# RÉACTIVITÉ DES GLACES ENVIRONNEMENTALES ET SPATIALES

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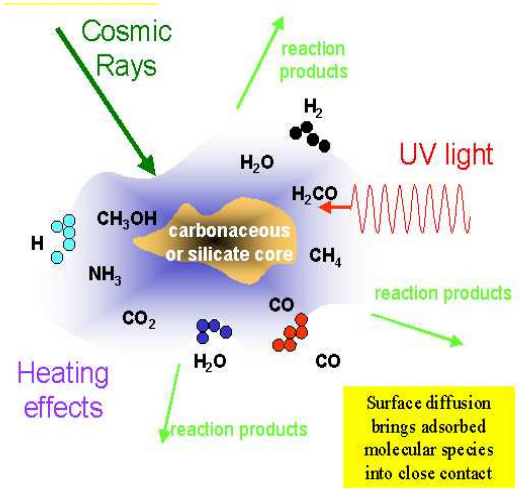
  - C. Laffon, CR CNRS section 06 (Matière condensée, structure et propriétés électroniques), INP
  - J. Lasne, Doctorant 3ième année.




## Milieu interstellaire

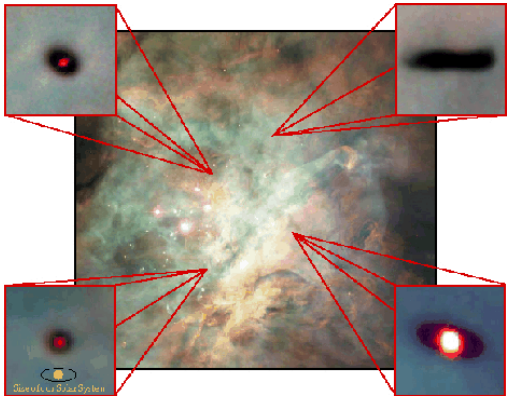
1-Réactions d'hydrogénation sur la glace, photochimie

