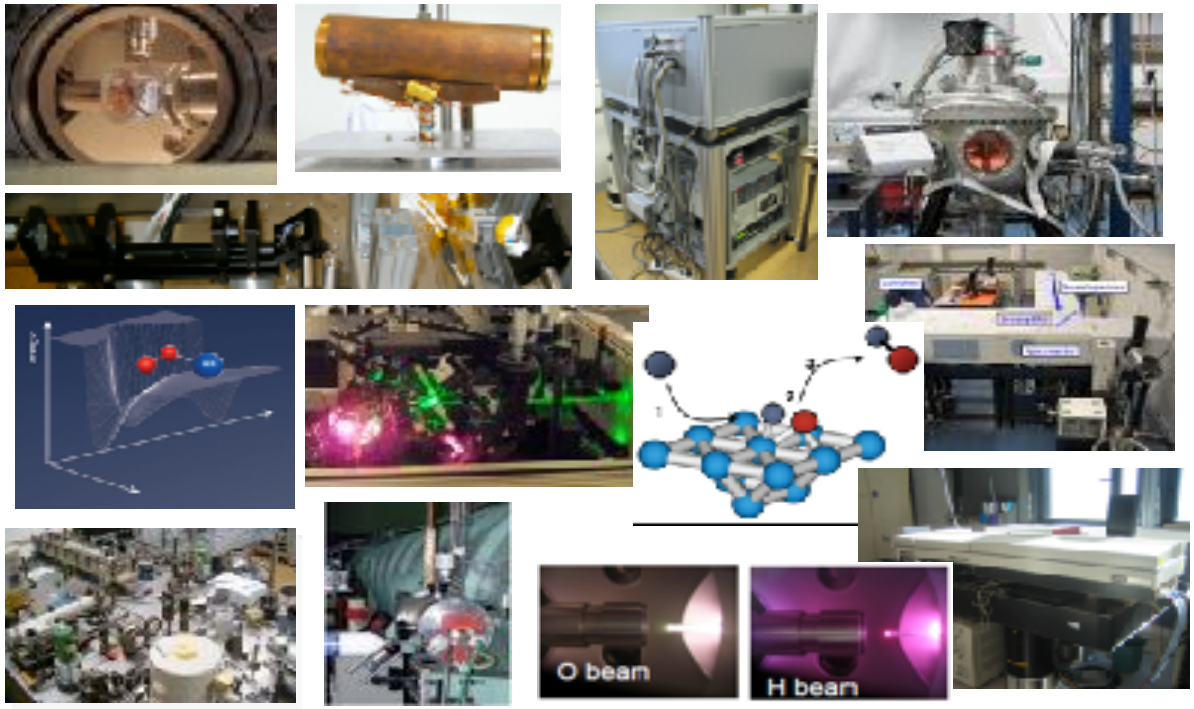
Molecules in the Universe

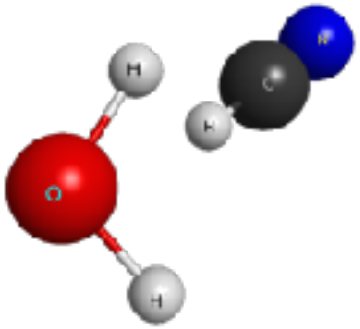
C. Janssen

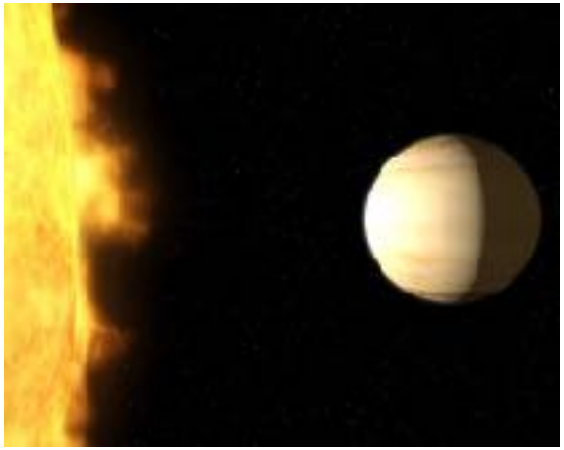
F Dayou, ML Dubernet, F Dulieu, X. Michaut



Various laboratory experiments and theoretical developments dedicated to the study of molecular interactions in the gas & on surfaces for astrophysical and atmospheric applications

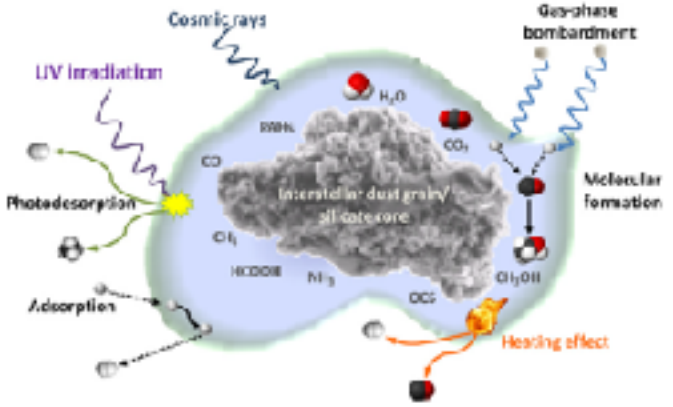
Why study the macroscopic world on the microscale ?



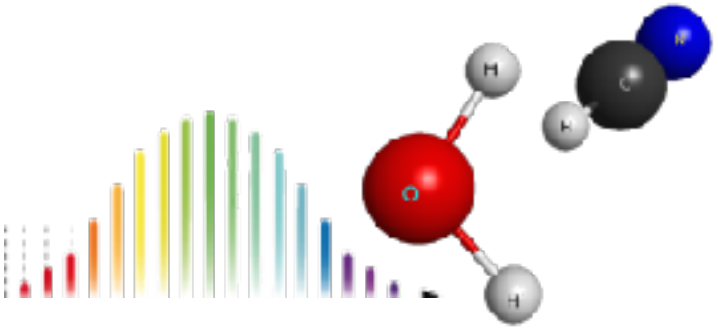


Research axes

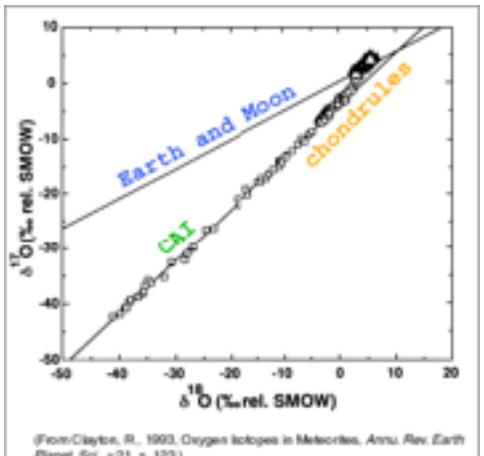
Reactivity and interaction at gas-solid interface and in the ice

