H atoms in the former clouds [14]. Thus, it has been suggested that water molecules are formed in the gas phase in the former clouds by the reaction of O atoms with carbonaceous grains at around 10 K [5–7].

The first possible process for H₂O formation is the sequential hydrogenation of O atoms on grains:

$$\begin{aligned} \text{O} + \text{H} &\rightarrow \text{OH}, & (1) \\ \text{OH} + \text{H} &\rightarrow \text{H}_2\text{O}, & (2) \end{aligned}$$

It is well known that O atoms have an activation barrier [6]. The second possible process is the reaction of OH with hydrogen molecules adsorbed on the surface of grains:

$$\text{OH} + \text{H}_2 \rightarrow \text{H}_2\text{O} + \text{H}. & (3)$$

* Corresponding author. Fax: +81 11 790 7142.
E-mail address: n Miyachi@nasda.ac.jp (N. Miyachi).

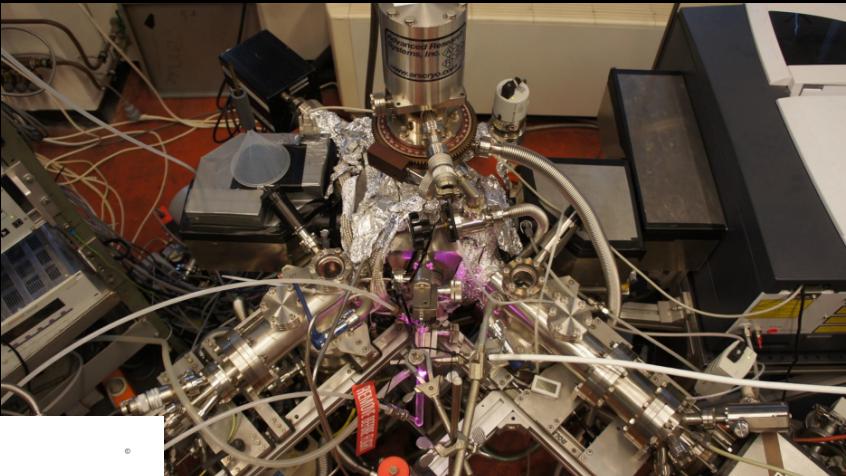
0009-2614/\$ – see front matter © 2008 Elsevier B.V. All rights reserved.
doi:10.1016/j.cplett.2008.04.007



Miyauchi et al., CPL (2008)



Ioppolo et al., ApJ (2008)



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LABORATORY EVIDENCE FOR EFFICIENT WATER FORMATION IN INTERSTELLAR ICES
S. Kewley, E. M. Cugia, C. Bouquet, E. F. van Dishoeck, and H. Linz
Raymond and Beverly Sackler Laboratory for Chemical Astrophysics, Leiden University,
P.O. Box 9513, 2300 RA, Leiden, Netherlands
Received 2008 April 16; accepted 2008 June 30

ABSTRACT
Even though water is the main constituent in interstellar ices, its chemical origin is not well understood. Three different formation routes have been proposed following hydrogenation of O₂ or O₃ on ice grains, but experimental evidence is largely lacking. We present a *solid-state* astrophysical laboratory study in which one of these routes is tested. We find that H atoms react with O₂ on porous amorphous water ice surfaces at temperatures relevant to interstellar ices, ranging from 12 to 28 K. The use of reflection absorption infrared spectroscopy (RAIRS) allows us to monitor the formation of H₂O₂ and H₂O in the gas phase, which is independent of temperature. This formation route converts O₂ into H₂O via H₂O₂ and is found to be orders of magnitude more efficient than previously assumed. It should therefore be considered as an important channel for interstellar water formation. We also discuss the model calculations.

Subject headings: astrochemistry — infrared: ISM — ISM atoms — ISM: molecules — methods: laboratory
Online material: color figures

A&A 492, L17–L20 (2008)
DOI: 10.1051/0004-6390.2008010434
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Astronomy & Astrophysics

LETTER TO THE EDITOR

Mobility of D atoms on porous amorphous water ice surfaces under interstellar conditions

E. Matar, E. Cugia, F. Dulieu, A. Momen*, and J.-L. Lemaitre
Université de Cergy-Pontoise & Observatoire de Paris, LERMA, UMR 8112 du CNRS, 95000 Cergy-Pontoise, France
e-mail: E.Matar@astropc.org (E. Matar)
Received 20 June 2008 / Accepted 21 October 2008

ABSTRACT
The mobility of H atoms on the surface of interstellar dust grains at low temperature is still a matter of debate. In dense clouds, the hydrogenation of adsorbed species (i.e., CO) as well as the subsequent desorption of the adsorbed molecules depend on the mobility of H atoms. Infrared observations of the interstellar medium (ISM) have shown the presence of large amounts of convective water ice. We present here direct experimental evidence of the mobility of H atoms on porous water ice surfaces at 10 K. Mobility is measured by the diffusion of H atoms in a porous water ice surface at 10 K. The diffusion is measured by Temperature Programmed Desorption (TPD) of H atoms and desorption of O₂ and D₂ simultaneously monitored by RAIRS. The diffusion coefficient of H atoms is found to be $D = 1.7 \times 10^{-10} \text{ cm}^2/\text{s}$ at 10 K. The diffusion of H atoms is enhanced by a factor of 10 compared to the diffusion of D atoms. The diffusion of H atoms is enhanced by a factor of 10 compared to the diffusion of D atoms even though these molecules have previously diffused inside the pores of thick water ice. Our results can be explained by the fact that the diffusion of H atoms is governed by the diffusion of H₂O₂ molecules. The diffusion of H atoms is enhanced by a factor of 10 compared to the diffusion of D atoms even though these molecules have previously diffused inside the pores of thick water ice. Our results can be explained by the fact that the diffusion of H atoms is governed by the diffusion of H₂O₂ molecules.

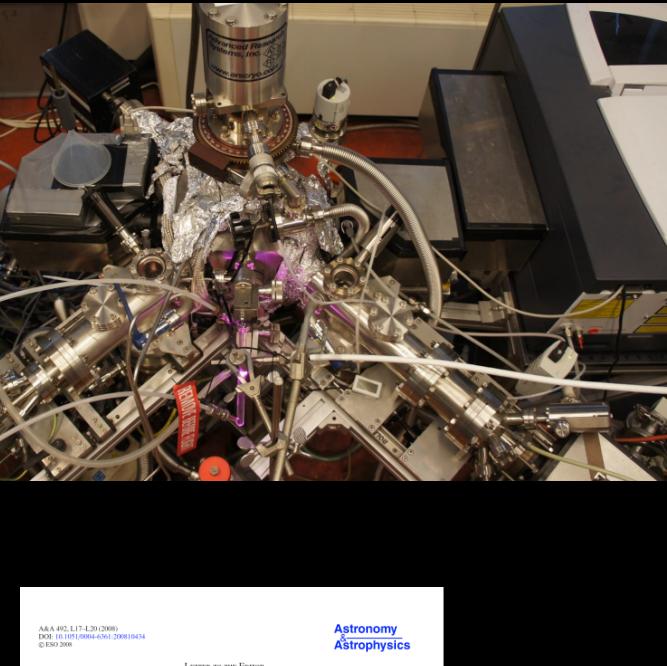
Key words: astrochemistry — ISM atoms — dust, extinction — methods: laboratory

Article published by EDP Sciences

Matar et al., A&AL (2008)



UNIVERSITÉ
de Cergy-Pontoise



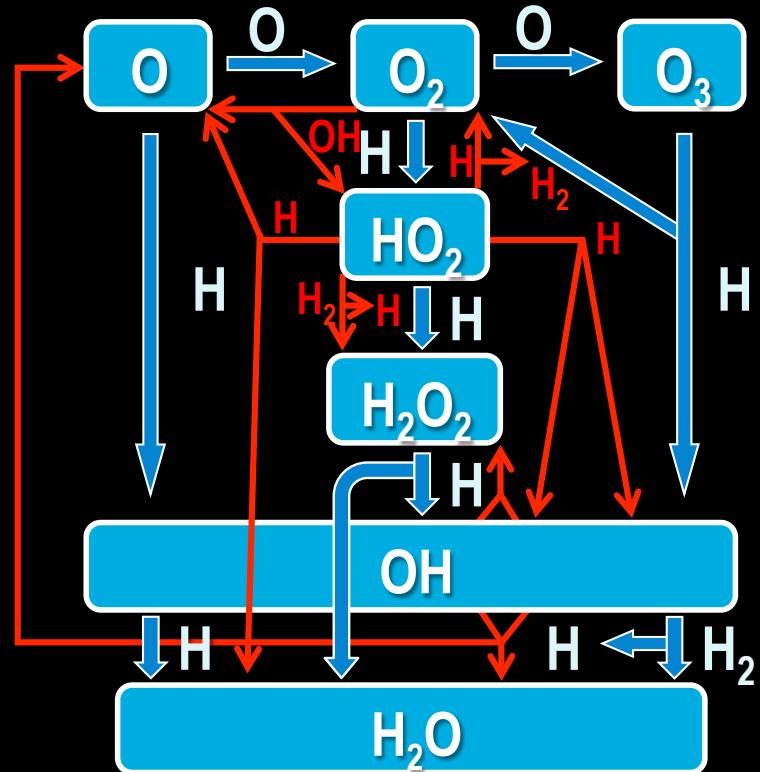
THE ASTROPHYSICAL JOURNAL, 689:1200–1203, 2008 August 10
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Received 2008 April 16; accepted 2008 June 30

1. Introduction
Among the numerous molecules detected in different interstellar environments, H atoms are a large fraction in a complex of hydroxyl species (Chung et al. 2007, and references therein). It has been established that H atoms are a major component of the interstellar medium (ISM) (van Dishoeck et al. 1999; Ioppolo et al. 2006). In the dense interstellar medium where most of the hydroxyl species are formed, H atoms are the most abundant species. The formation stage (Tegmark et al. 1997; Caselli & Tielens 2004; Caselli et al. 2007) of the interstellar medium is still not well understood. The formation of H atoms is not yet fully understood. It is mainly composed of water ice (i.e., all the theoretical chemical models predict that H atoms are mobile on water ice surfaces) (Tielens & Hagen 1982; Cugia & Herbst 2007), mobility of hydrogen is dependent on the presence of O₂ (Cugia & Herbst 2007) and modeling of experimental data (Miyachi et al. 2008) are still not available. The mobility of H atoms on the surface of porous amorphous water ice (PAW) has been studied by several authors (Nishimura et al. 1993) and interpretation of experimental data (Herbst et al. 1993; Ioppolo et al. 2006). The mobility of H atoms at low temperature supposed to be due to that of the O atoms in interstellar ices (Tielens & Hagen 1982; Cugia & Herbst 2007). It has been already demonstrated that O atoms are mobile at 10 K on our PAW samples (Ioppolo et al. 2006; Bouquet et al. 2006). The mobility of H atoms on the surface of porous amorphous water ice, as is estimated by the diffusion of H atoms in a porous water ice surface, is not yet available. In Sect. 2, we briefly describe the experimental setup and the method used to measure the diffusion coefficient of H atoms on porous water ice surfaces. In Sect. 3, we present the results and explain them assuming that D is mobile on PAW ice at 10 K. In Sect. 4, we discuss a simple rate equation model for the diffusion of H atoms on PAW ice. In Sect. 5, we discuss other interpretations before concluding.

2. Experimental section
The FOFIRICE instrument in the InterStellAR Medium (ISM) simulation setup has been developed with the purpose of the reaction and interaction of atoms and molecules on porous water ice surfaces under interstellar conditions (the relevance of substrate, low density, and very low temperatures: >10 K). FOFIRICE is composed of an ultra-high vacuum chamber with a base pressure of $\sim 10^{-11}$ torr, about

* Present address: LCAM, Université Pan-Sud, Orsay, France.

