Electronic structure and reactivity of astrochemically relevant inorganic hydrides

Nathan J. DeYonker, Marco Fioroni
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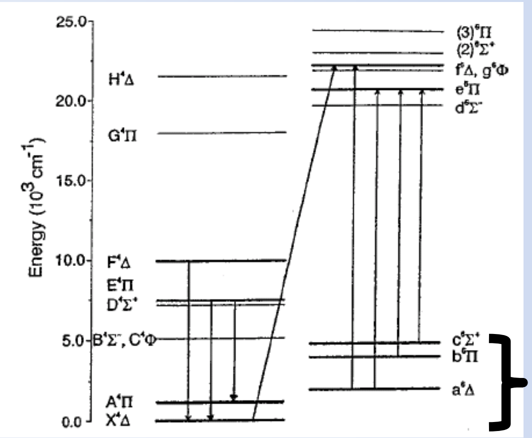
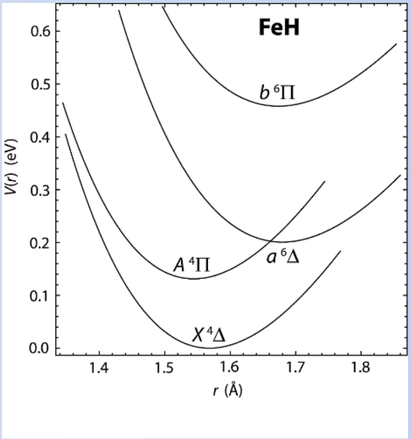
High-accuracy electronic structure of FeH

- Controversial identity of ground electronic state
- Line lists used in dwarf star/gas-giant population ratios, extrasolar planetary atmospheres and cores
- Single reference theories vs. multireference theories?

- "Chemical accuracy" for T_e of all spin components for $X\ ^4\Delta$, $a\ ^6\Delta$, $A\ ^4\Pi$, $b\ ^6\Pi$
- Improved Bond Dissociation Energy

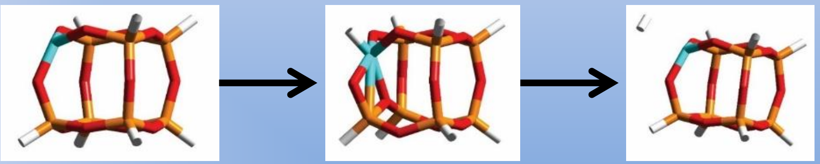


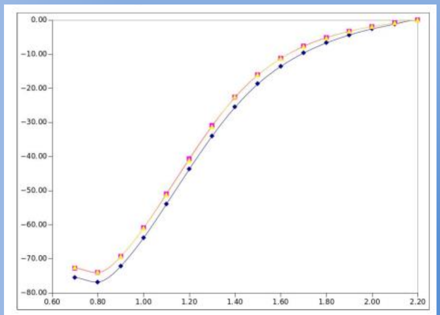


POSS H_2 Formation

- High universal abundance of molecular hydrogen is not well-explained
- Do TM defects on siliceous grains (Fe^+- POSS) catalyze H_2 formation in ISM?

- Barrier-less POSS-H, POSS-H_2 formation
- Agreement between double-hybrid DFT and MP2-F12
- Chemisorption of H to Si or O centers is not thermodynamically favorable





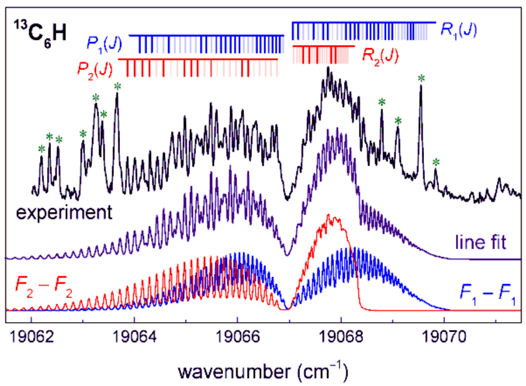
FeH: N. J. DeYonker, W. D. Allen, *J. Chem. Phys.*, **137**, 234303 (2012).
POSS H_2 Formation: M. Fioroni, N. J. DeYonker, *ChemPhysChem*, **17**, 3390 (2016).

THE UNIVERSITY OF MEMPHIS.