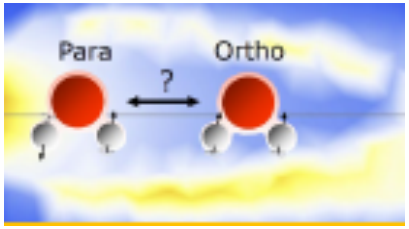


Molecular processes and parameters for atmospheres and ISM



Molecular anomalies





Molecules in the Universe

Jussieu Spin, photons and ices :	3.5 C/EC + 1 PHD	+ 2 IR + 1 IE + 1 tech
Jussieu SMILE (Molecular Spectroscopy and Laser Instrumentation for Environment)	5 EC+1Em + 2 PHD	
Cergy Reactivity on cold surfaces :	5 EC+1IR + 3 PHD	+ 1 IE+1 tech
Meudon van der Waals systems for Astrophysics and for Planetology	1.5 EC+ 1 IR 1 P.Doc	+ 2 IE
Collisional excitation, reacticity and high resolution VUV spectroscopy of interstellar molecules Meudon	2 EC + 2 Em	+ 1 IE+1 tech

Total 22. C/EC and 12 Ing. & Tech.
6 PHD students
1 post-doc

Scientific animation

Molecules in the Universe workshops

- Every two months: ~ 4 per year
- Location is cycling : Jussieu-Cergy-Jussieu- Meudon-Jussieu-Cergy-...
- 2 - 3 seminars
  + 1 « interpole » meeting per year

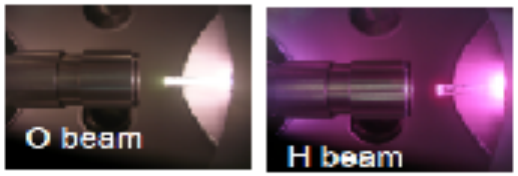
  - Permanents of the pole
  - PHD students
  - Others poles LERMA
  - External
  - + news or short coms

T. Zanon, Meudon, 2015

Discussion continues during our homemade buffet

June 14, Cergy: Bron & Minissale speakers

Gaz-surfaces interactions : reactivity

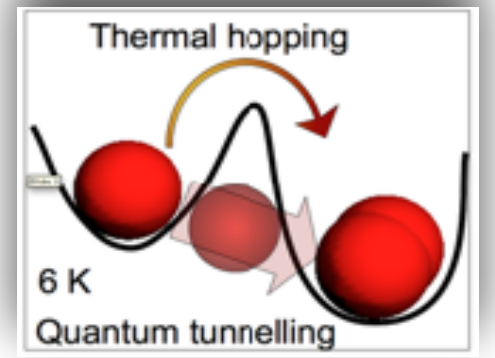


Plasmas Discharges
Atomic beams

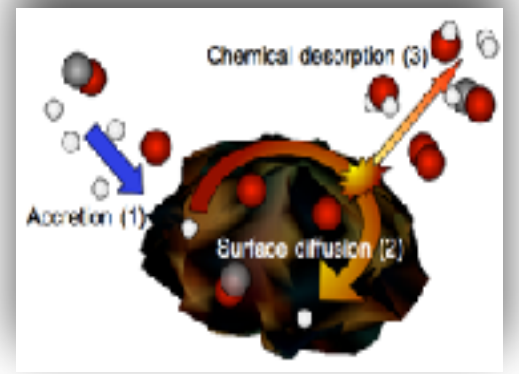
Cold substrate (10 K)
(graphite, water ice, silicate)

Analysis chamber
- IR Reflexion-Absorption
- Mass spectr.