Interstellar water ice



O + H

Dulieu et al. 2010; Jing et al. 2011

O₂ + H

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

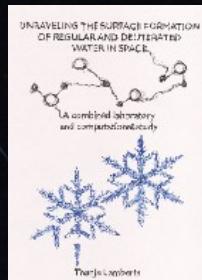
O₃ + H

Mokrane et al. 2009; Romanzin et al. 2011

Sackler Laboratory for Astrophysics



Prof. Harold Linnartz



(TALK @ 10:50)

Dr. Thanja Lamberts



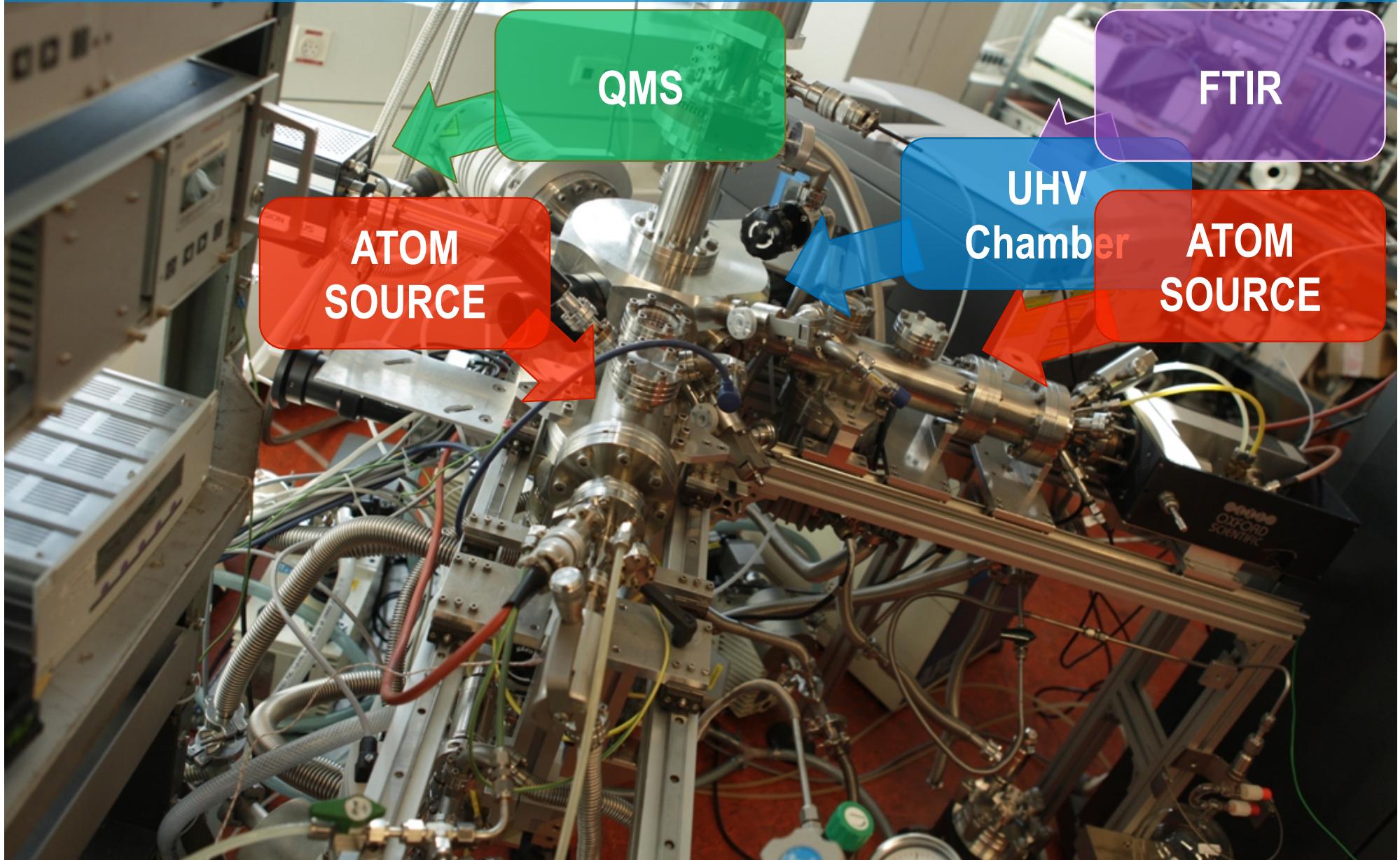
Prof. Ewine van Dishoeck

Dr. Herma Cuppen
(Radboud University Nijmegen)



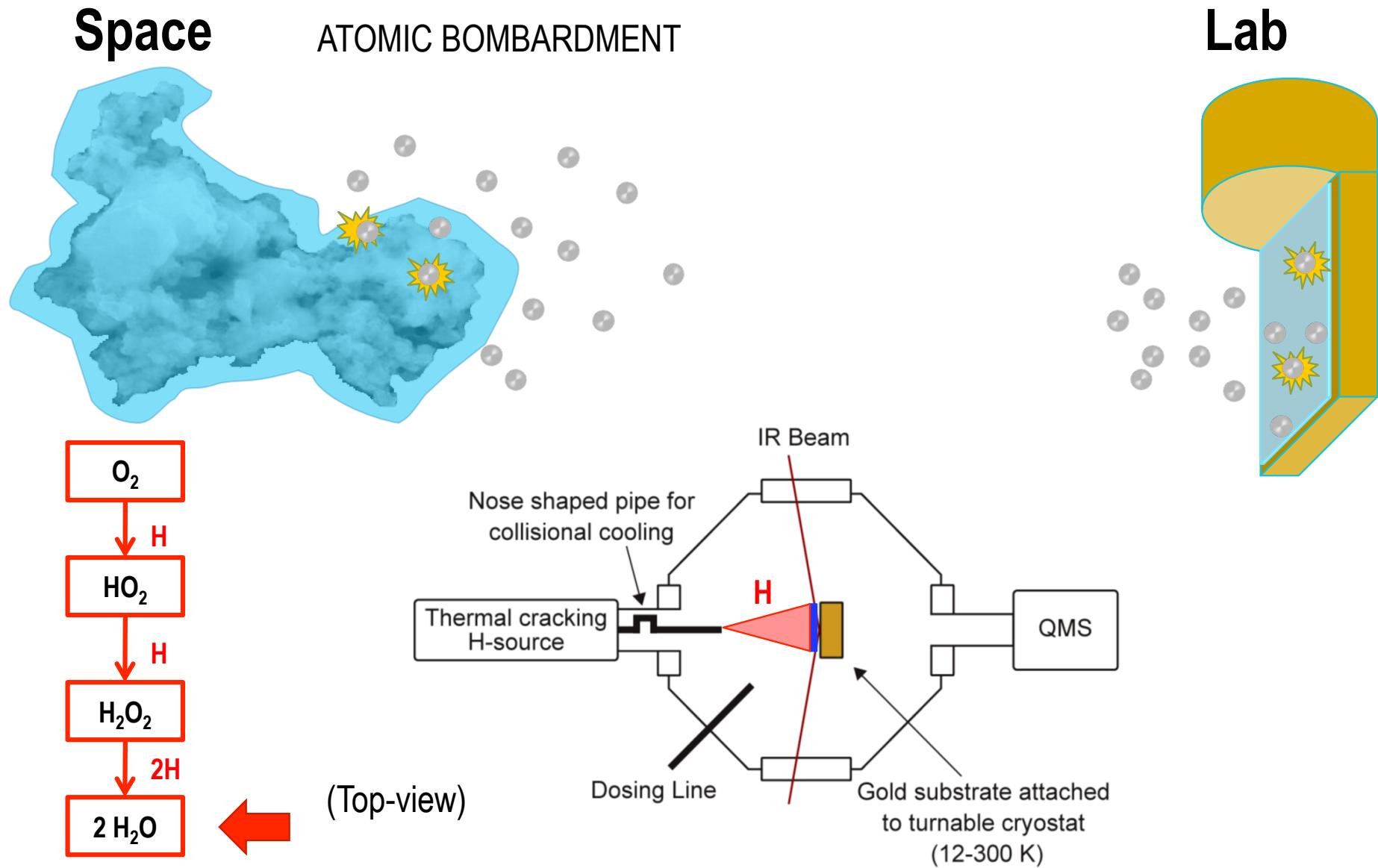
SURFRESIDE²

SURFace REaction SImulation Device 2



Experimental Procedure

Pre-deposition Experiments



Surface Hydrogenation of O₂

Pre-deposition Experiments

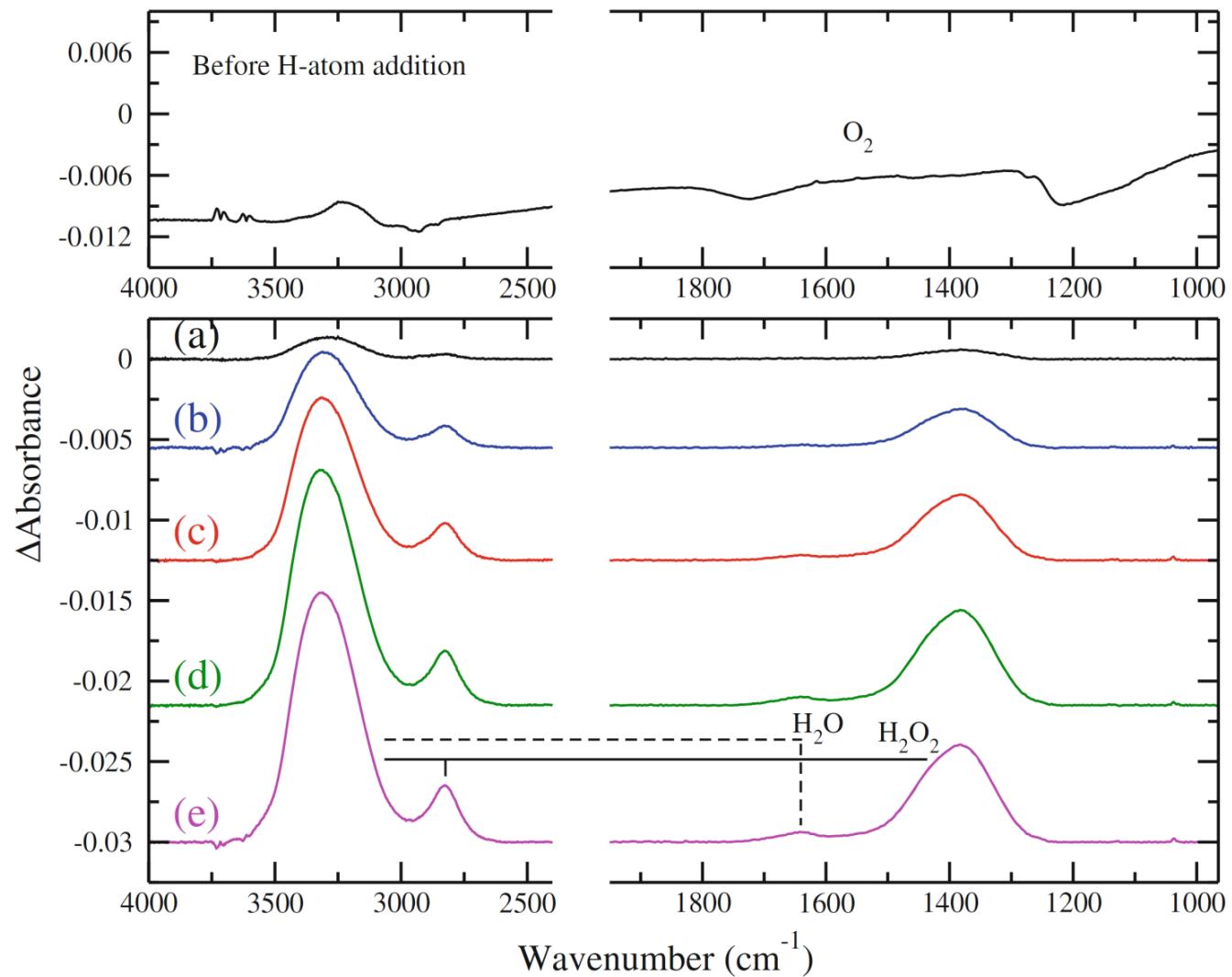
Ioppolo et al., RFAL (2011)