Spectroscopic survey of electronic Transitions of C_6H, $^{13}C_6H$ and C_6D

X. Bacalla, E.J. Salumbides, H. Linnartz, W. Ubachs, D. Zhao

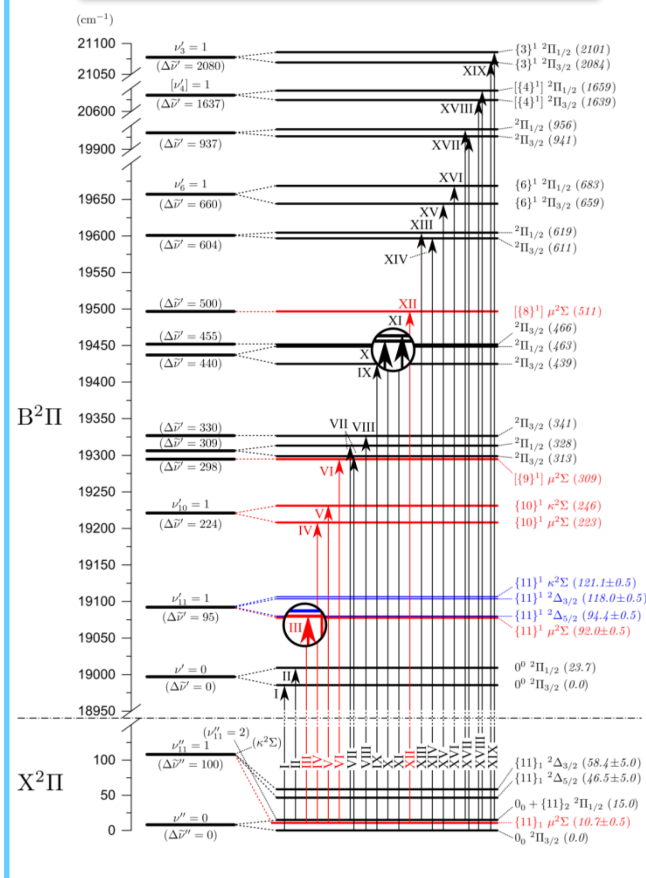
Department of Physics and Astronomy, VU University, De Boelelaan, 1081 HV, Amsterdam, The Netherlands
Sackler Laboratory for Astrophysics, Leiden Observatory, Leiden University, The Netherlands
University of Science and Technology China, Hefei, China



- Measurement of optical absorption spectra
- $B^2\Pi$-$X^2\Pi$ system 473 – 527 nm
- Isotopic substitution H/D, 12C/13C
- Renner-Teller analysis of bending modes
- Analysis of rotational structure 19 bands

Details at the poster #2

Final Result: level diagram of $B^2\Pi$ state



Poster 3

Inner-shell photo-excitation as probe of the molecular ions CH^+, OH^+, and SiH^+: Measurements and theory

J.-P. Mosnier *et al.*
School of Physical Sciences and NCPST, Dublin City University, Dublin 9, Ireland

- Photoionization cross-sections were measured for the processes

$$AH^+ + h\nu \rightarrow A^{2+} + H^+ + \bar{e}$$

$$A^+ + h\nu \rightarrow A^{2+} / A^{3+} + \bar{e}$$

K-shells CH^+ (290 eV), OH^+(550 eV) and L-shell SiH^+(110 eV)