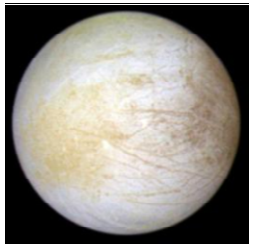
$CO+H$, $CH_3OH/H_2O$, $CN+H$

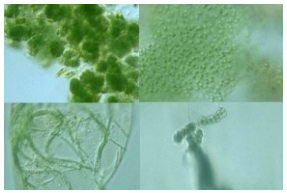
2-Formation de la glace

$OH+H \rightarrow H_2O$

SMART
UPMC
PCMI
ANR







## Systèmes planétaires

1-Résistance au rayonnement des acides aminés

Irradiation de la glycine/glace

2-Persistance de la chiralité

Alanine/glace

3-Photochimie des glaces planétaires

Irradiation de glaces $H_2O$, $NH_3$

OPV
EOPV

## Terre

1-Chimie stratosphérique

HCl et $ClONO_2$/glace

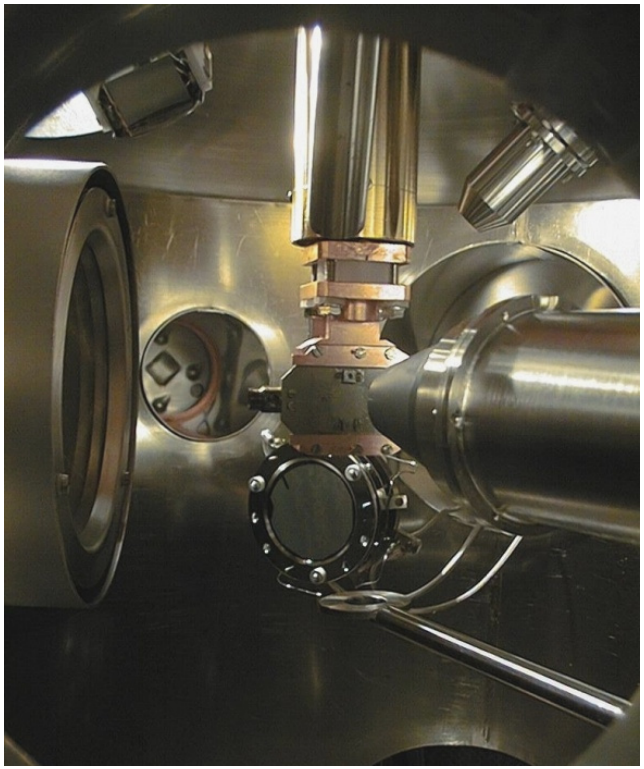
2-Chimie troposphérique

Transports des COV vers UTLS

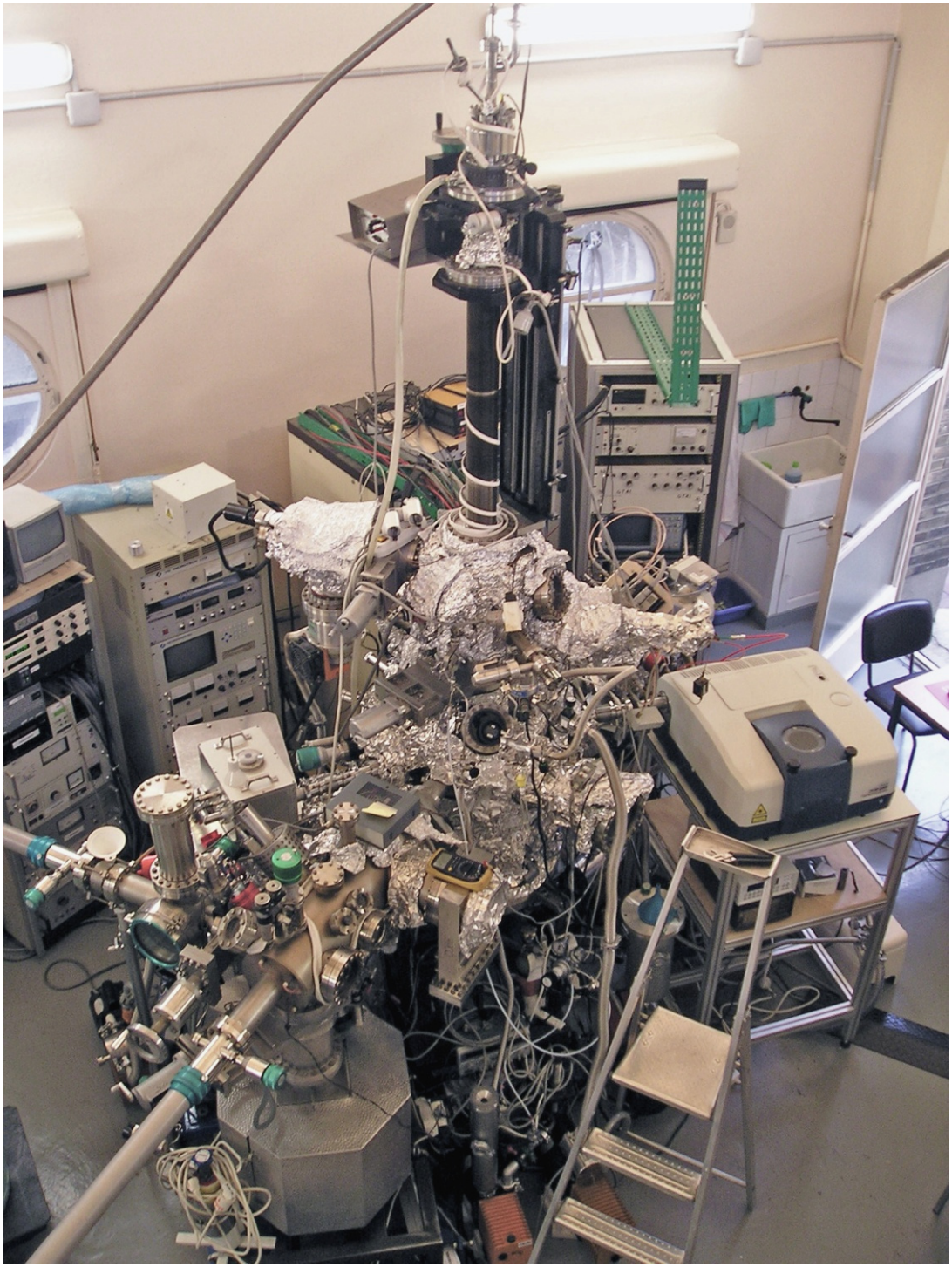
Photochimie des nitrates

LEFE
CHAT