Pre-deposition:
35 ML of O₂ ice

Temperature:
 $T = 25\text{ K}$

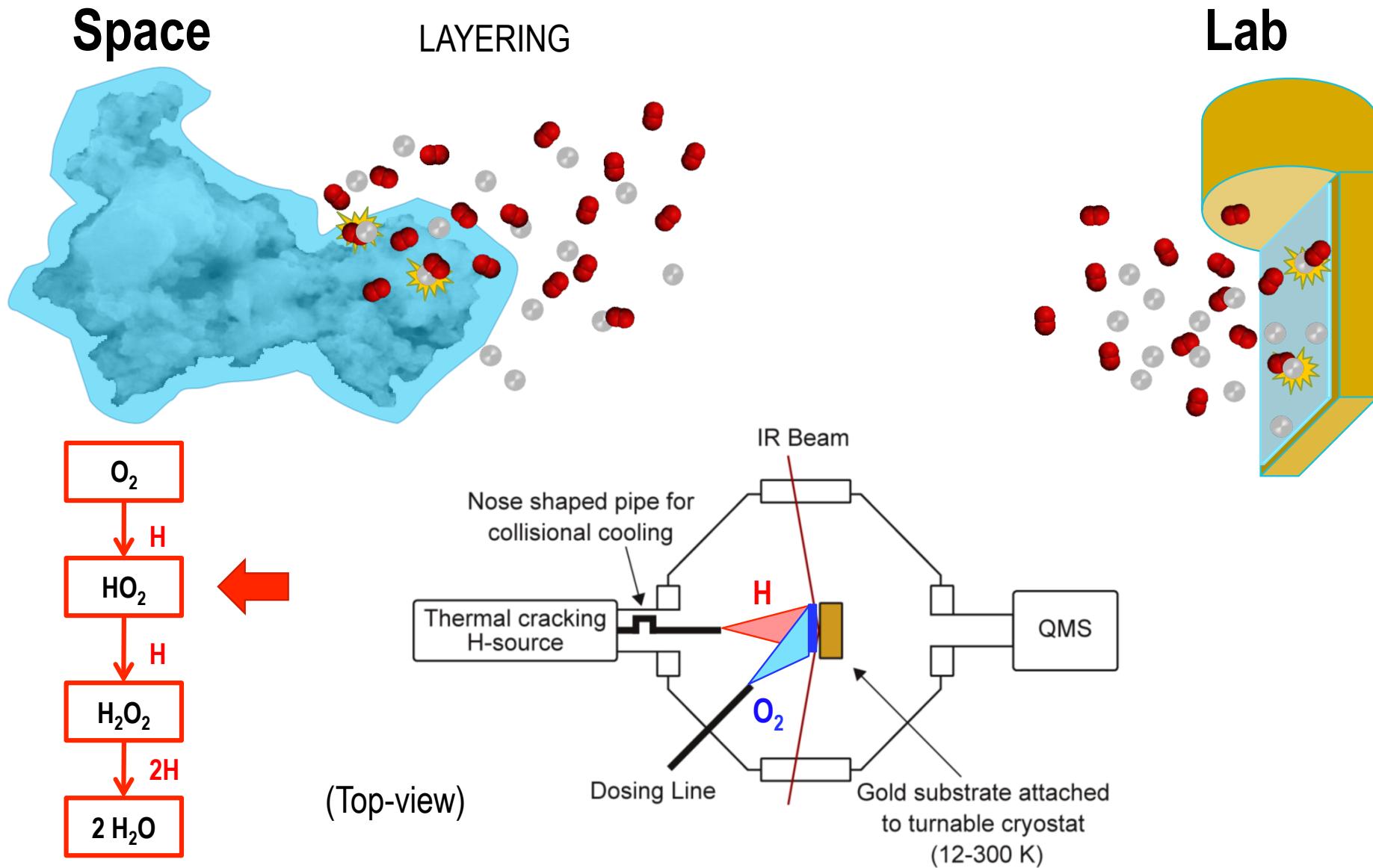
H-atom flux:
 $2.5 \times 10^{13}\text{ cm}^{-2}\text{ s}^{-1}$

H-atom fluences:
(a) $4 \times 10^{15}\text{ atoms cm}^{-2}$
(b) $4 \times 10^{16}\text{ atoms cm}^{-2}$
(c) $7 \times 10^{16}\text{ atoms cm}^{-2}$
(d) $1 \times 10^{17}\text{ atoms cm}^{-2}$
(e) $2 \times 10^{17}\text{ atoms cm}^{-2}$



Experimental Procedure

Co-deposition Experiments



Surface Hydrogenation of O₂

Co-deposition Experiments

Cuppen et al., PCCP (2010)

Co-deposition:

O₂ + H ice

Temperature:

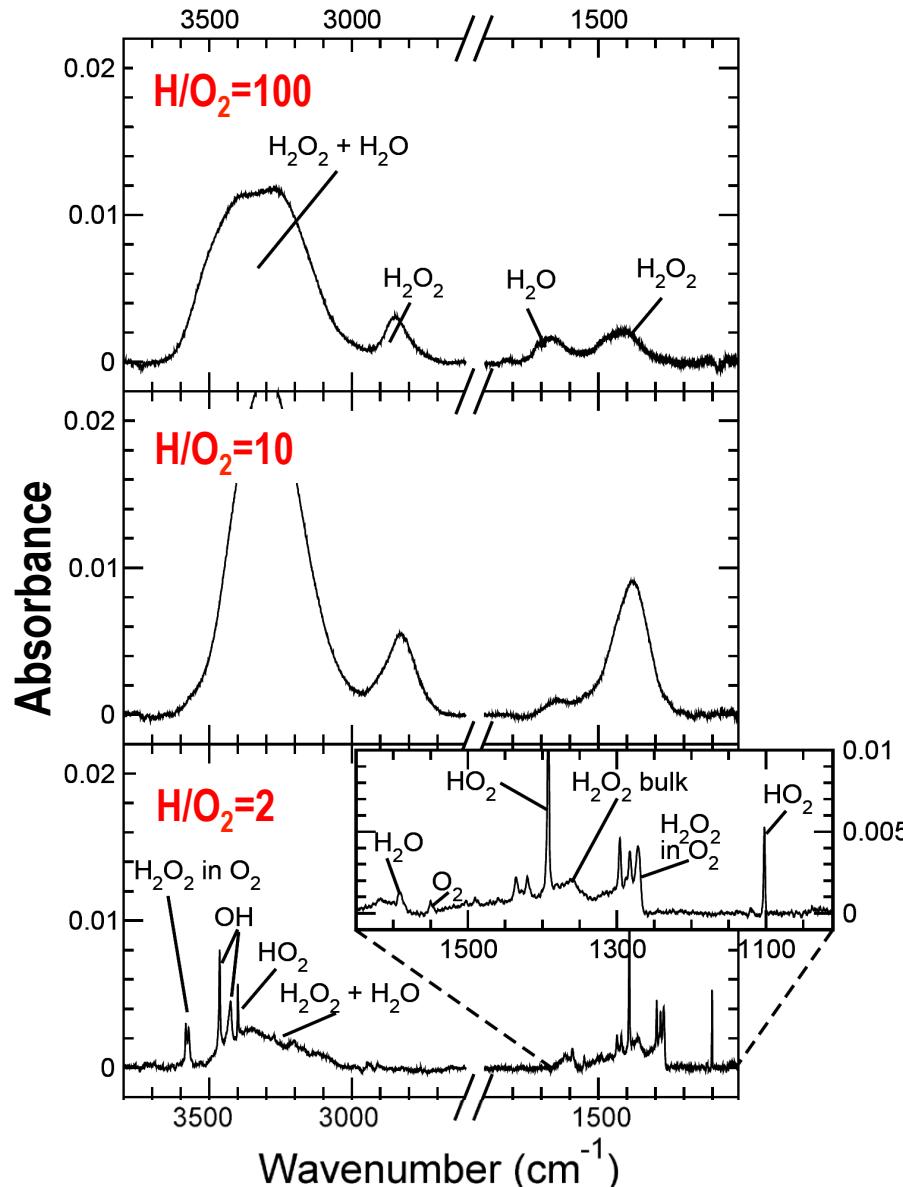
T = 20 K

H-atom flux:

2.5x10¹³ cm⁻² s⁻¹

H-atom fluences:

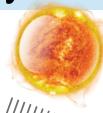
3x10¹⁷ atoms cm⁻²



Experimental Procedure

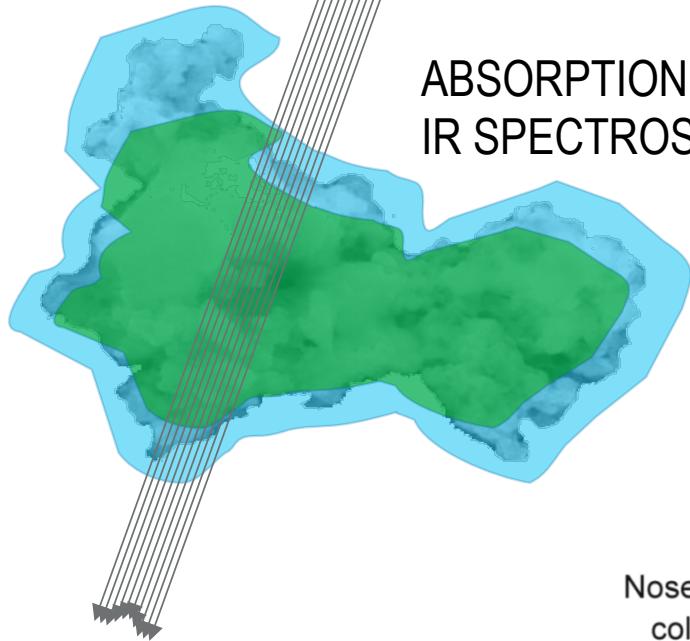
Analytical Tools

Space

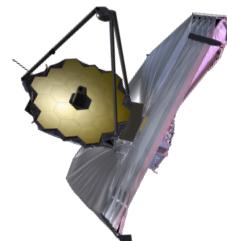
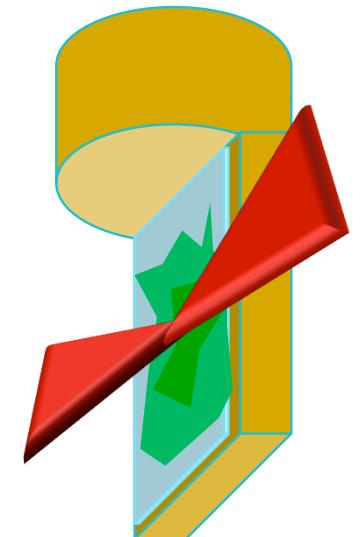


NEW SPECIES FORMED

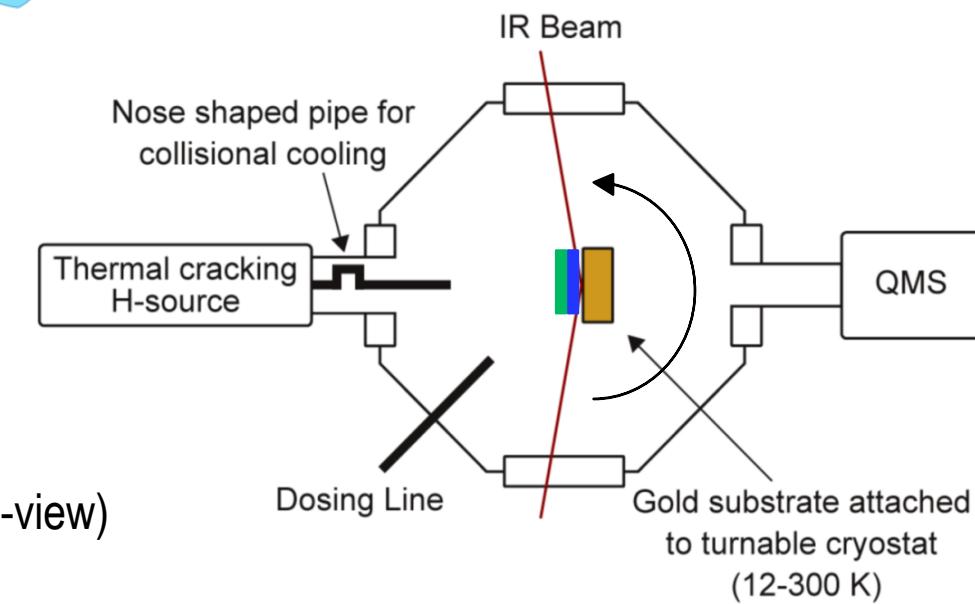
ABSORPTION
IR SPECTROSCOPY



Lab



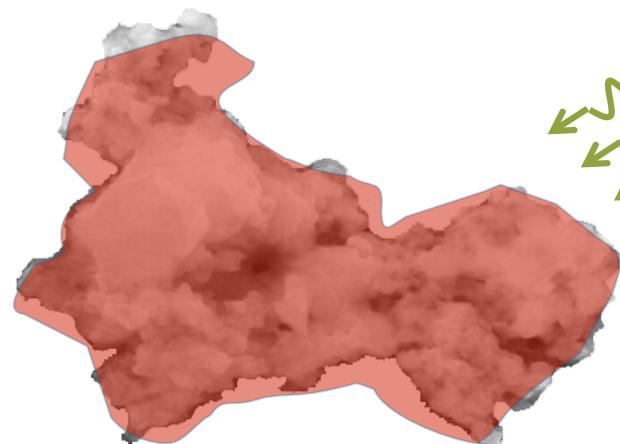
(Top-view)



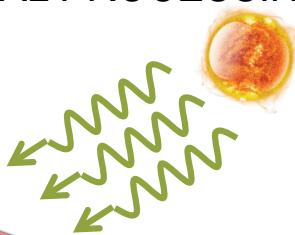
Experimental Procedure

Analytical Tools

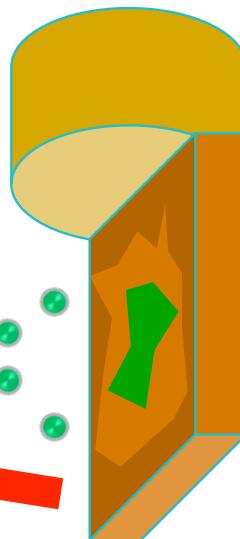
Space



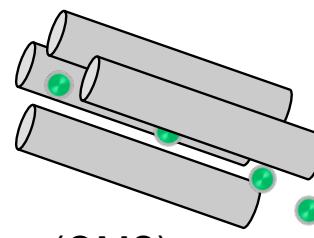
THERMAL PROCESSING



Lab



TEMPERATURE
PROGRAMMED
DESORPTION



(QMS)