- Ion-photon merged-beam technique at SOLEIL synchrotron

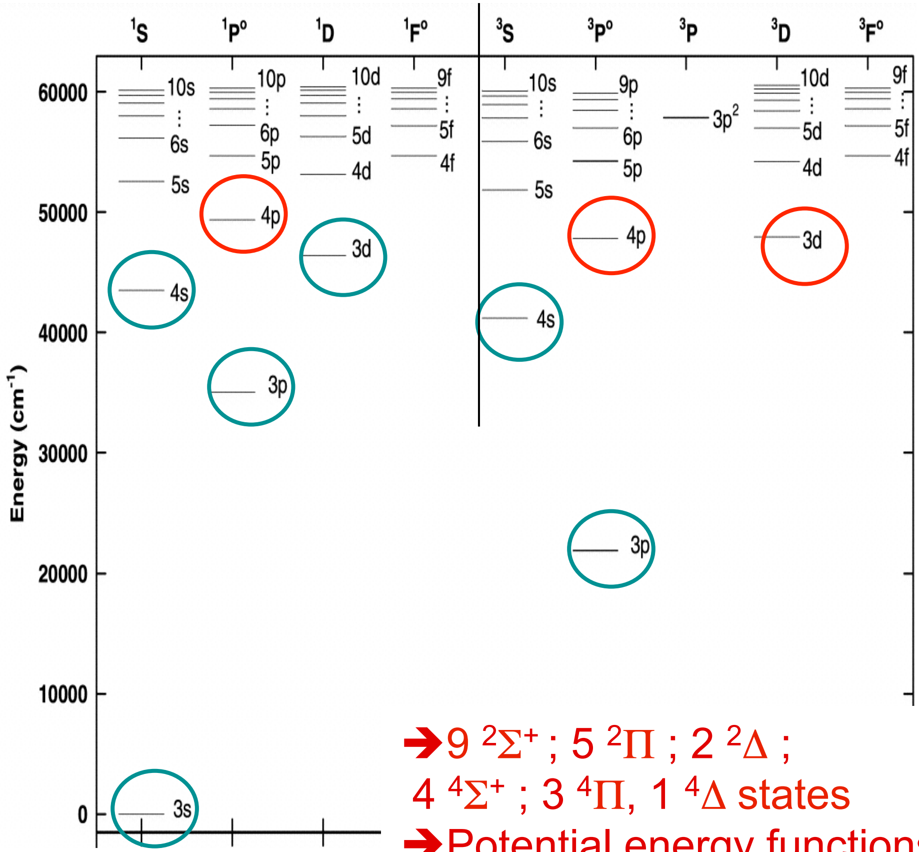
- Data interpreted by ab initio calculations of the core-excited molecular energy level structures and corresponding dipole transition moments

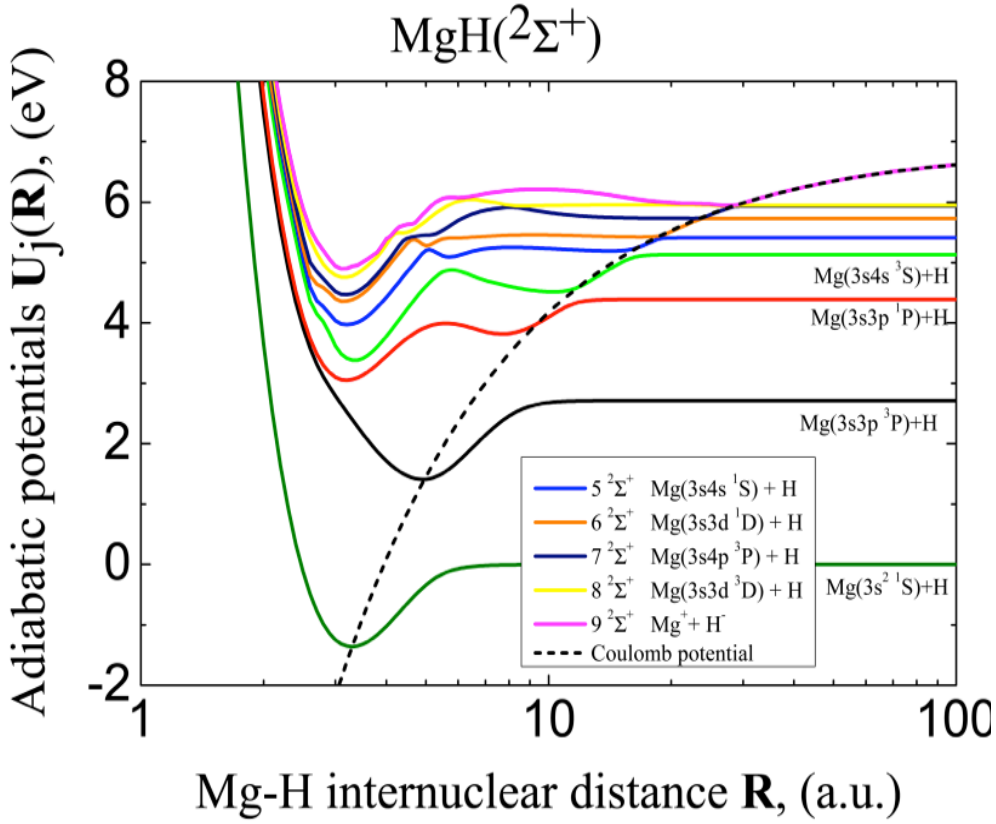
- Contributions from ground and excited valence electronic states.