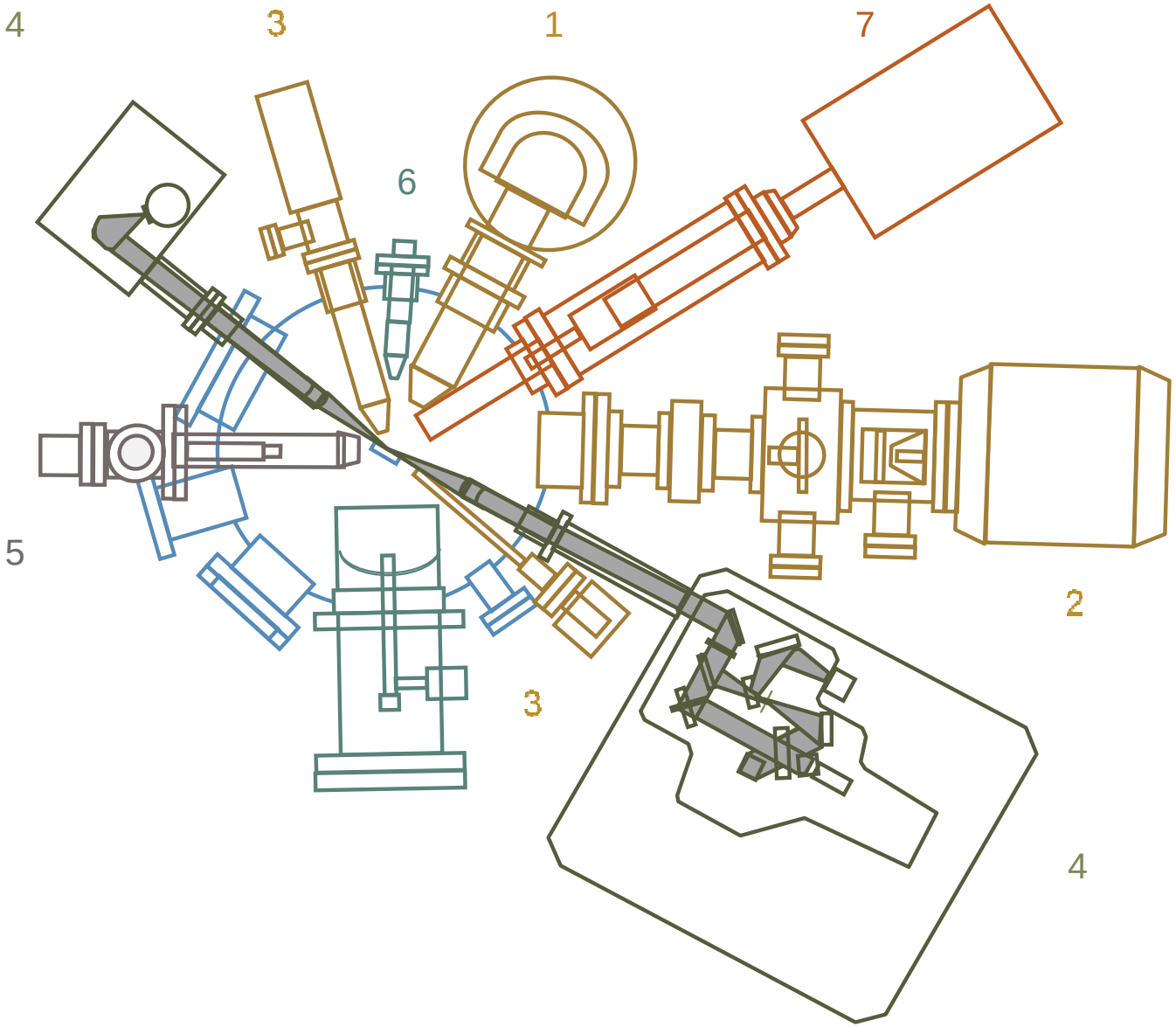
# SUMO



NEXAFS en synchrotron (Elletra, Max, SLS, SOLEIL)



# SUMO




1-Analyseur d'électrons

2- Source d'atome métastable (MIES)

3- Source X (Mg, Al Ka) et UV (He I, HeII)

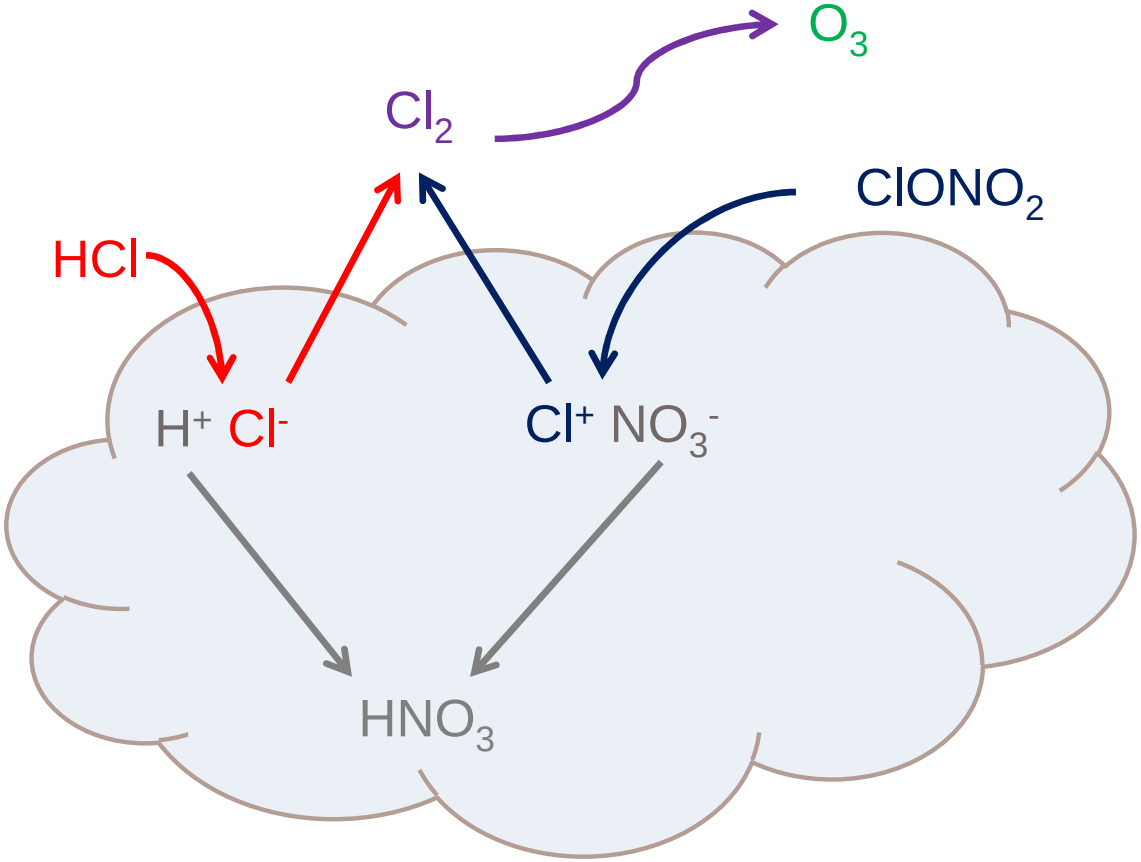
4- FTIR de surface, sous vide

5- Spectromètre de masse quadripolaire (TPD)