IR Beam

Nose shaped pipe for
collisional cooling

Thermal cracking
H-source

(Top-view)

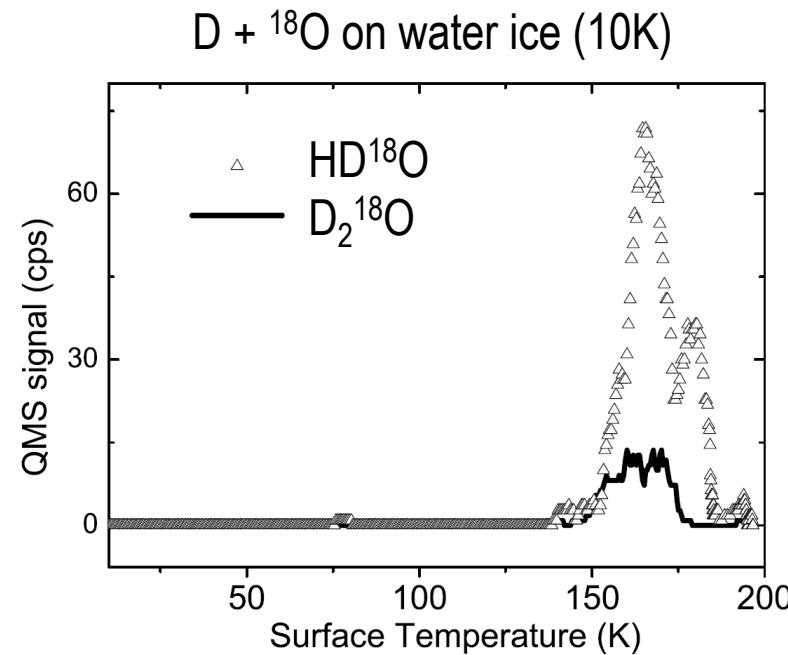
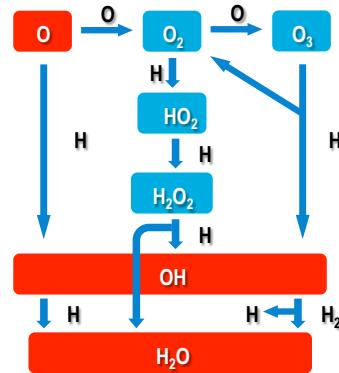
Dosing Line

Gold substrate attached
to turnable cryostat
(12-300 K)

QMS

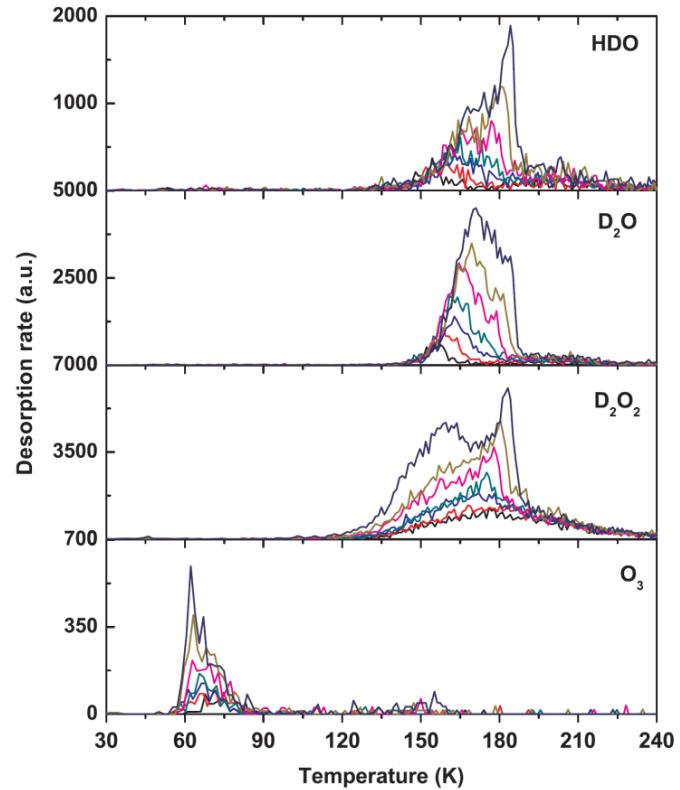
Hydrogenation of O Atoms

Transition from Diffuse to Dense Clouds ($A_v \sim 1-5$)



Dulieu et al., A&A (2010)

D + ¹⁶O on bare grain analogs (15K)

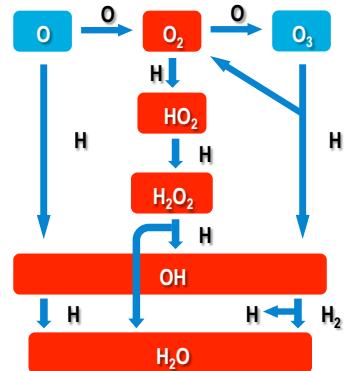


Jing et al., ApJL (2011)

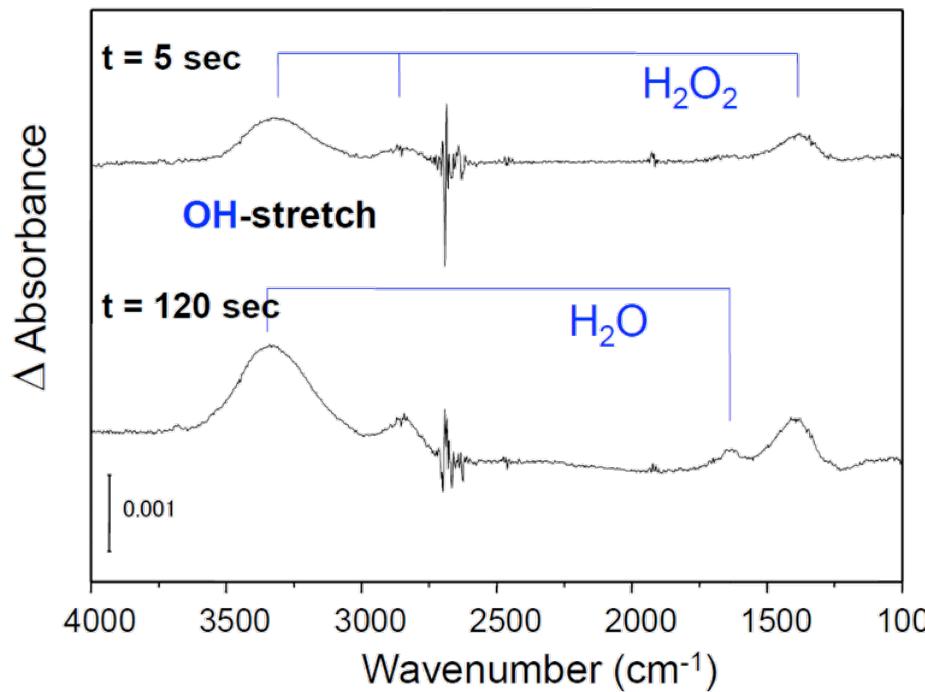
Hydrogenation of O₂

Dense Molecular Clouds ($A_v > 5$)

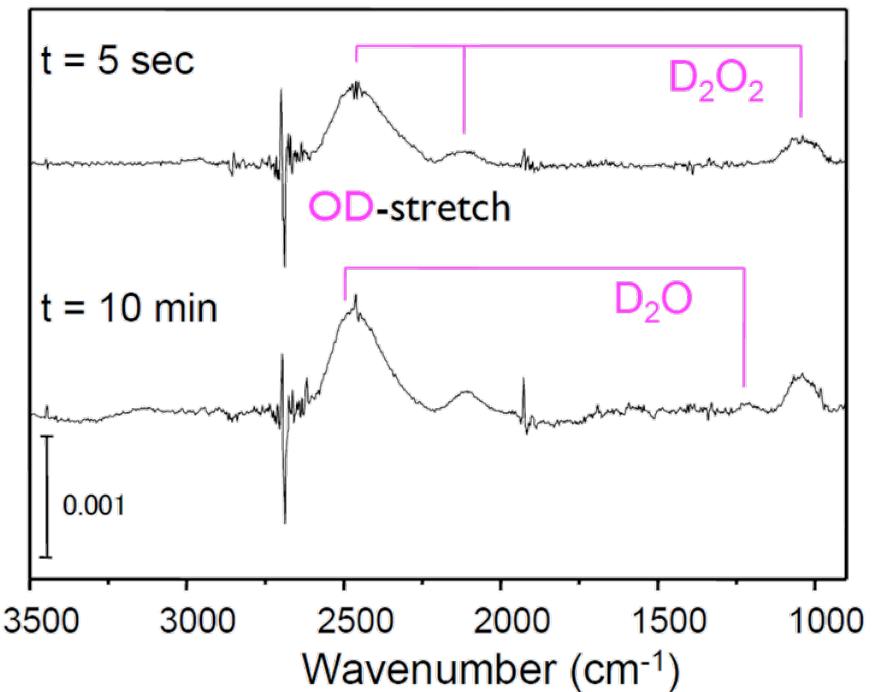
Miyauchi et al., CPL (2008)



Solid O₂(10K) + H



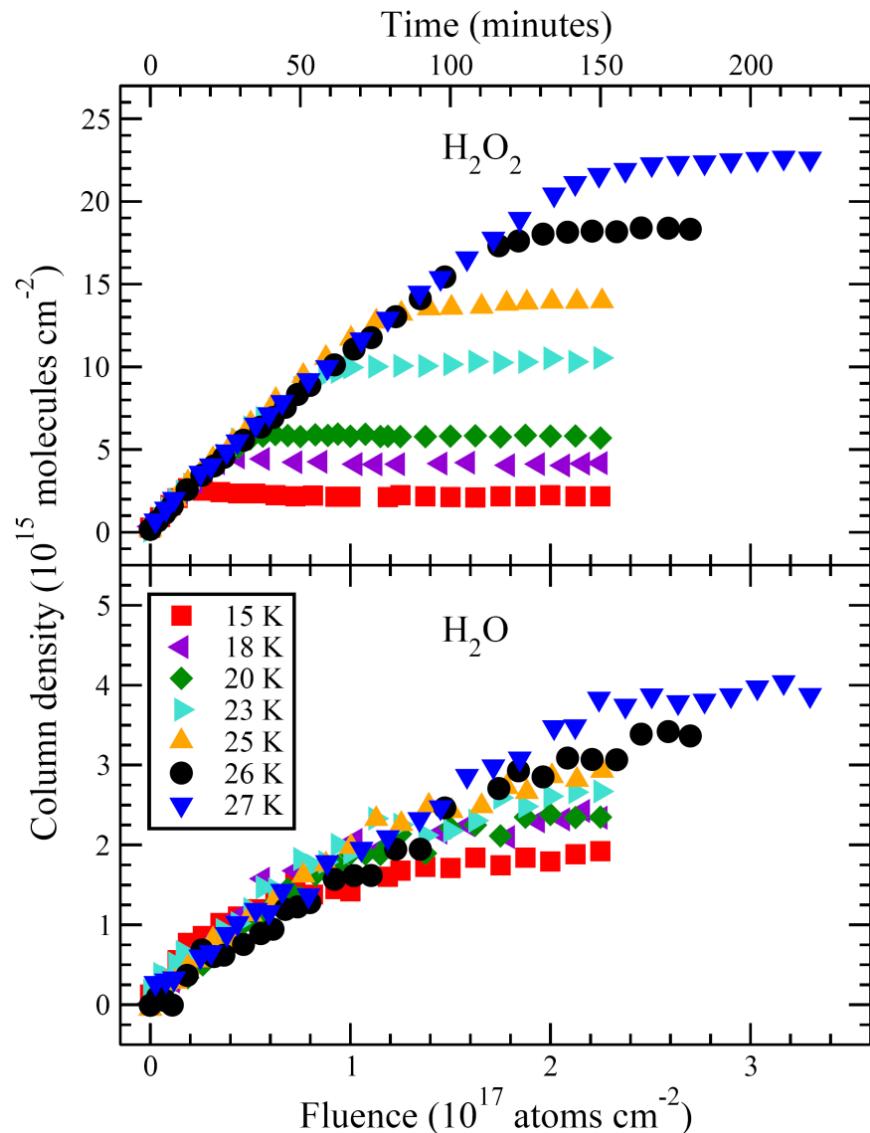
Solid O₂(10K) + D



Hydrogenation of O_2

Temperature Dependence

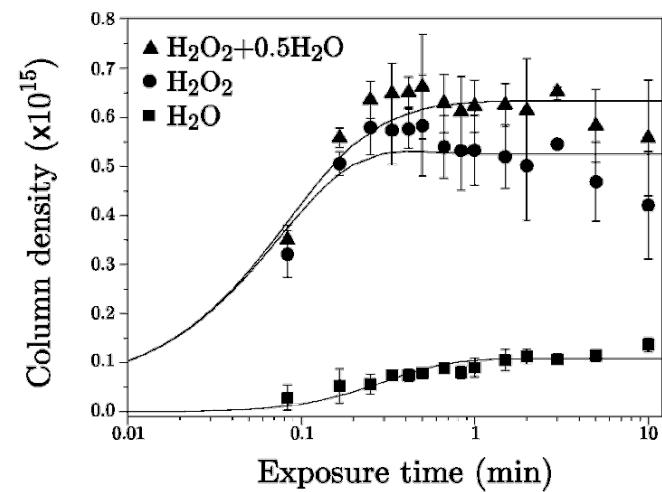
Ioppolo et al., ApJ (2008); PCCP (2010)



Formation rates are temperature independent → linear behavior.