Quantum calculations on diatomic hydrides for stellar atmosphere modelling

M. Guitou[a,*], A. Mitrushchenkov[a], A. Spielfiedel[b], N. Feautrier[b]
S. A.Yakovleva[c], A. K. Belyaev[c]

Mg + H $\underset{\text{désexcitation}}{\overset{\text{excitation}}{\rightleftarrows}}$ Mg* + H $\underset{\text{neutralisation}}{\overset{\text{ionisation}}{\rightleftarrows}}$ $Mg^{+} + H^{-}$





➔ 9 $^2\Sigma^+$; 5 $^2\Pi$; 2 $^2\Delta$; 4 $^4\Sigma^+$; 3 $^4\Pi$, 1 $^4\Delta$ states

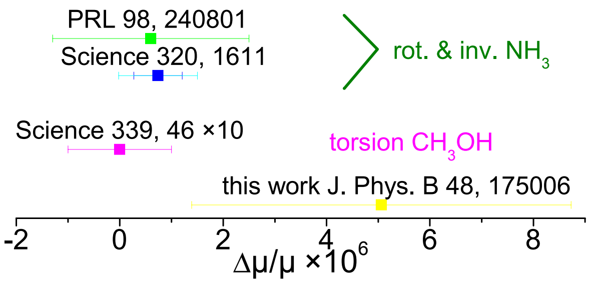
➔ Potential energy functions

➔ Radial and rotational couplings

➔ inelastic collisions treatment

Sensitivity from frequency splittings in the molecular spectra to a variation of the fundamental constants

Florin Lucian Constantin, Laboratoire PhLAM CNRS UMR 8523 Villeneuve d'Ascq France



Cosmological variation of the fundamental constants

-Possible spatial and temporal variations of $\mu = m_p/m_e$, α, g_N

-Sensitivity of a molecular frequency to a variation of μ : $df/d(\ln\mu)$

-Comparison of astrophysical lines with different sensitivity coefficients

-Address here the comparison of frequency intervals in the quasar spectra

Molecular modelisation

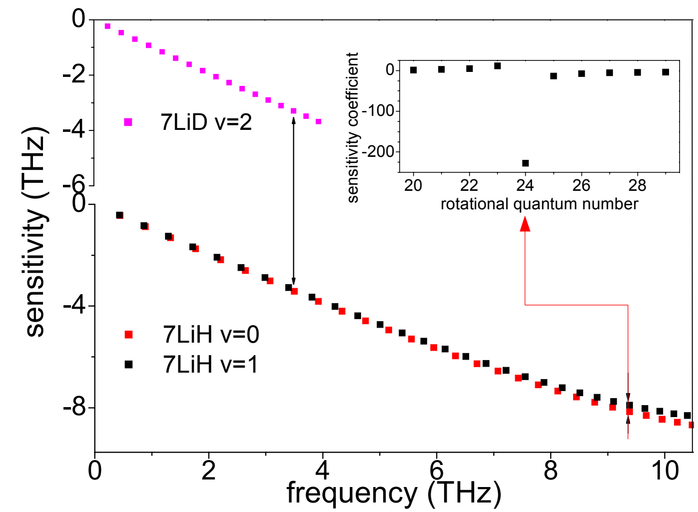
-Dunham expansion model of isotopic LiH, CO energy levels