O-atom diffusion at very low temperature

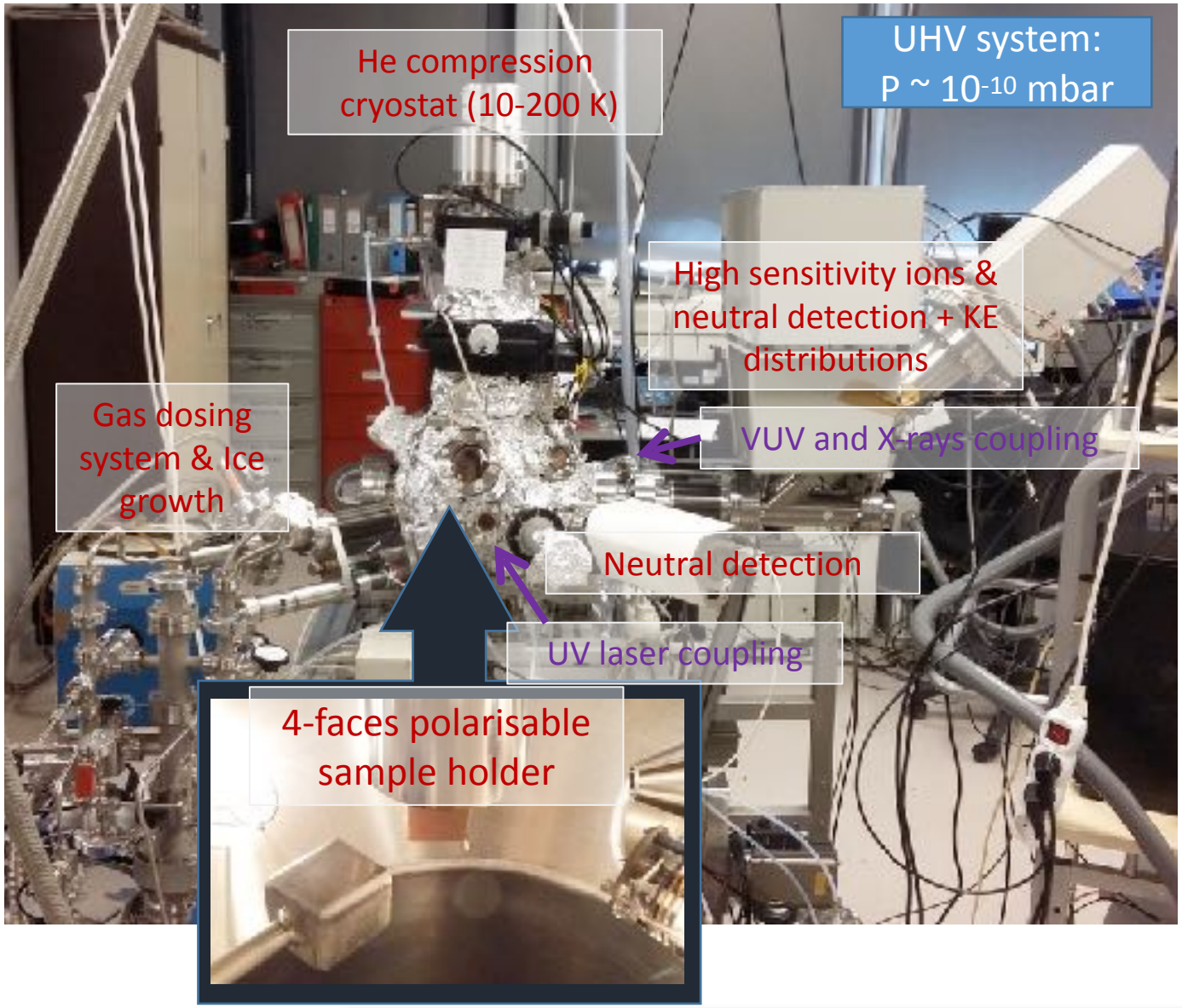


Towards Oxygenation reactions (not only hydogenation)



Desorption after reactions

« SPICES 2 » set-up : Surface Processes and ICES 2



Higher Sensitivity

- *Increase vacuum perfomance*
- *New analysis Chamber*
- *New mass spectrometer*

New achievements

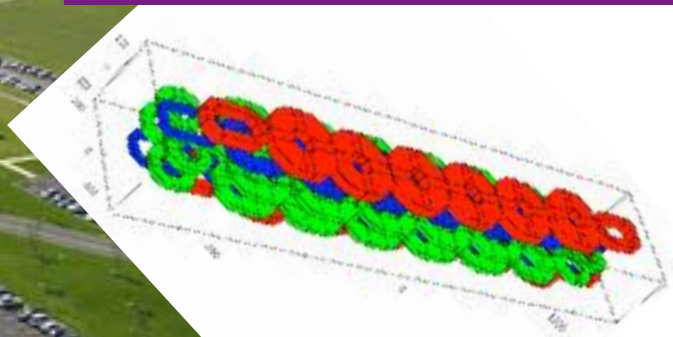
- Ion/neutral detection
- Kinetic energy measurement
- Compatible with : continuous (synchrotron) Or pulsed (laser) sources

-> internal energy

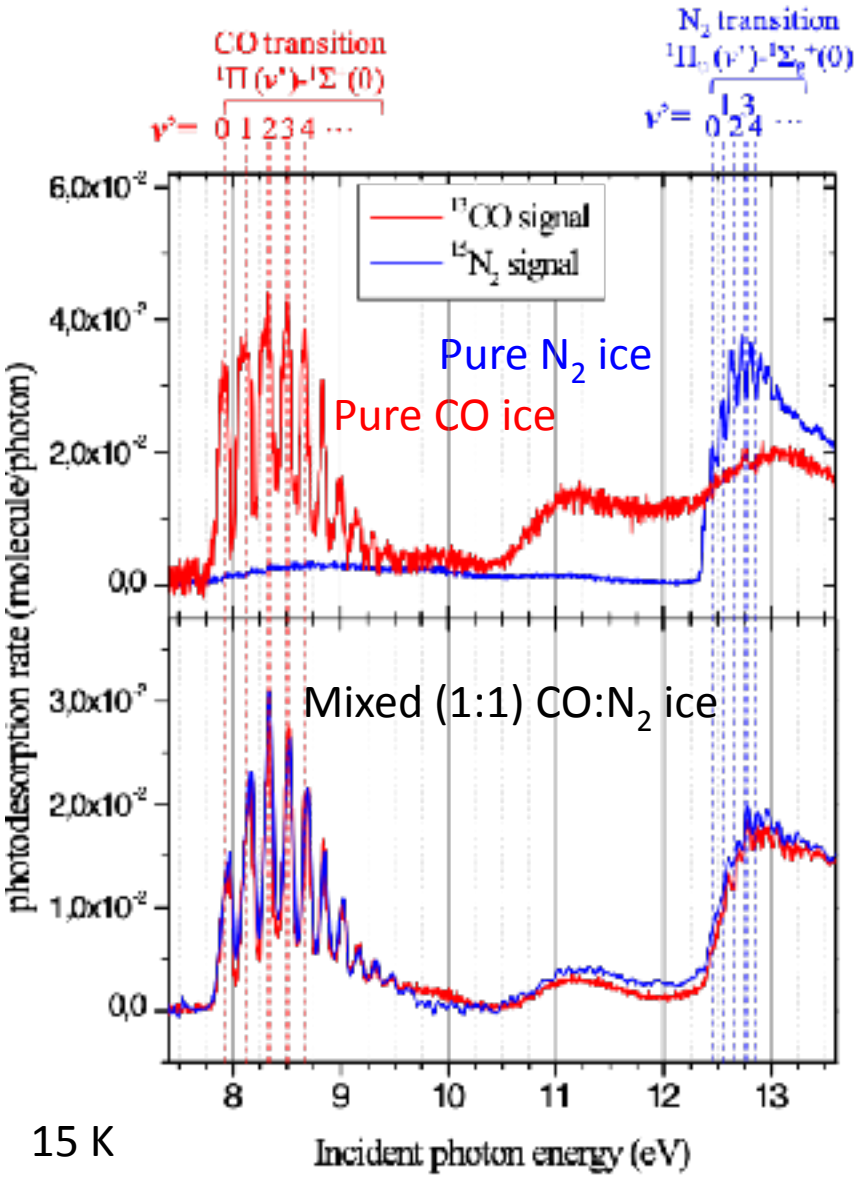
DESIRS BEAMLINE

Fully tailored polarization

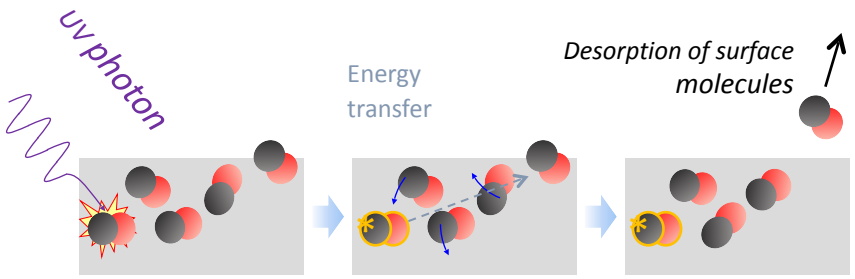
Undulator : 4.5 – 40 eV



Gas-surfaces interactions : UV Photon Stimulated Desorption



15 K



Bertin et al., ApJ 2013

- Surface process : top few ML

E_{des} < 100 meV

@ 8.2 eV

- Yields ~ X 10^{-2} molecules/ photons
- Decrease with ice deposition Temp
- σ_{abs} ~ 1.5 10^{-17} cm^2