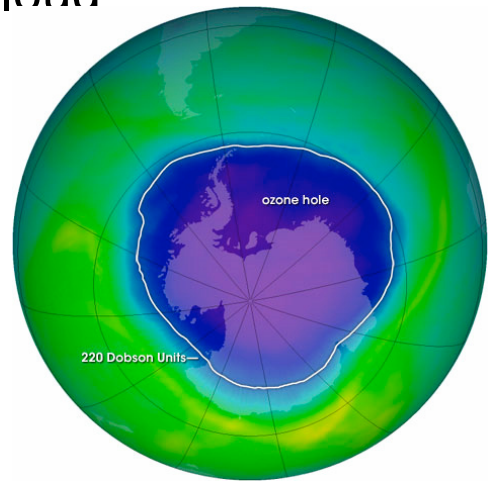
6- Canons électrons 0-100 eV et 0-4 keV (LEED)

7- Source ECR de radicaux (H, OH…)

# Ex: chimie hétérogène de la stratosphère




Polar Stratospheric Cloud




$HCl \rightarrow Cl^- + H^+$

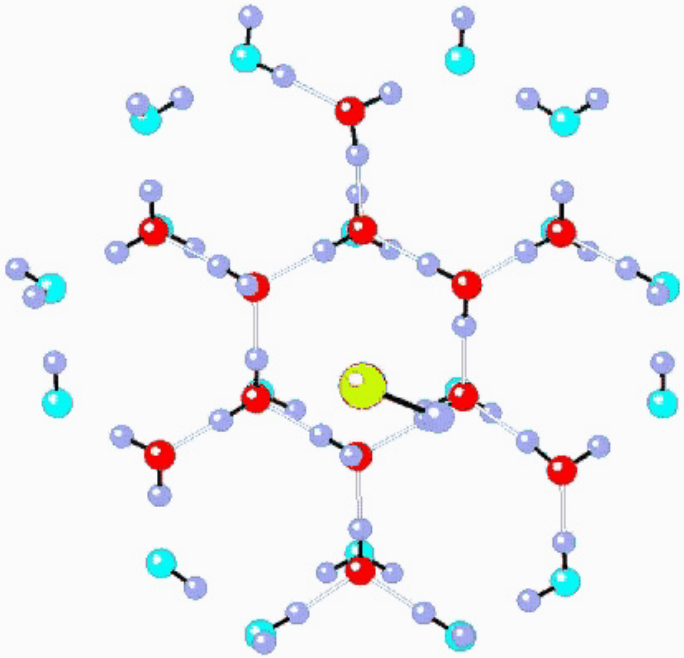
$Cl^+ + Cl^- \rightarrow Cl_2$

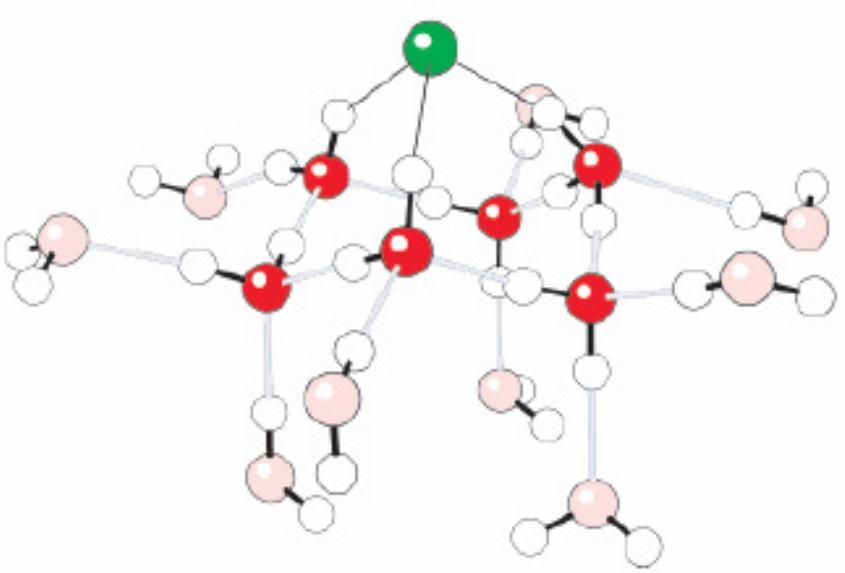
$Cl + O_2 \rightarrow ClO + O_2$

$ClONO_2 \rightarrow Cl^+ + NO_3^-$