-Calculations of the sensitivities of rotational transitions

-Interest for near-resonant transitions in the LiH spectra

rotational intervals / isotopic effect, rovibrational interactions

-Frequency splittings with sensitivity coefficients at $\pm 10^2$ level



Constraint on $\Delta\mu/\mu$ from the microwave spectra of B0218+357

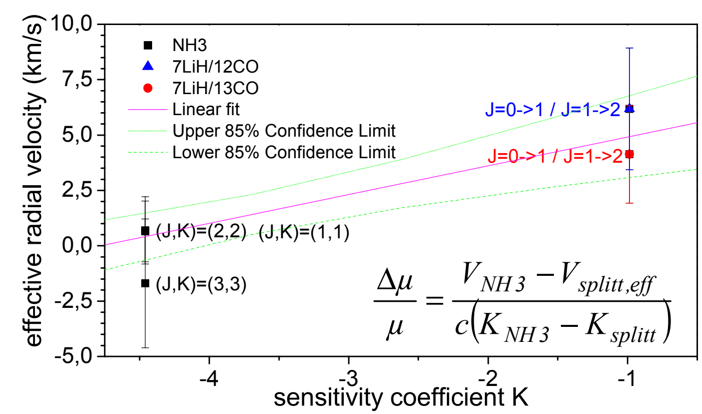
-Comparison between $^{14}NH_3$ inversion lines (J,K)=(1,1),(2,2),(3,3) [1] with frequency intervals between rotational lines J=0->1 of ^{7}LiH [2] and respectively J=1->2 of $^{12}C^{16}O$ or $^{13}C^{16}O$ [3].

-Effective radial velocity for a frequency interval

$$V_{splitt,eff} = \left(f_{LiH} V_{LiH} - f_{CO} V_{CO}\right) / \left(f_{LiH} - f_{CO}\right)$$

-Constraint based on the unweighted average of V_{NH3}-$V_{splitt,eff}$

$\Delta\mu/\mu = (5.06 \pm 3.67) \times 10^{-6}$ at z=0.68466 (6.4 Gyr look-back time)



References

[1] C. Henkel *et al*, A&A 440, 893 (2005)

[2] D. N. Friedel *et al*, Astrophys. J. 738, 37 (2011).

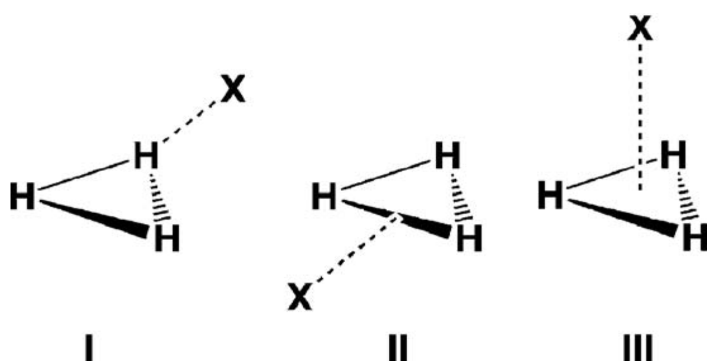
[3] spectra provided by F. Combes; T. Wiklind and F. Combes, A&A 299, 382 (1995).

Formation of cationic hydrides of noble gases in the protosolar nebula

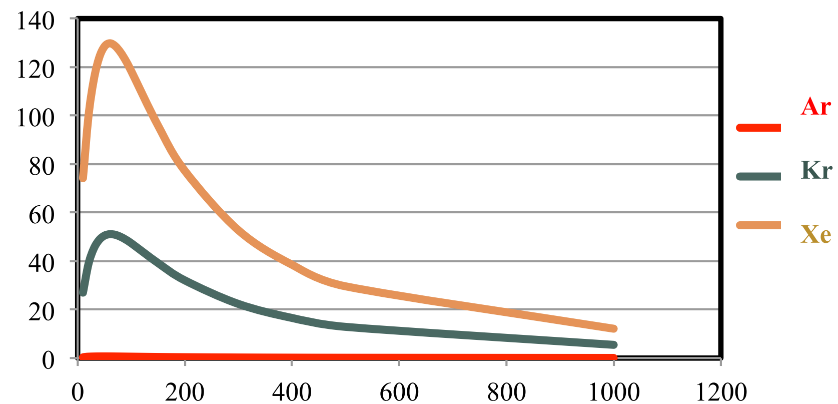
O. Ozgurel, E. Zicler, F. Pauzat, Y. Ellinger, M-C. Bacchus-Montabonel

- Non observation of HeH^+ in ISM → Small HeH_n^+ clusters as a proper target?
- Deficiency of noble gases (Ar, Kr , Xe) in Titan's atmosphere → Were the buildings blocks already poor in noble gases ?