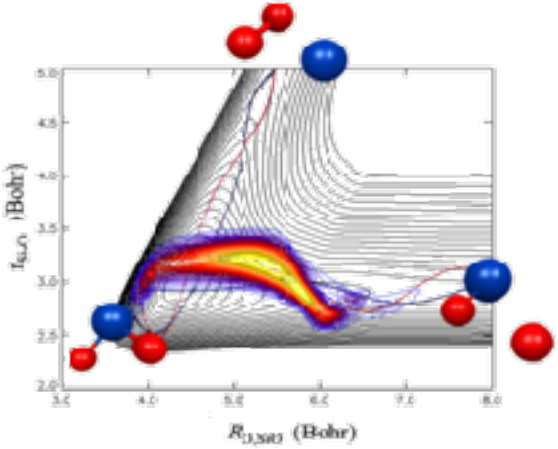
Quantum Yield

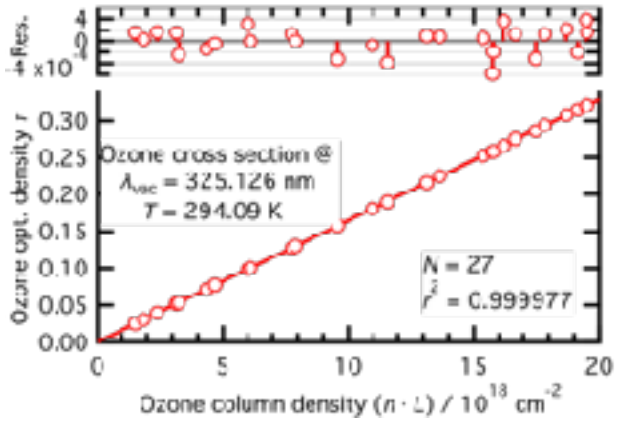
~1 molecule /absorbed photon

in top 3 ML (10-20 K)

Molecular processes and parameters for atmospheres and ISM

- *Unique tools for providing traceable spectroscopic data: Molecular Metrology*
  - *High accuracy measurements*
    - *Theory and simulations*
      - *Reference data for physical and atmospheric research*





$\sigma = 16.470\ 10^{-20}\ cm^2\ (\pm 0.2\%)$

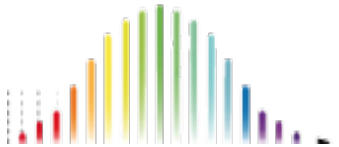
Janssen et al, AMT, 2017

Driving force:

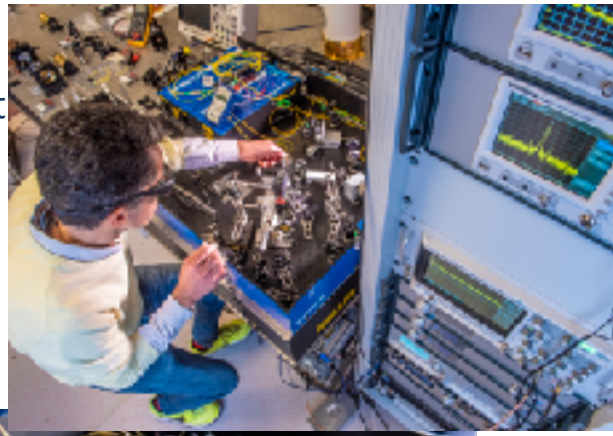
- *Provide fundamental molecular data for*
  - *understanding and studying climate and atmospheric composition change*
  - *modelling cometary and stellar atmospheres as well as the interstellar medium*
  - *fundamental physics*
- *Study terrestrial & planetary atmospheres*
  - *understanding and studying climate and atmospheric composition change*
  - *develop new analytical tools and techniques of observation (axis III)*

Molecular processes and parameters for atmospheres and ISM

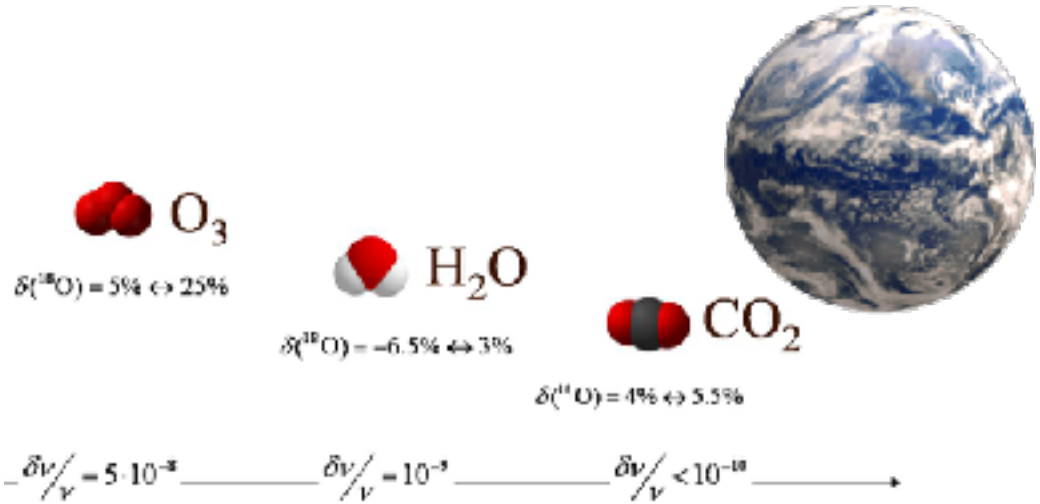
Towards traceable IR spectroscopic data for planetary research (PRESPASS)



- Frequency-comb stabilised laser spectrometer @ 10 µm (FCS-DL)
- Michelson interferometer stabilised diode laser (MIS-DL)
- Coupling to UV and VIS laser : most precise absolute cross section of ozone so far (more than 10 x better than actual reference, Janssen et al. AMT, 2017)