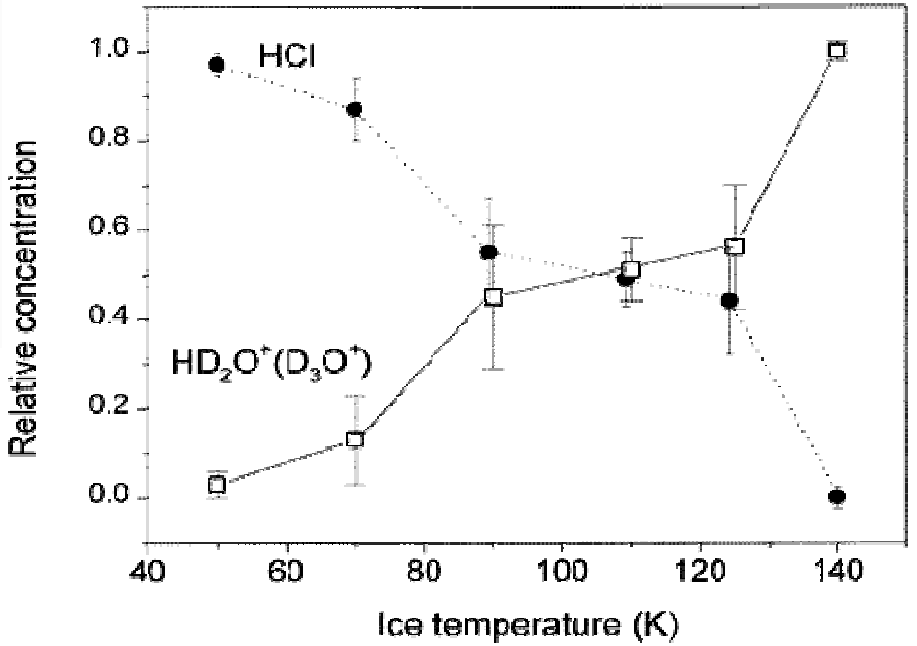
$H^+ + NO_3^- \rightarrow HNO_3^-$

# Réaction de HCl sur $H_2O$ ?





QM/MM (PM3/Classical MD)
ice TIP4P, 0K

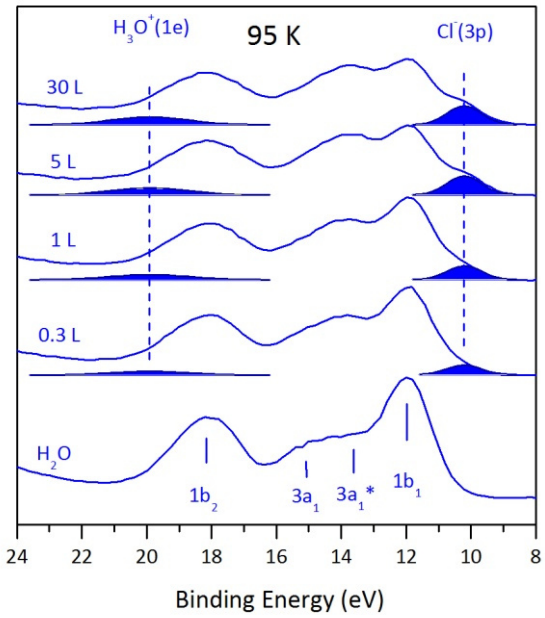


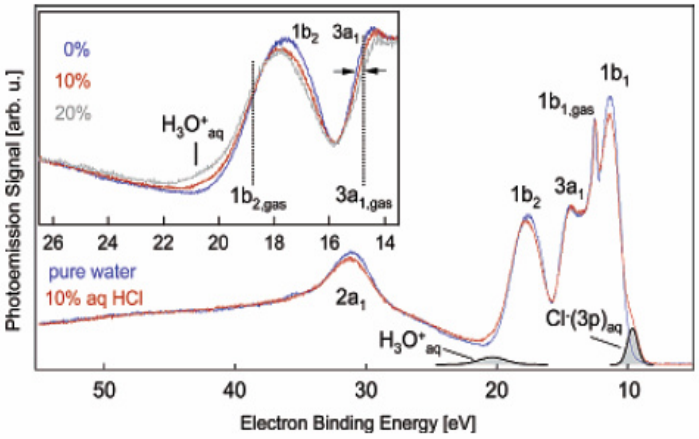

-Ionisation spontanée (pasd'activation T)
-Saturation des dH @ 0.3 MC

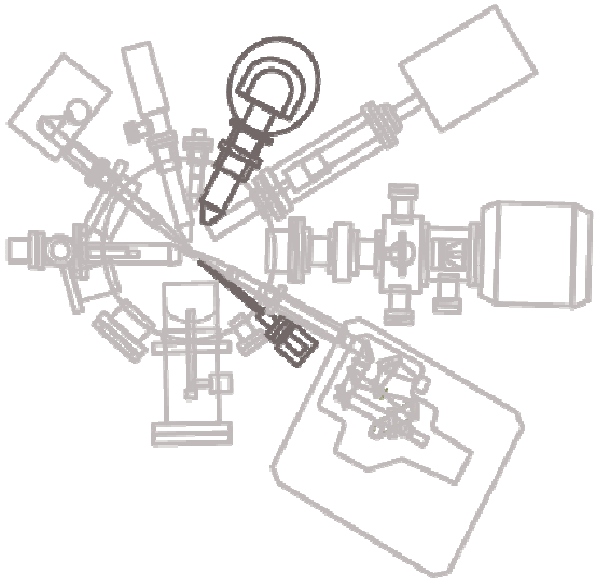
M. Svanberg, J. B. C Pettersson, K. Bolton, J. Phys. Chem. A 2000, 104, 5787