$$H_3^+ + X \rightarrow XH_3^+$$

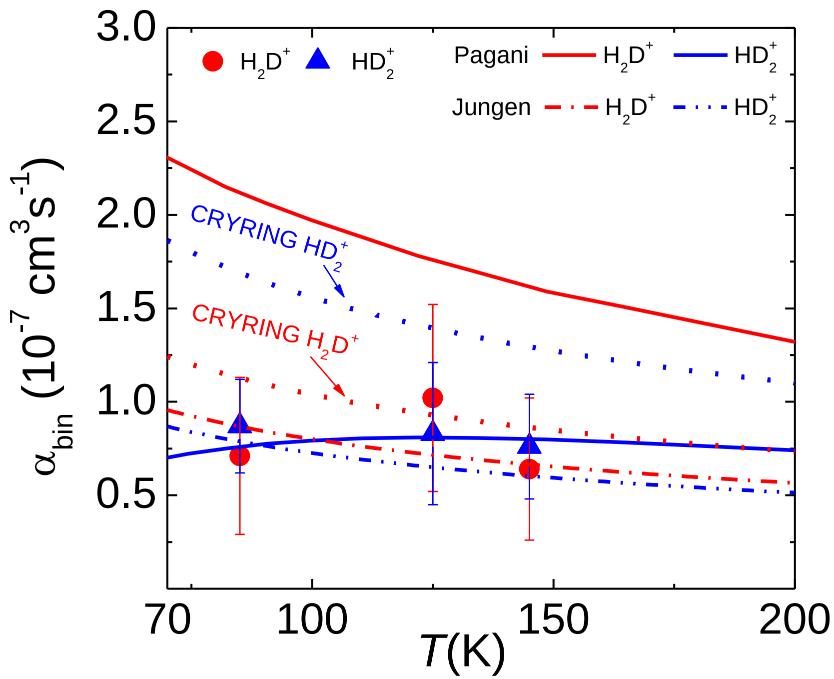


Stationary points on the XH_3^+ potential energy surface



The rate constant for the radiative association ($X + H_3^+$) as a function of the temperature

Temperature dependence of H_2D^+ and HD_2^+ recombination with electrons



Overtone spectroscopy of N_2H^+ ($2v_1$ band)

J	v_{calc} (cm^{-1})	v_{exp} (cm^{-1})	v_{exp} - v_{calc} (cm^{-1})
4	6320.6316	6320.6312	-0.0004
5	6317.2686	6317.2683	-0.0003
6	6313.8549	6313.8550	0.0001
7	6310.3904	6310.3900	-0.0004
8	6306.8753	6306.8752	-0.0001
9	6303.3096	6303.3099	0.0003
10	6299.6935	6299.6940	0.0005
11	6296.0269	6296.0280	0.0011

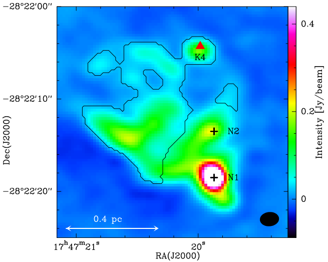
Small-scale physical and chemical structure of diffuse molecular clouds along the line of sight of Sgr B2

Max-Planck-Institut für Radioastronomie

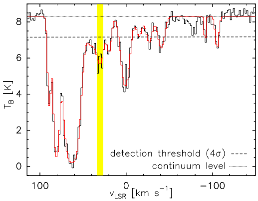
V. Thiel, A. Belloche, K. M. Menten (MPIfR)

IMPRS astronomy & astrophysics Bonn and Cologne

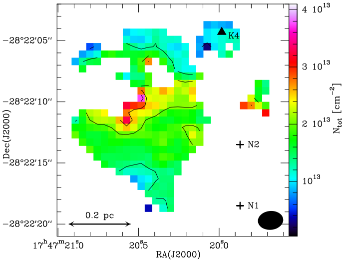
c-C_3H_2 in absorption along the line of sight to Sgr B2 as probed with ALMA