Very high final yield, temperature dependent.

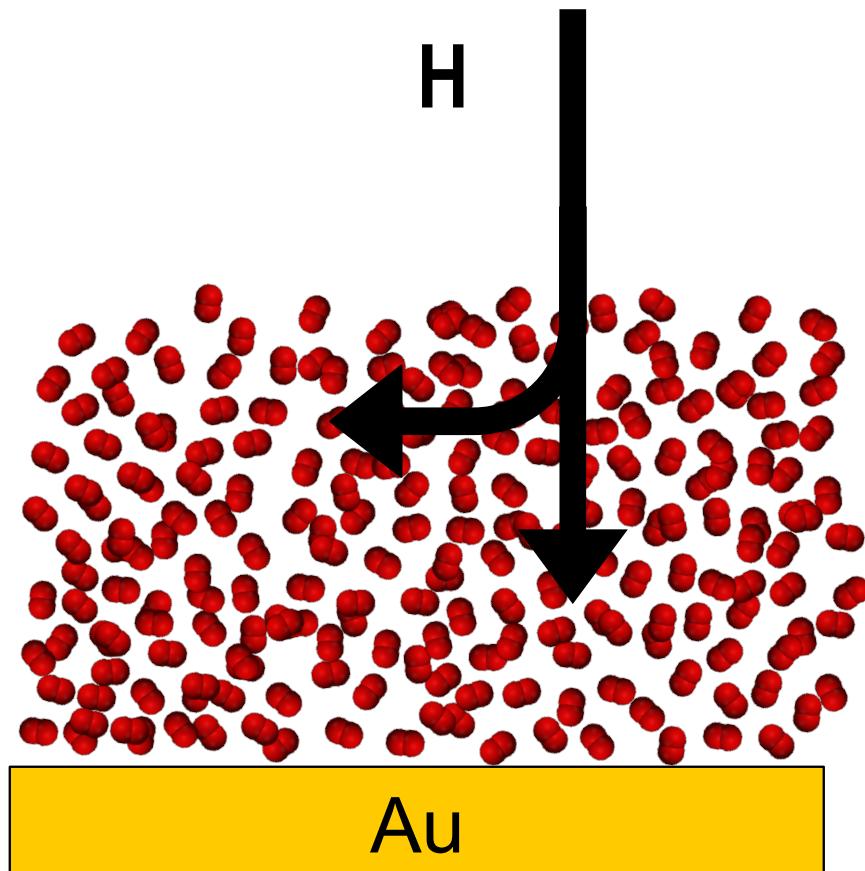
At low temperature, in agreement with Miyauchi et al. (2008) (10 K).



Hydrogenation of O₂

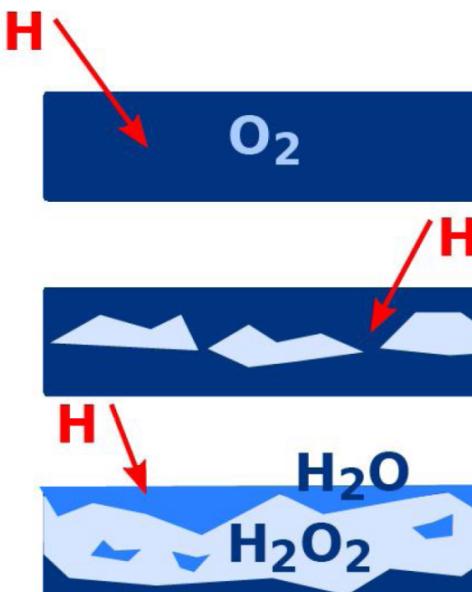
Temperature Dependence

Ioppolo et al., PCCP (2010)



Competition

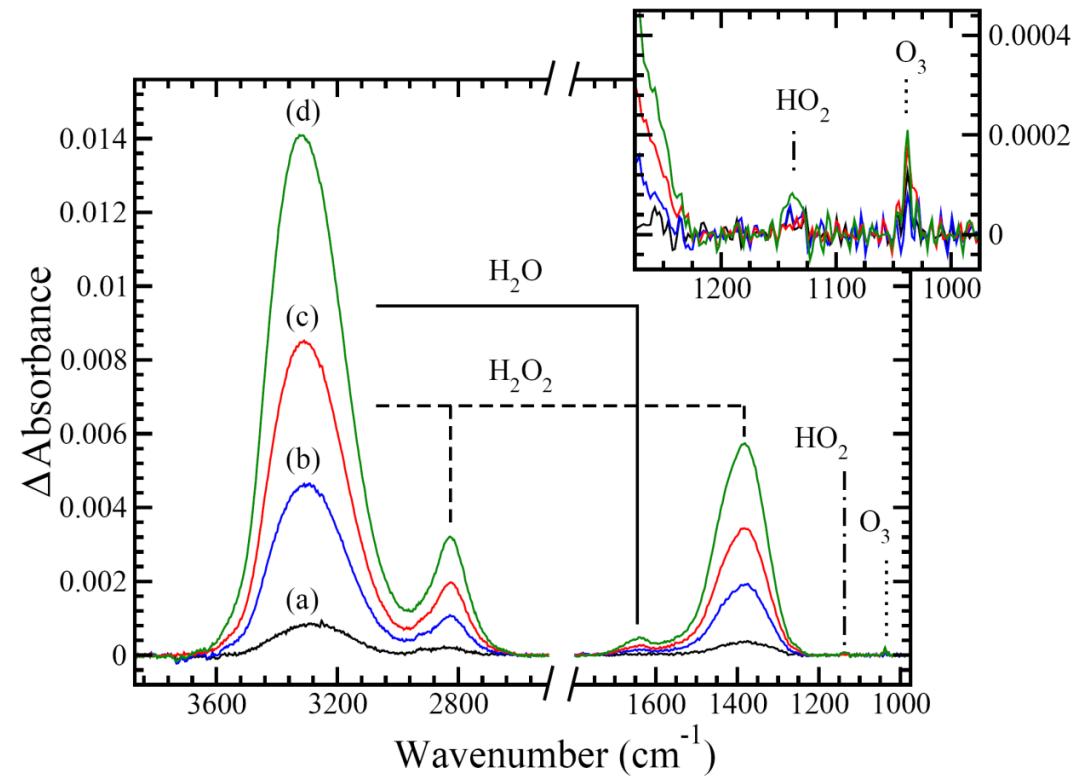
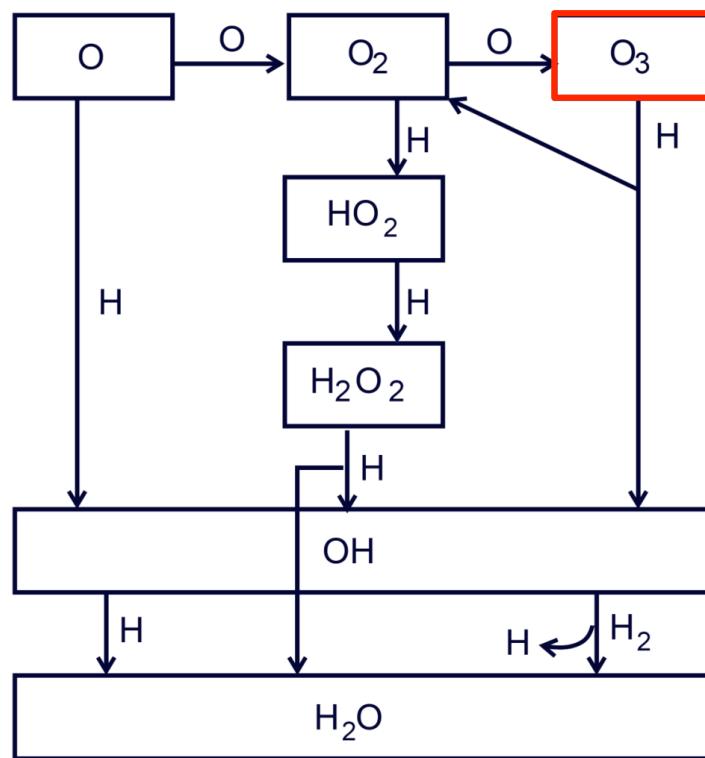
Competition between **reaction** H + O₂ (*T* independent) and **diffusion** of H atoms into O₂ ice (*T* dependent).



Hydrogenation of O_2

Incomplete Reaction Scheme

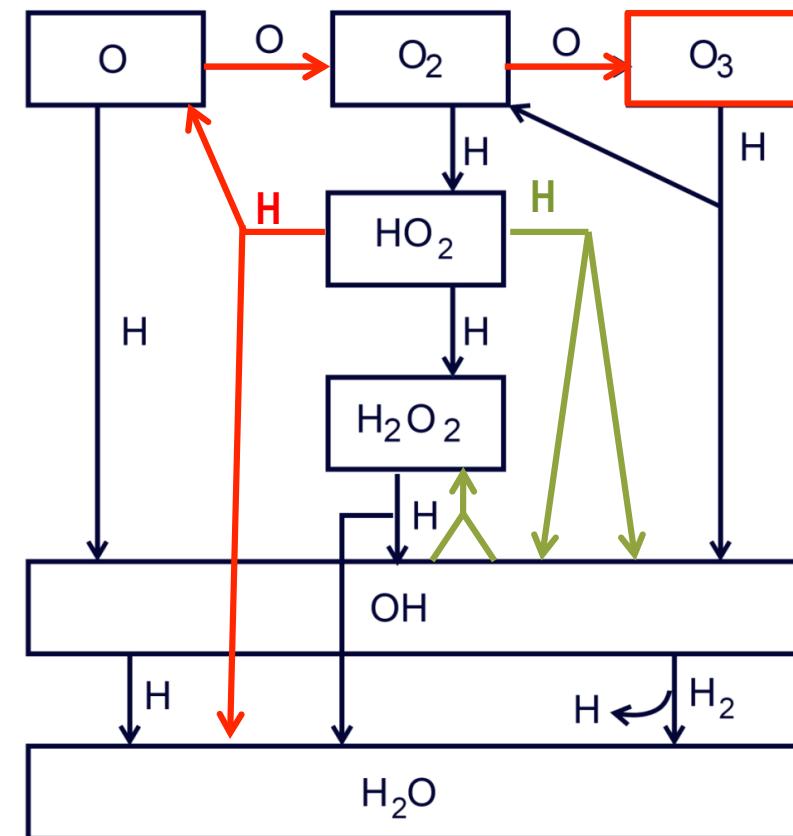
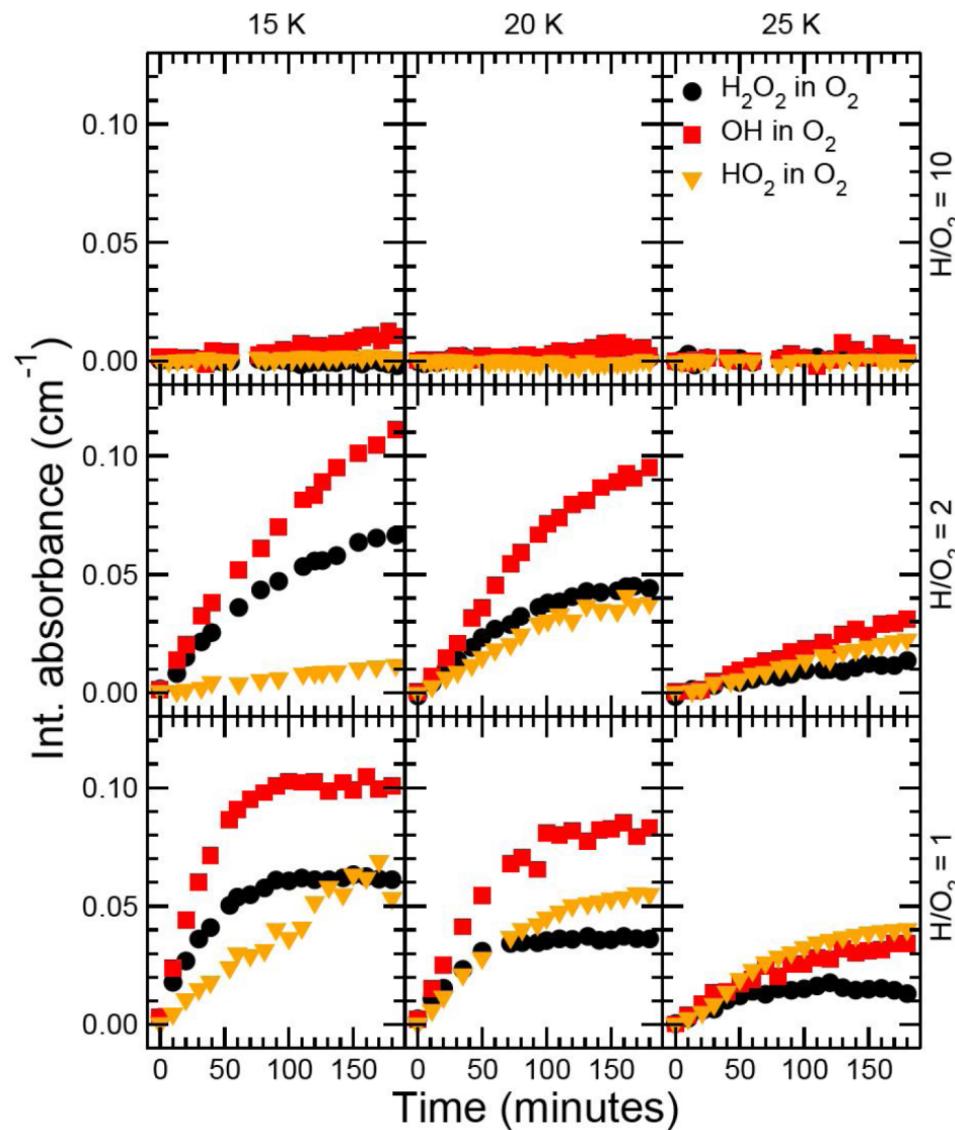
Ioppolo et al., PCCP (2010)