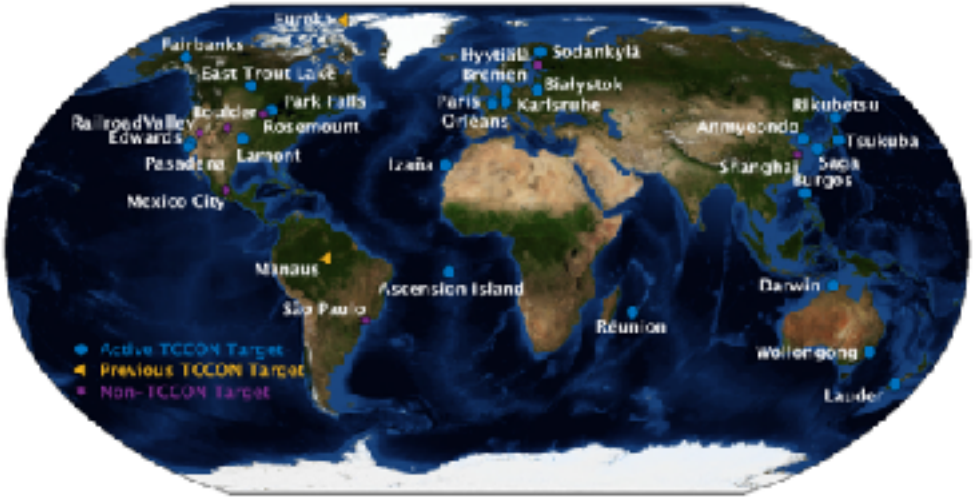
- Provide very high resolution data for remote sensing of isotopes
- Retrieve line parameters and line profile information on oxygen bearing key compounds: O_3, H_2O and CO_2

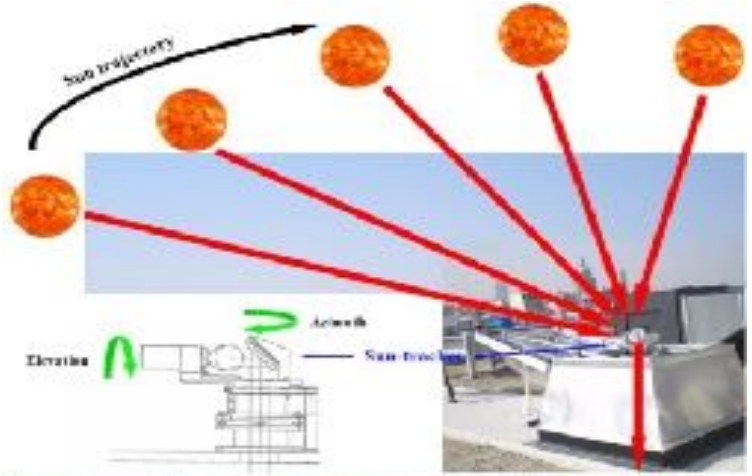


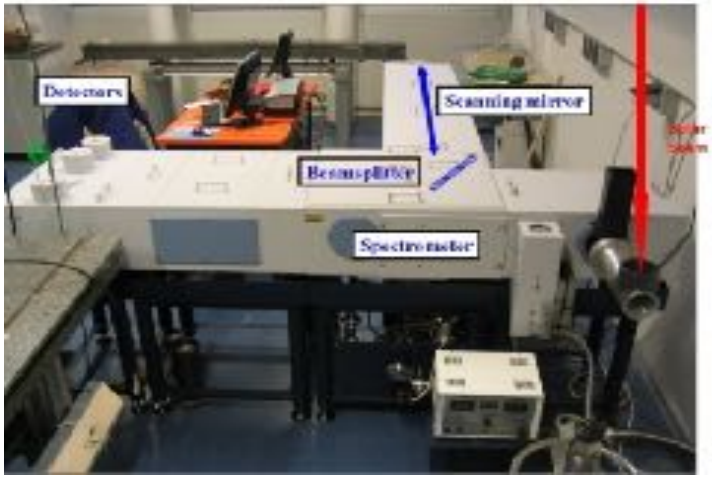
Frequency comb, Jussieu

Atmospheric observation

Only European TCCON observation site in a large city (2015)



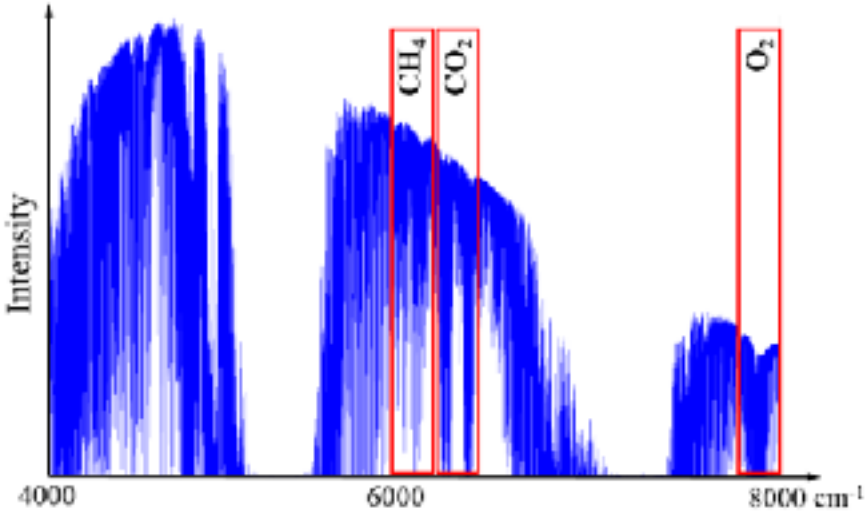


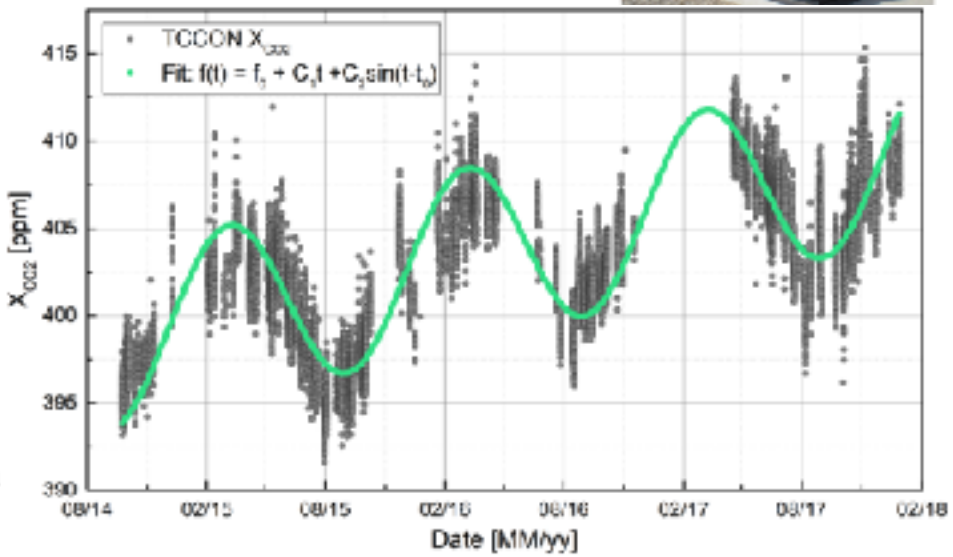


- High resolution FTS-Paris is in operation since 2007
- Part of international TCCON network (since 2015)
- Part of OCAPI (IPSL observation network) & QualAir (UPMC)
- Provides unique data: only one other mega-city station worldwide
- Validation target for on-going and future satellite missions