continuum map at 85 GHz, black contour: region selected for analysis



spectrum towards K4



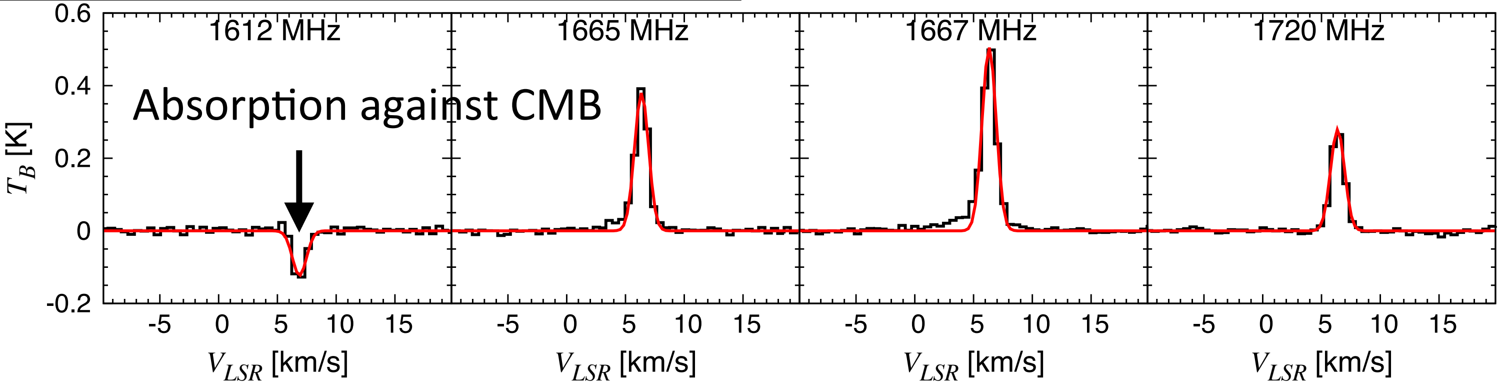
c-C_3H_2 column density map integrated from 27.0 to 33.9 km s^{-1} (yellow range in spectrum)

#9

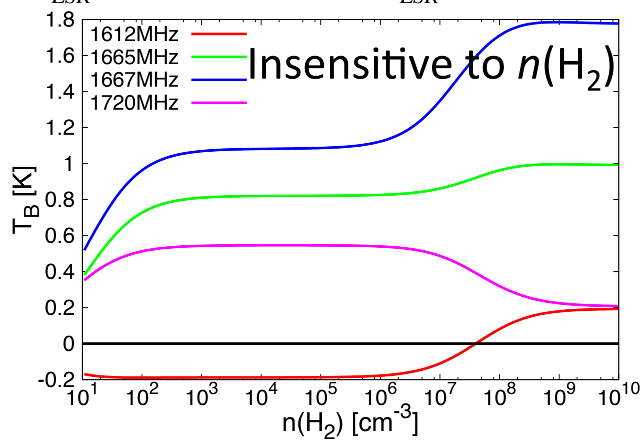
Exploring Molecular-Cloud Formation with OH 18 cm Transition

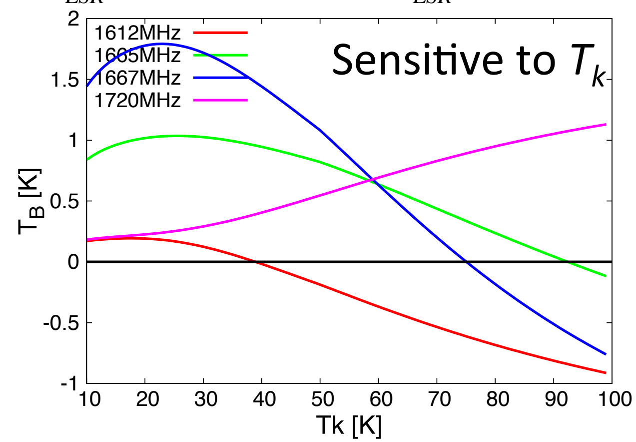
Y. Ebisawa, H. Inokuma, Y. Watanabe (University of Tokyo), N. Sakai (RIKEN)
H. Maezawa (Osaka Prefecture University),K. M. Menten (MPIfR), S. Yamamoto (University of Tokyo)

Observed spectra toward HCL2 East



Model





fitting → T_k = 60 ± 3 K, N(OH) = (4.4 ± 0.3) x 10^{14} cm^{-2}, o/p of H_2 = 3.5 ± 0.9

OH 18 cm transition as a thermometer for warm molecular cloud over wide range of H_2 density (10^2 - 10^6 cm^{-3})

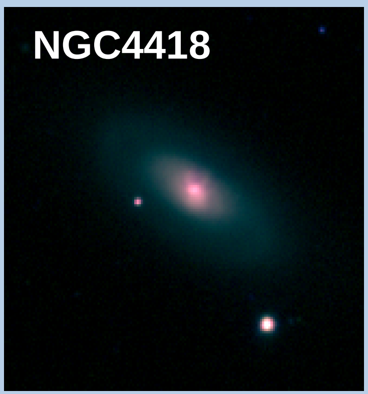
Extragalactic molecular complexity
Multi-band ALMA observations in obscured AGN