Kang et al., JACS 122 (2000) 9842

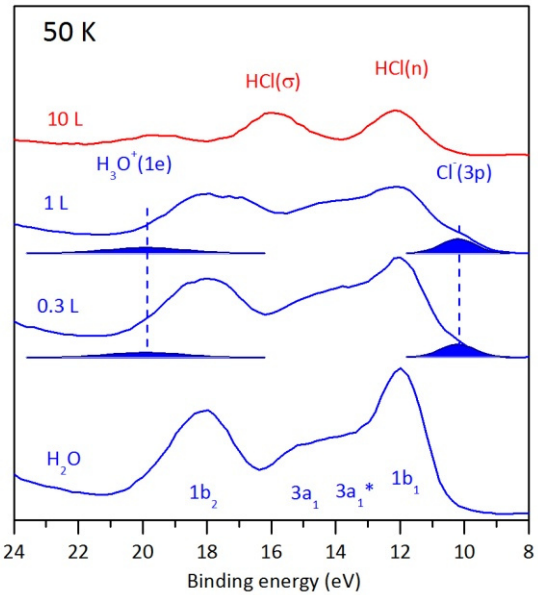
# UPS

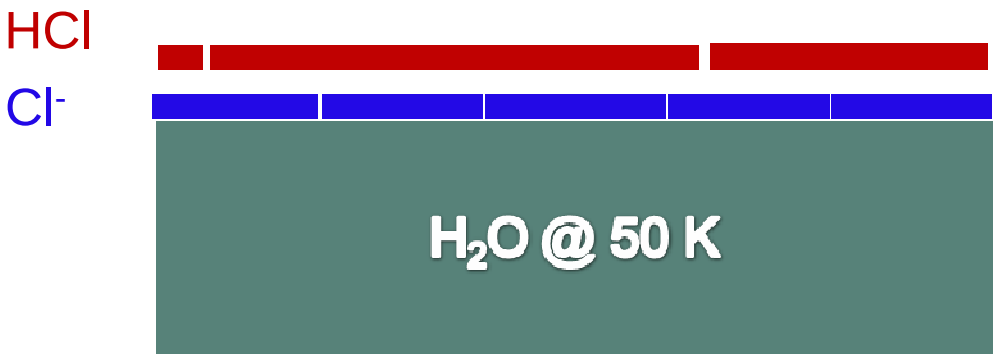


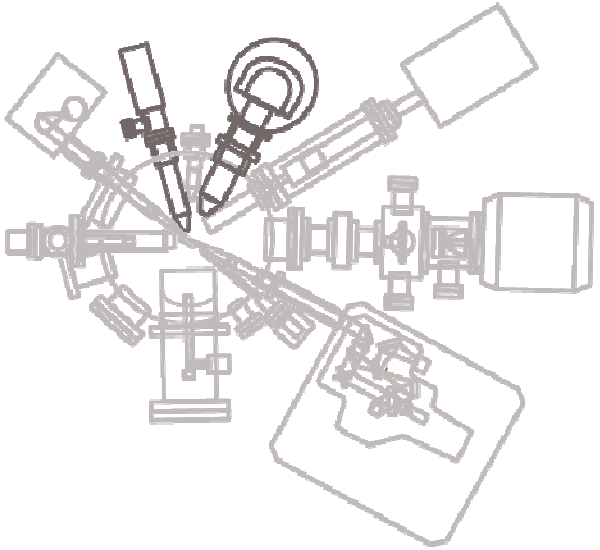



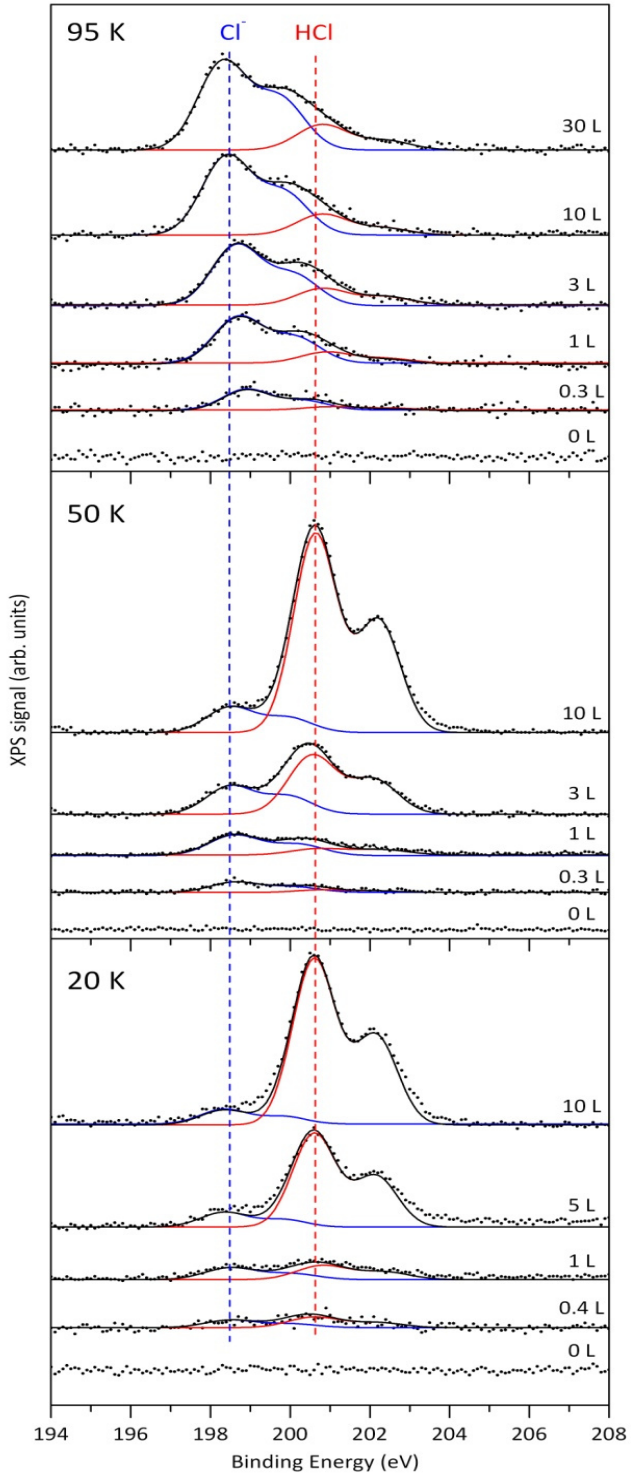
Winter, B. et al., *JACS* **128**, 3864 (2006)