Atmospheric observation : CO_2 at Paris

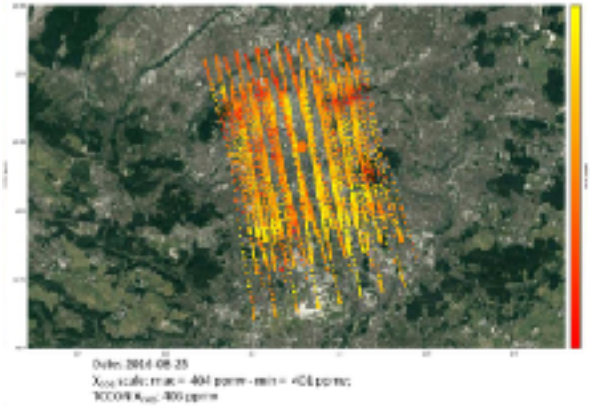
- CO2 record from autumn 2014 on





- Comparison with OCO satellite

OCO-2 Paris overflight



Wunch et al, AMT 2017

Molecular processes and parameters for atmospheres and ISM

VUV spectra of molecules and multiply charged heavy element ions

- High resolution (R = 150000) VUV normal incidence spectrograph Meudon
- Image plates with 5 decades of linear intensity response
- Penning discharge or HV vacuum sparks
- Wavelength range 200-3000 Å

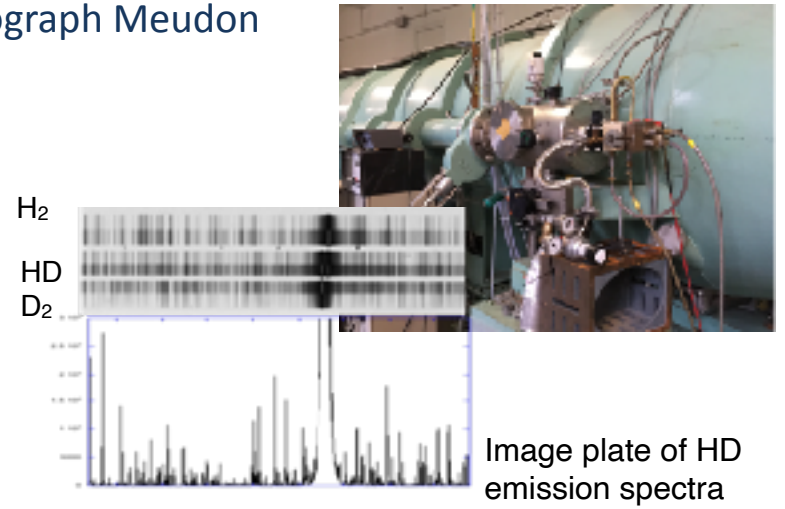
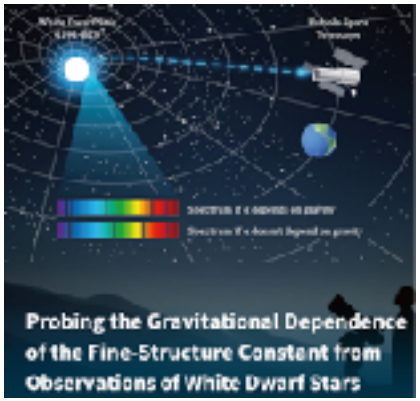


Image plate of HD emission spectra



Bainbridge et al, Universe 2017

Projects

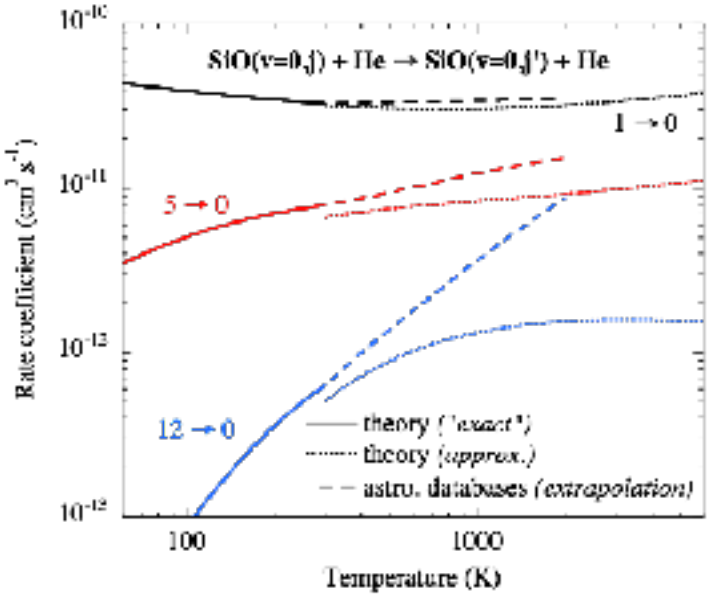
- Emission spectra of the hydrogen isotopologue HD (theory & experiment)
- Emission spectra of iron group multiply charged ions (Fe-V, Ni-V) as laboratory references for possible change of the fine structure constant α in white dwarfs observed by HST
- Study of transition energies and probabilities of heavy element (Eu, Er, Tm) ions for abundance studies and radiative transfer simulations of Neutron Star Merger Ejecta

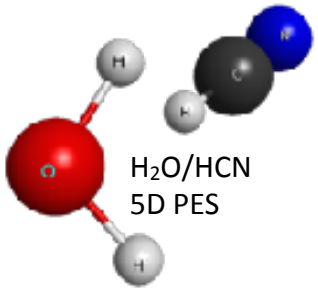
Molecular processes and parameters for atmospheres and ISM