Hydrogenation of O_2

New Reaction Scheme

Cuppen et al., PCCP (2010)

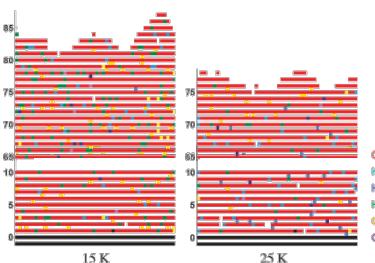
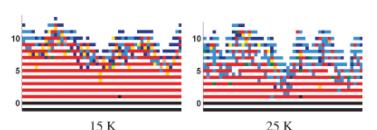
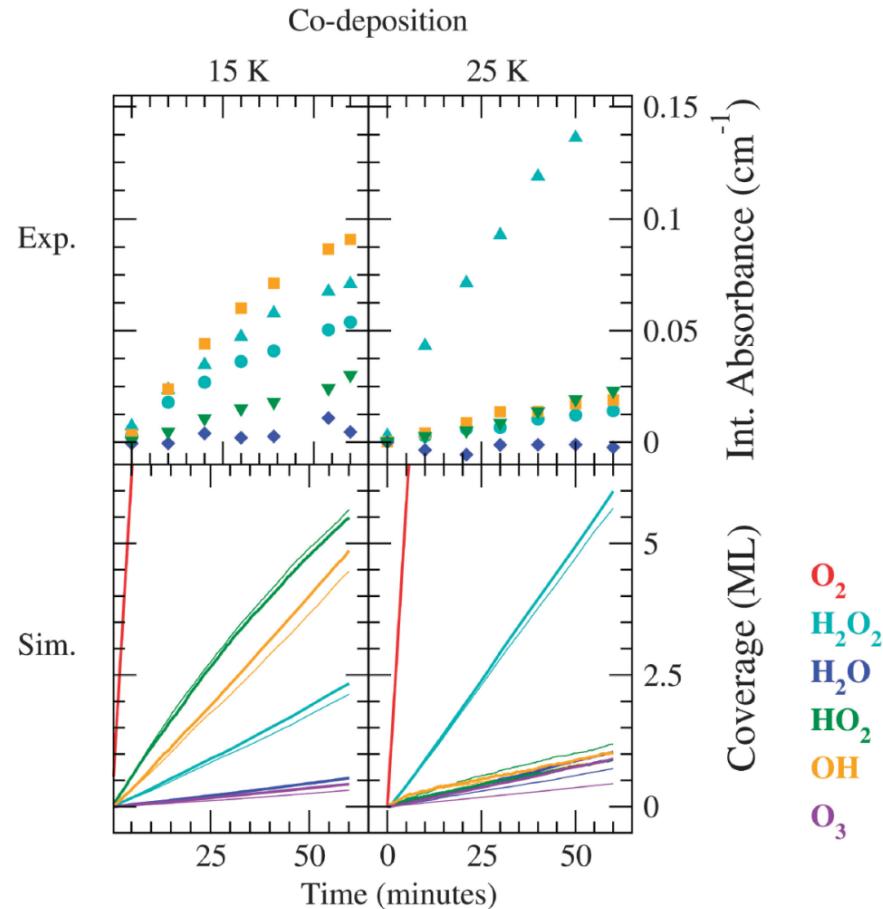
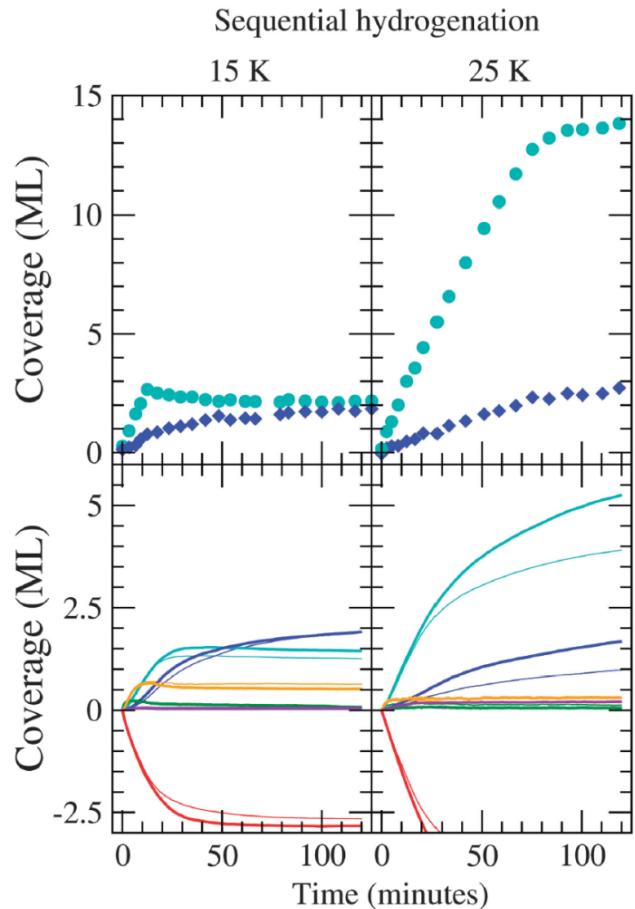


OH is formed together with H_2O_2

Hydrogenation of O_2

Monte Carlo Simulations

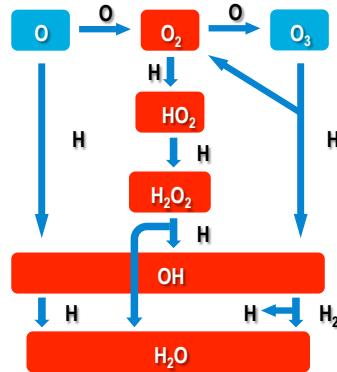
Lamberts et al., PCCP (2013)



Hydrogenation of O₂

Monte Carlo Simulations

Lamberts et al., PCCP (2013)



- Key reactions for the O₂ channel are in red
- Slow destruction of H₂O₂ explains its high accumulation
- High H diffusion rate reproduces large penetration depth of H into O₂ ice
- Diffusion of radical species (OH and H) is a key parameter

Table 5 Parameters that reproduce the selected experiments the best. A comparison to (mean) gas-phase literature values is also included. Key reactions are listed in bold face

Reaction	R^a (s ⁻¹)	Lit. E_a (K)
Temperature independent reactions		
H + H → H ₂	1×10^{12}	—
H + O₂ → HO₂	1.1×10^5 ^b	$\sim 0^{28,43}$
H + HO₂ → products	1×10^{12}	T indep. ²⁹
OH + OH	56%	
H ₂ O ₂	35%	
H ₂ + O ₂	2%	
H ₂ O + O	7%	
H + O → OH	1×10^{12}	—
O + O → O ₂	1×10^{12} ^c	—
H + O ₃ → O ₂ + OH	1.1×10^5	450 ⁴⁴
H + OH → H₂O	1.1×10^5	$\sim 0^{43}$

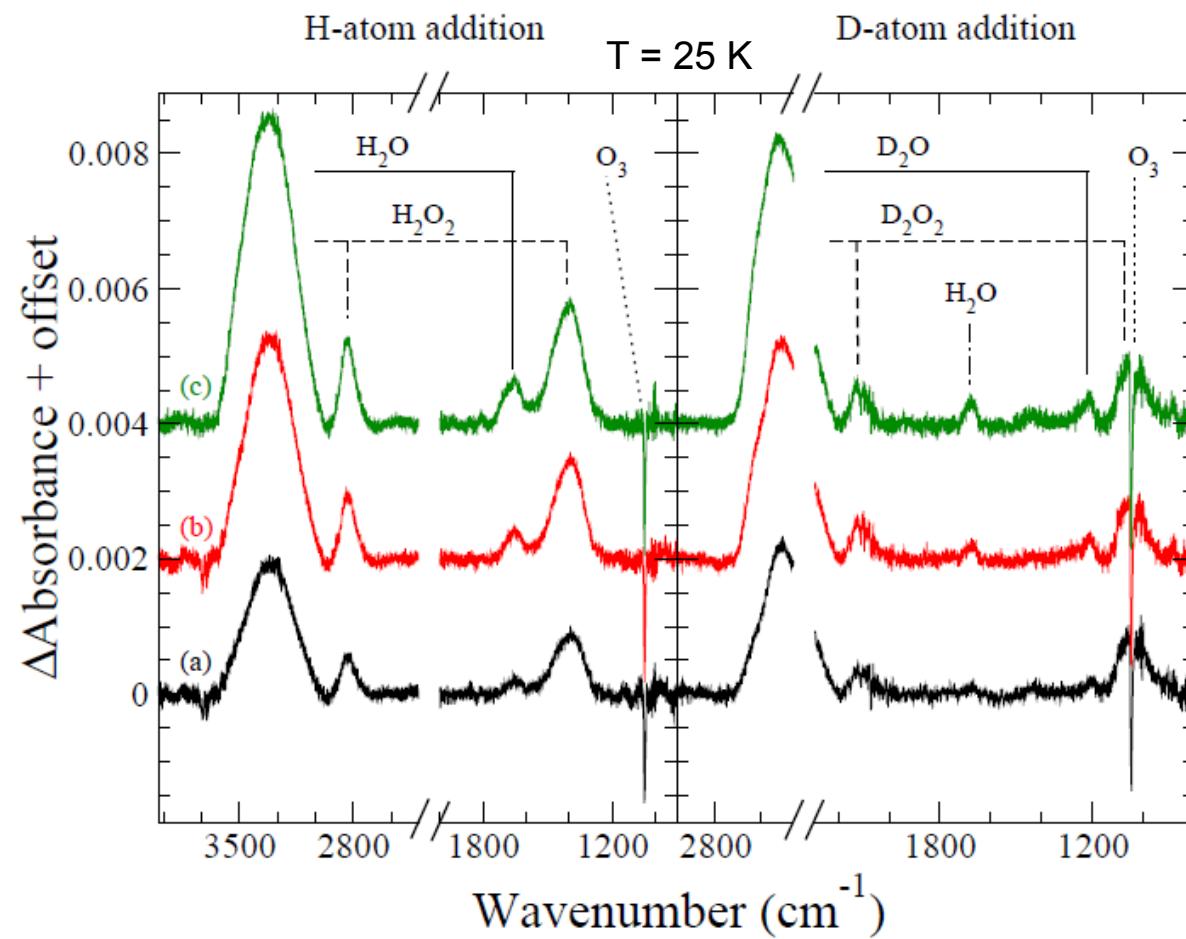
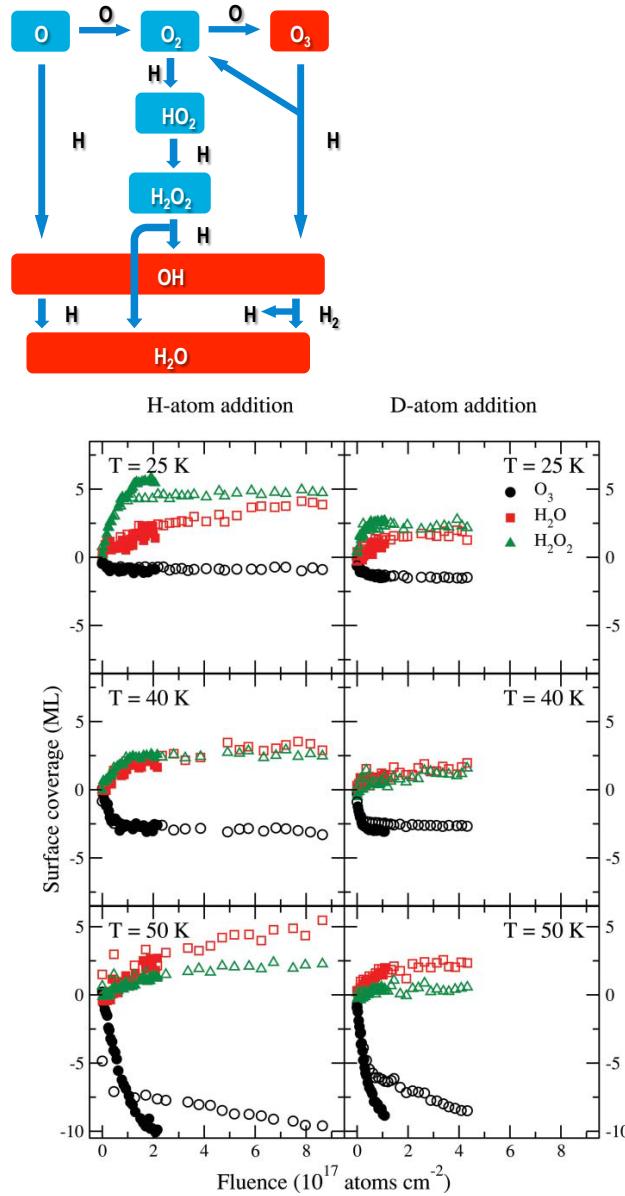
Temperature dependent reactions