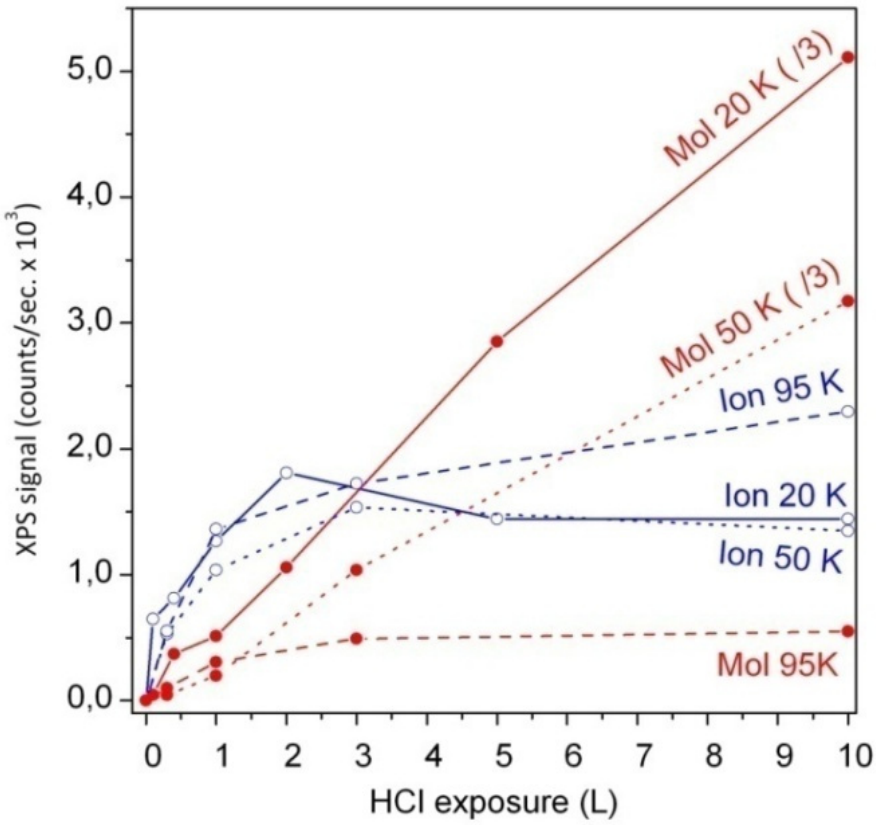


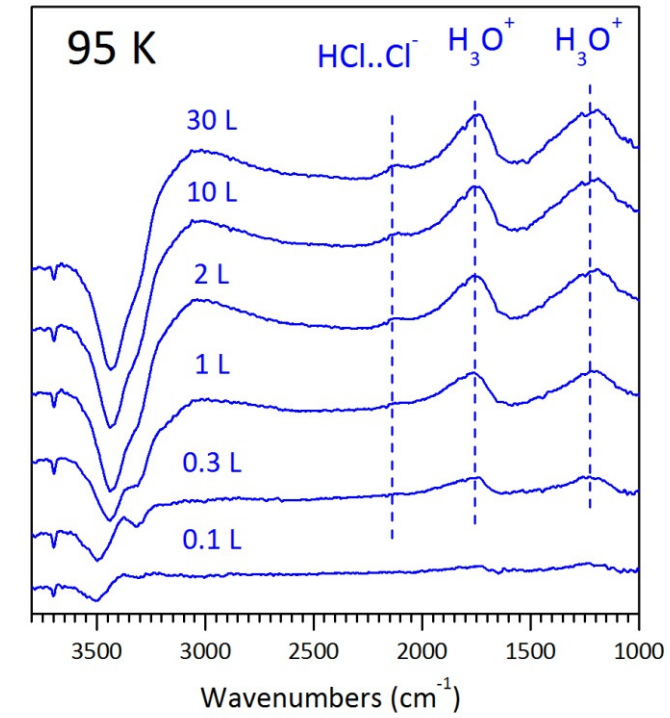



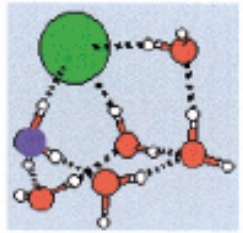
# XPS




95 K
Cl⁻
HCl
30 L
10 L
3 L
1 L
0.3 L
0 L
50 K
10 L
3 L
1 L
0.3 L
0 L
20 K
10 L
5 L
1 L
0.4 L
0 L
XPS signal (arb. units)
194
196
198
200
202
204
206
208
Binding Energy (eV)

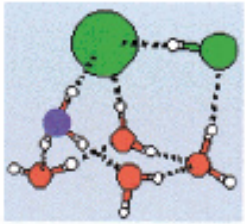

XPS signal (counts/sec. x 10³)
5,0
4,0
3,0
2,0
1,0
0,0
0
1
2
3
4
5
6
7
8
9
10
HCl exposure (L)
Mol 20 K ( /3)
Mol 50 K ( /3)
Ion 95 K
Ion 20 K
Ion 50 K
Mol 95K



$H_3O^+$

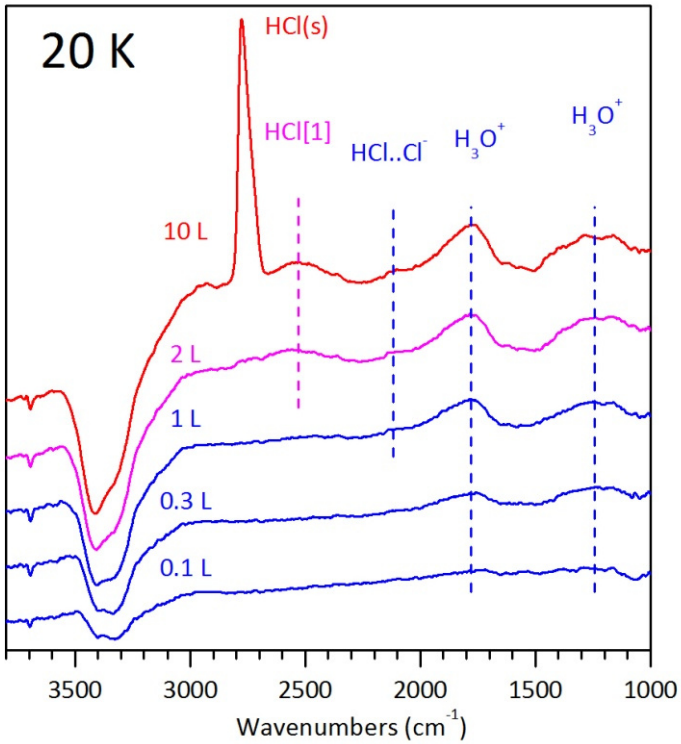
1730 $cm^{-1}$

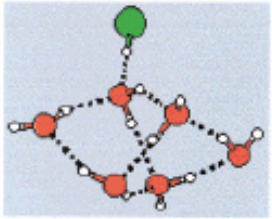


$HCl..Cl^-$

2140 $cm^{-1}$

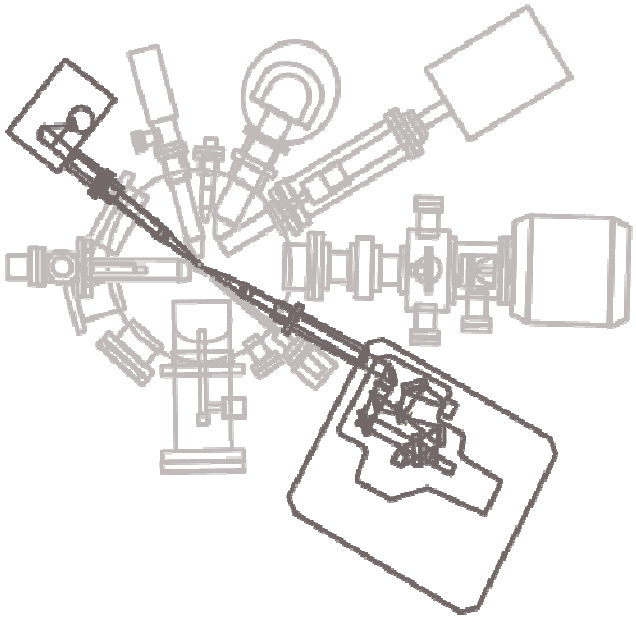
J. P. Devlin & al.
Nature 417 (2002)
269



HCl[1]

2550 $cm^{-1}$



FTIR

# Conclusion

- Pas d’activation thermique à l’ionisation de HCl/glace
- Validation des modélisations théoriques.