Collisional parameters for the modelling of non-LTE media

- Simulations based on quantum chemistry and quantum dynamics
- Rotational excitation of molecules (ISM)
- Electronic excitation of atoms (stellar atmospheres)
- Variety of systems and temperature conditions
- Development of the BASECOL database (since 2004)
- Creation of the worldwide VAMDC e-infrastructure

Balança et al., 2017





H_2O/HCN
5D PES

Quintas-Sanchez et al., 2017

Projects

- Support of ALMA, Herschel, NOEMA, GAIA, Rosetta, … exploitation
- Systems with more degrees of freedom (larger species, vibration,…)
- Improved description of processes for high-temperature media
- Collisions of molecules with water (cometary atmospheres)
- Update of BASECOL database and development of VAMDC platform

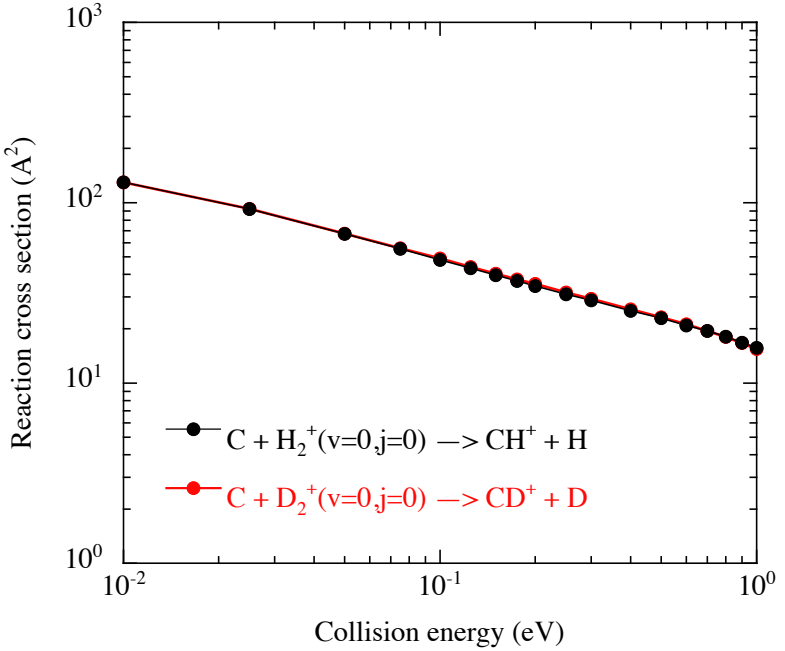
Molecular processes and parameters for atmospheres and ISM

Reaction rates for the chemical modelling of astrophysical media

- Simulations based on quantum chemistry and quantum dynamics
- Use variety of complementary approaches
- Low-temperature reactions between unstable radicals
- Deep insight into reaction mechanisms
- State-to-state reaction rates

Merged-beams apparatus (Columbia Univ.)

COLUMBIA UNIVERSITY



Dayou (2018)

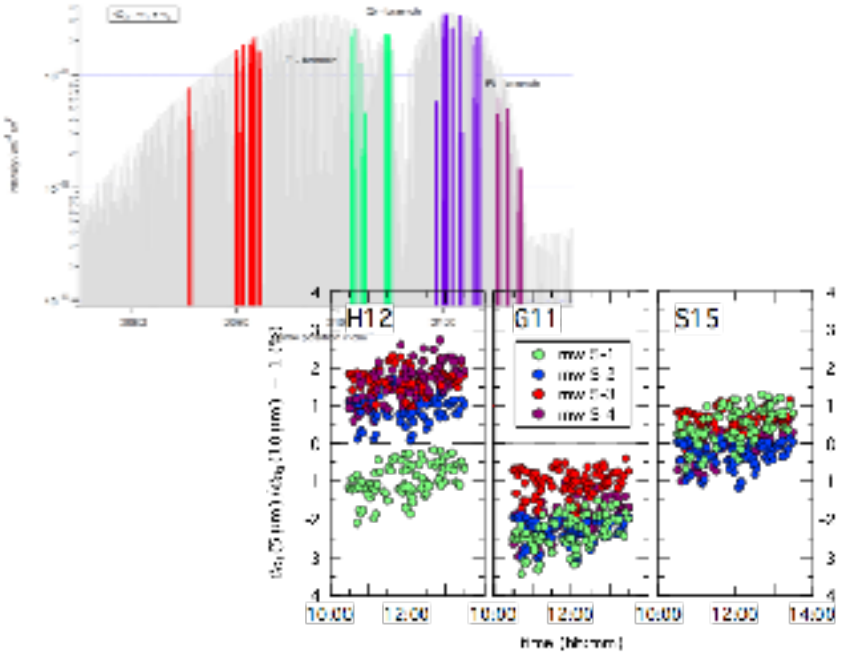
- Study of low-temperature isotopic effects ($C+H_2^+/HD^+/D_2^+$ reactions)
- Joint experimental/theoretical study (D.W. Savin group, Columbia Univ.)
- Study of state-resolved photodissociation processes (diffuse ISM)

Molecular processes and parameters for atmospheres and ISM

Close links between observation, simulation, laboratory studies and databases

- Molecular VUV data (H_2, CO) are fed into MOLAT database
- Calculated collision rates are directly integrated into BASECOL
- Consistency of spectroscopic data bases (HITRAN, GEISA, S&MPO) is verified through remote sensing