H + H₂O₂ → H₂O + OH	800	1280	2000 ³²
H ₂ + O → OH + H	3165 ^c	3165 ^c	3165 ⁴⁵
H ₂ + HO ₂ → H ₂ O ₂ + H	5000 ^c	5000 ^c	13 100 ³³
H ₂ + OH → H ₂ O + H	500 ^c	800 ^c	2100 ^{31,36}
OH + OH → products	— ^d	— ^d	0 ³¹
H ₂ O ₂	90%	90%	0 ³¹
H ₂ O + O	10%	10%	0 ³¹
O + O ₂ → O ₃	500	500	0 ³¹

NOTE: the hydrogen diffusion barrier used was 53 K instead of the value listed in Table 3. ^a This work. ^b A value of 8.3×10^5 is used for the co-deposition simulations. ^c Reaction practically does not take place in our simulations. ^d See Section 4.2.3.

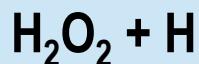
Hydrogenation of O_3

Romanzin et al., JCP (2011)

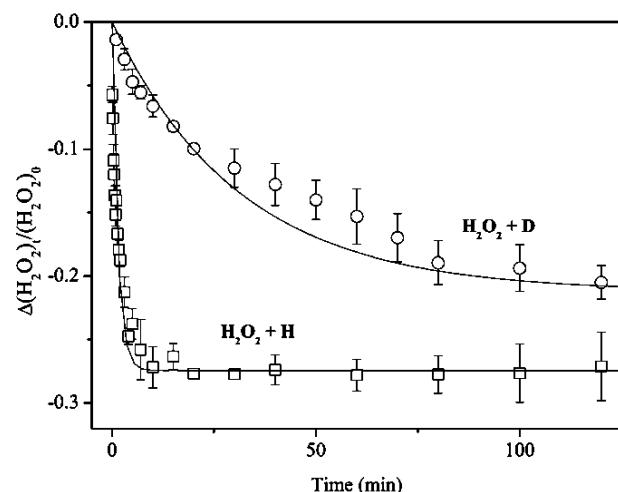
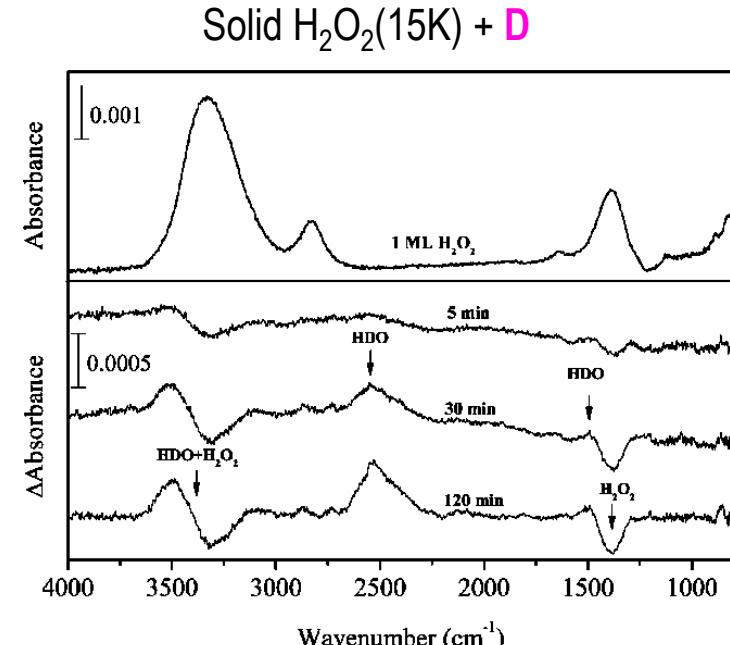
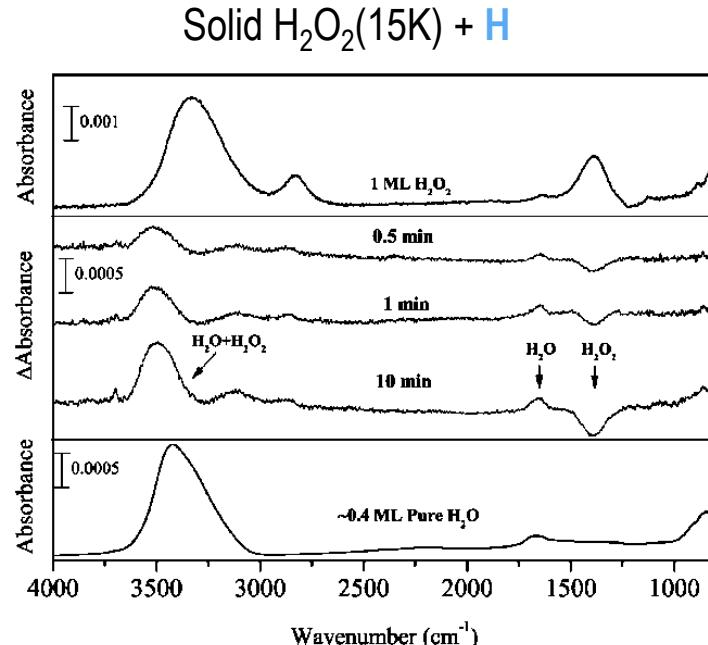
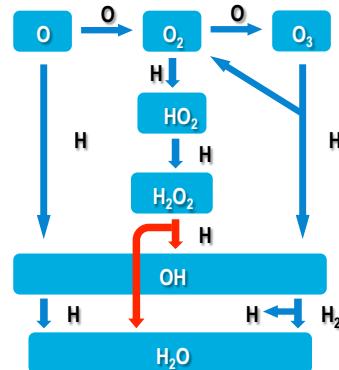


Selected Reactions to Water

(Thanja's Talk)

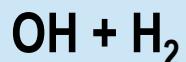


Oba et al., FD (2014)

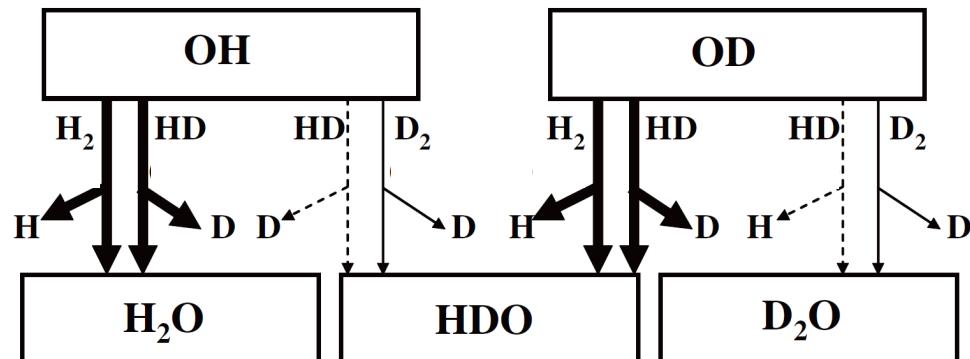
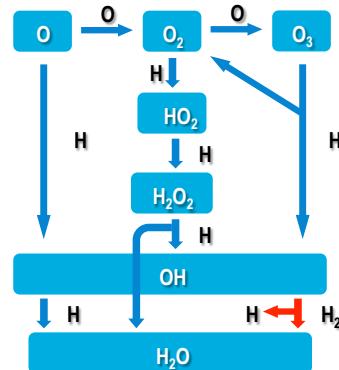


- Large activation barrier in gas phase (>2000 K)
- Large isotope effect (reaction rate H >> D atoms)
- Reactions proceed through quantum tunneling (10-30 K)

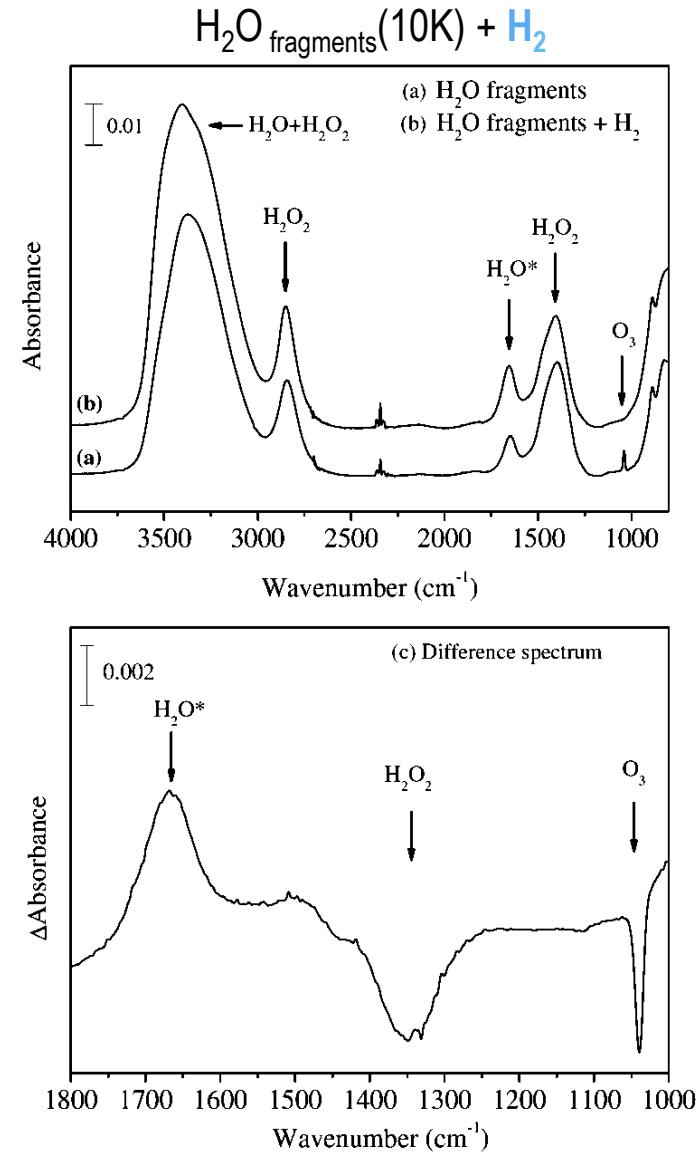
Selected Reactions to Water



Oba et al., ApJ (2012)