  ➡ triggers new laboratory studies



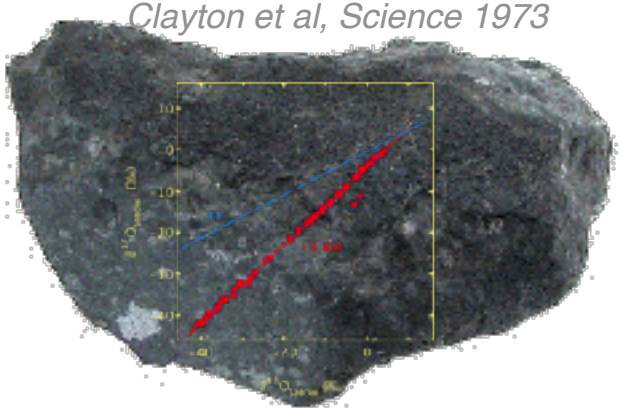
Janssen et al, JMS 2016

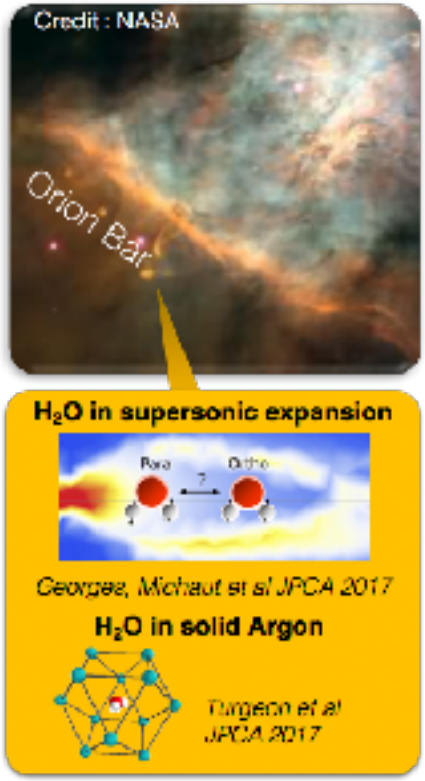
ortho-NH_2D + H_2 (*Daniel et al MNRAS 2014*) added to BASECOL database *(Dubernet et al, A&A, 2013)* in 2016

Molecular anomalies

- *Unusual and unexplained molecular signatures, such as ortho-para ratios and anomalous isotope ratios, provide new and exciting probes for their environment*
  - *New and highly sensitive tools for laboratory studies are developed*

Clayton et al, Science 1973



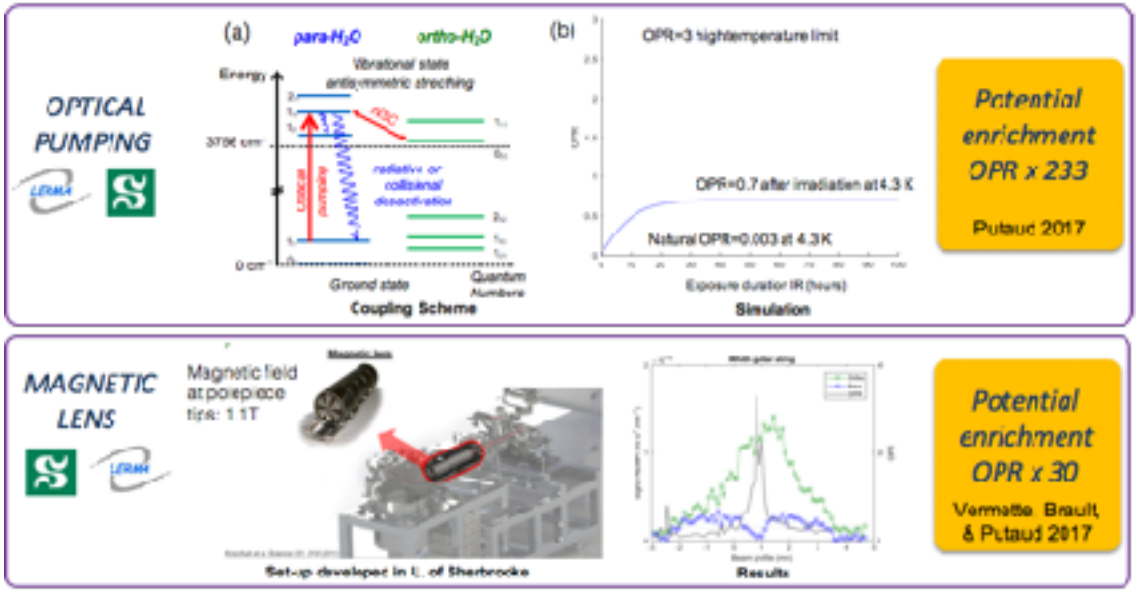


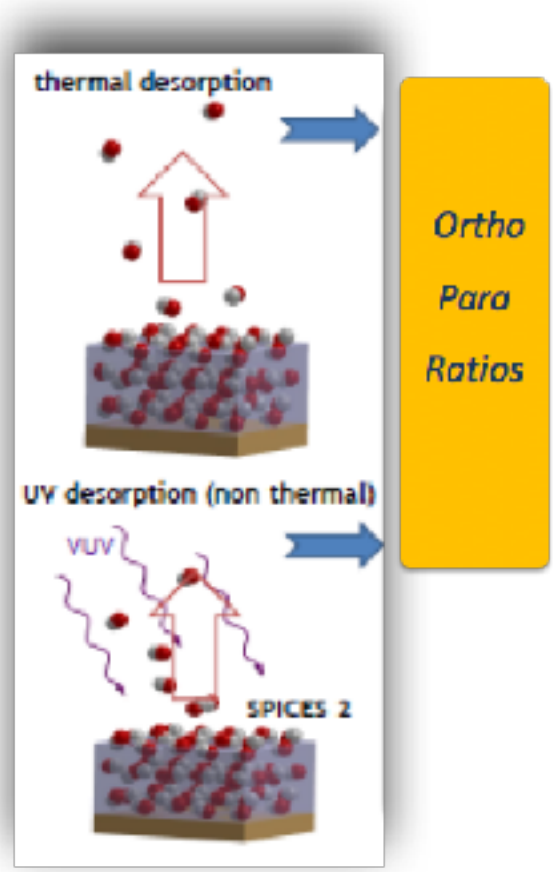
Key questions:

- *Understand physico-chemical origin of unusual isotope and ortho-para ratios (OPRs)*
- *Why do observed OPRs in cometary atmospheres, protoplanetary disks, PDRs and diffuse clouds often differ from what is expected from these environments ?*
- *Can we understand low T isotope fractionation on icy films : tunnelling and large isotope effects ?*
- *Where does heterogeneity of oxygen isotopic composition of the solar system come from ?*
- *What can we learn from isotope signatures of multiply substituted isotopologues ?*

Molecular anomalies

What is the link between the thermal history of ices and spin temperatures measured in space ?





Project & goals

- Develop new experimental tools
- Measure characteristic times for nuclear spin conversion on icy mantle
- Establish link between OPR on ice and OPR in gas phase
- Understand the influence of the desorption (thermal or non-thermal) on the OPR in the gas phase

Summary and highlights

- ***Fundamental physics approach for understanding mechanisms at the molecular level that can solve astrophysical and atmospheric research problems***
- ***Strong & unique laboratory astrophysics activity***
- ***Atmospheric observation and lab spectroscopy have strong social relevance and close link to gas metrology activities is established via participation in international WG***
- ***Activities span whole range from laboratory measurements/simulation to observation and results are distributed to the international community via databases***
- ***Development of new and unique technologies for using & studying molecular anomalies as probes:***
  - ***Rare (doubly substituted) isotope analyser for CO_2***
  - ***Nuclear spin state enrichment***