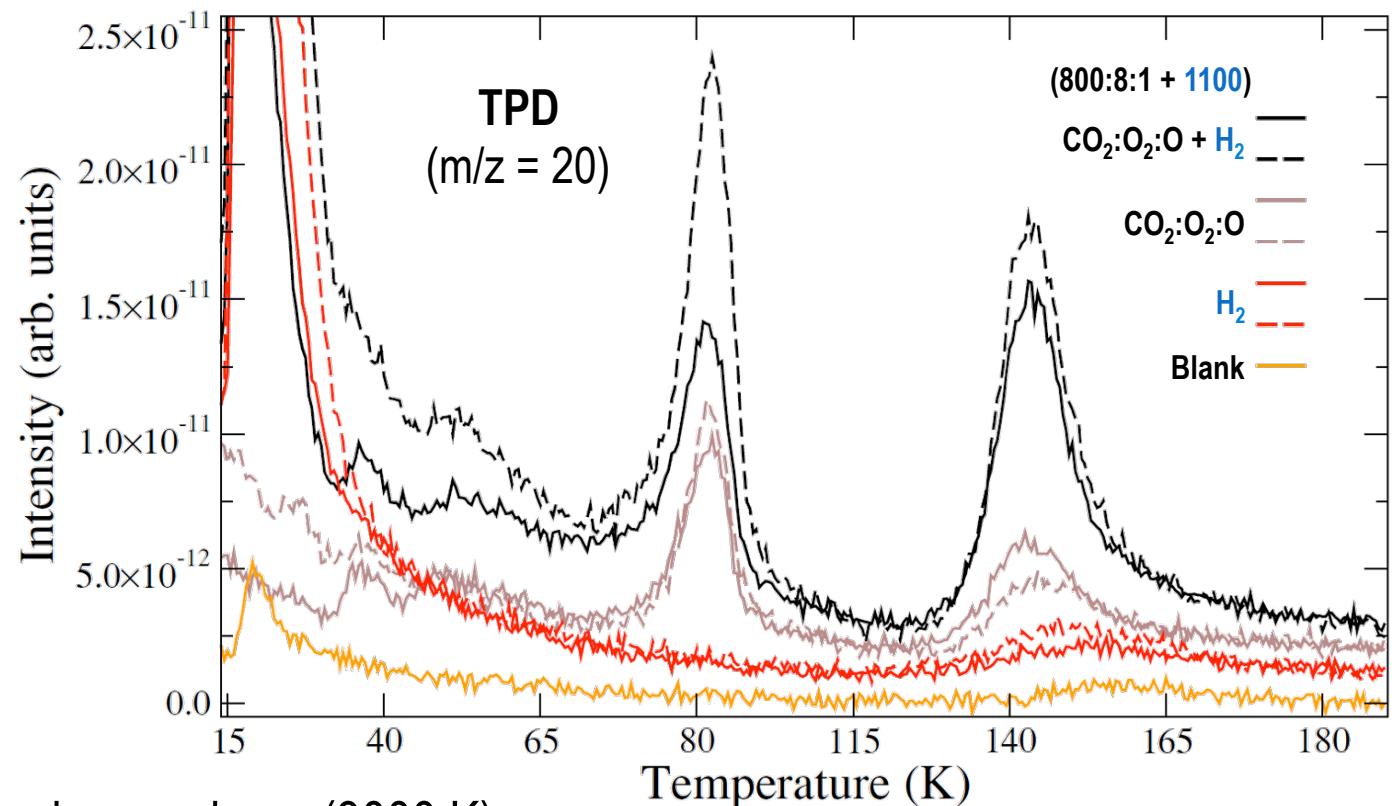
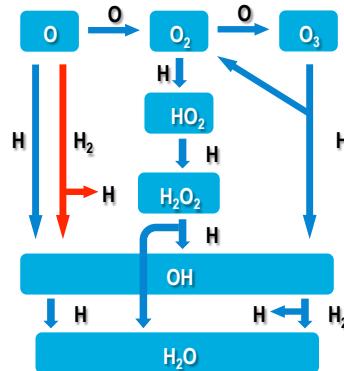
- Large activation barrier in gas phase (2100 K)
- Large isotope effect (H₂O form >> HDO form)
- Reactions proceed through quantum tunneling



Selected Reactions to Water



Lamberts et al., A&A (2014)



- Large activation barrier in gas phase (3000 K)
- Reaction is endothermic by 960 K
- Combined classical & tunneled reaction mechanism
- **<11% of water in MC formed through $\text{O} + \text{H}_2$ channel**

Modelling Grain Surface Chemistry

The Effect of Exothermicity

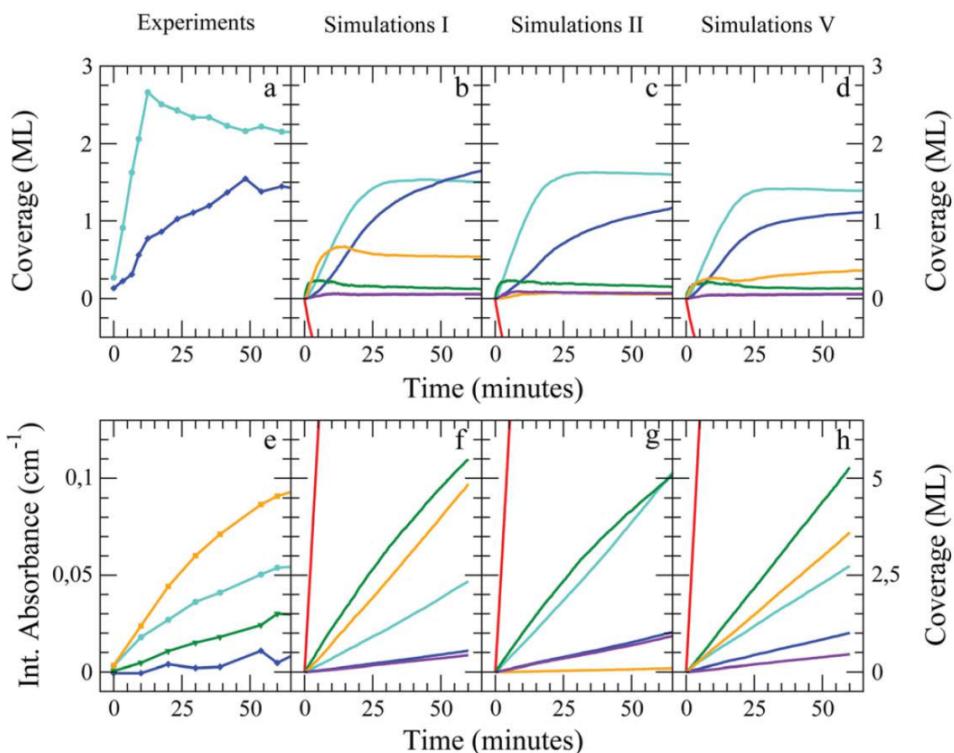
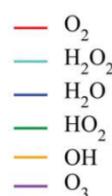
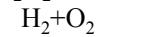
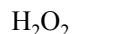
Lamberts et al., FD (2014)

- Exothermal reactions with two or more products lead to diffusion and desorption
- Exothermicity also leads to compaction of the ice
- Excess energy used to overcome chemical reactions (unclear mechanism)
- Kick-out mechanism unexplored here

Table 3 Summary of the parameters chosen for all experimental simulations

Run	H + HO ₂ (%) products	<i>E_{a,OH}</i> diff (K)	<i>E_{a,OH}</i> + OH react (K)	<i>T_{ex}</i> (K)	DIRECTIONALITY
I	56 : 32 : 2 : 7	105	600	100 ^a	off
II	91 : 0 : 2 : 7	210	0	100 ^a	off
V	91 : 0 : 2 : 7	210	0	1400	on

OH+OH



Modelling Grain Surface Chemistry

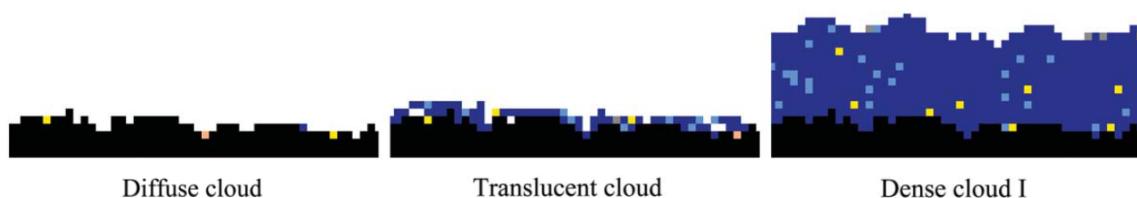
The Effect of Exothermicity

Lamberts et al., FD (2014)

- Final amount of produced H_2O is similar to the one found in Cuppen & Herbst, ApJ (2007)
- Results in good agreement with observations
- Main differences between the two studies are the formation routes for water ice
- Consequences for the deuterium fractionation of ice species at low T

Table 7 Contributions of the different reaction routes to H_2O formation in percentage

	T_{ex} (K)	$\text{H} + \text{OH}$	$\text{H}_2 + \text{OH}$	$\text{H} + \text{H}_2\text{O}_2$	$\text{OH} + \text{OH}$	$\text{H} + \text{HO}_2$
Diffuse	1400	99.5	0.0	0.0	0.5	0.0
	2000	99.8	0.0	0.1	0.1	0.0
Translucent	1400	85.4	2.4	10.4	1.8	0.0
	2000	87.6	2.2	8.7	1.5	0.0
Dense I	1400	76.7	17.6	4.0	1.0	0.7
Dense II	1400	22.5	61.6	11.3	2.4	2.2

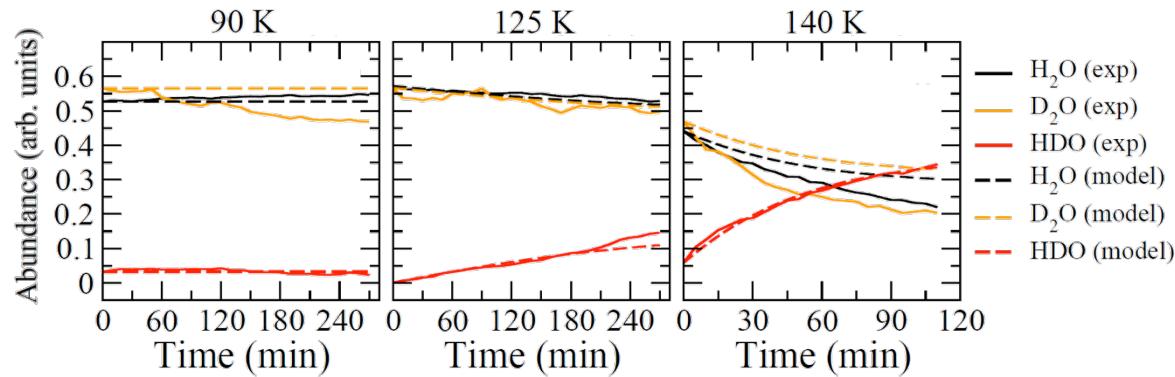
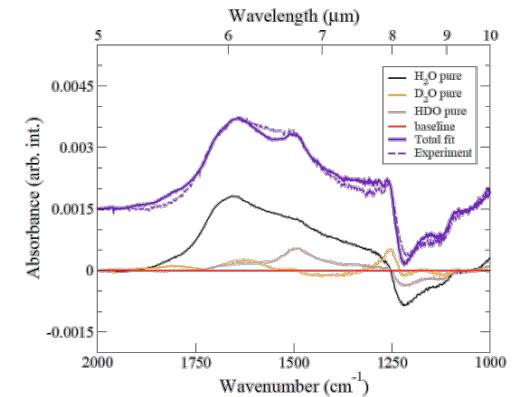
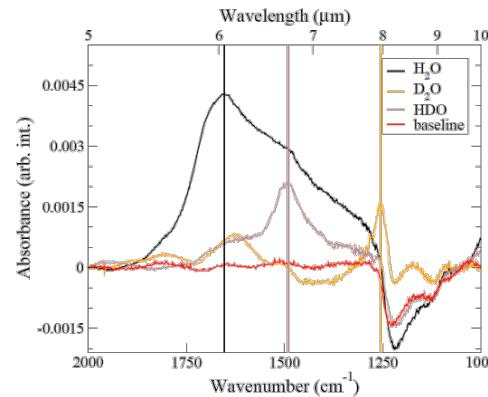
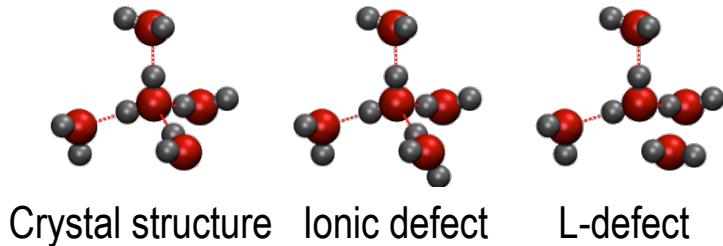


Before Thermal Desorption

Thermal H/D Exchange

Lamberts et al., MNRAS (2015)

Hop-and-Turn mechanism



- Activation energy for H/D exchange (3840 ± 125 K)
- Proton/deuteron swapping also in water ice mixtures (OH, NH groups)
- Reactive timescales ($< 10^4$ years at $T > 70$ K) relevant to interstellar environments

Take Home Message

- Laboratory work fundamental to investigate water formation in space
- Bottom-up approach highlighted a more complex surface reaction pathway
- Simulations can push results beyond laboratory possibilities



FUTURE CHALLENGES

Design new experiments to:

(Daniel Paardekooper's Talk)

- Better understanding of fundamental mechanisms (reaction, diffusion, desorption)
- Obtain more accurate surface reaction rates
- Investigate proton transfer and energy relaxation in ices in more detail