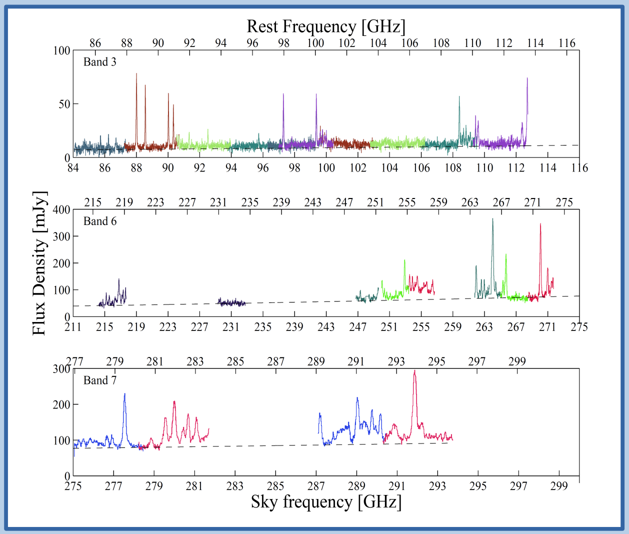
Francesco Costagliola

K. Sakamoto, S. Muller, S. Martín, S. Aalto, N. Harada, P. van der Werf, S. Viti, S. García-Burillo

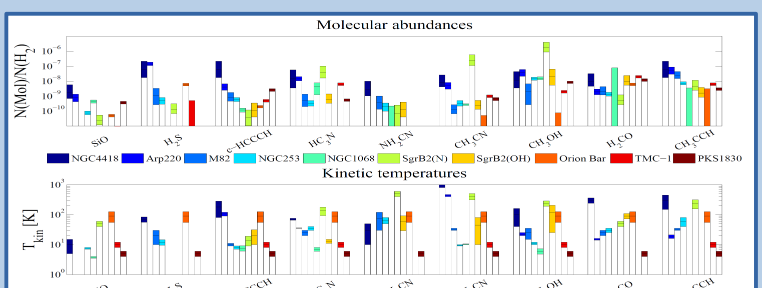
The circum-nuclear regions of obscured AGN combine large molecular columns with intense infrared, ultra-violet, and X radiation and represent ideal laboratories for the study of the chemistry of the interstellar medium under extreme conditions.

ALMA multi-band spectral scan of NGC4418

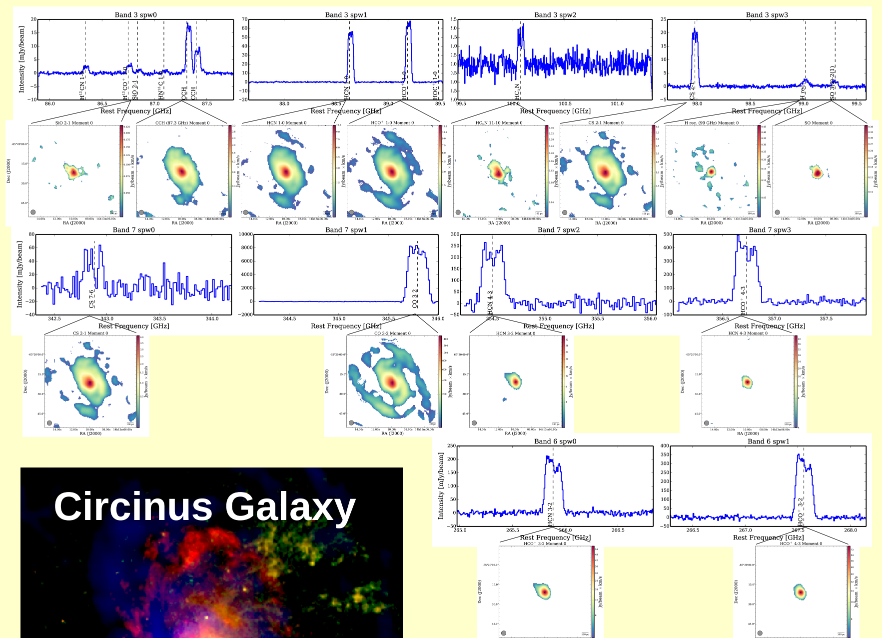


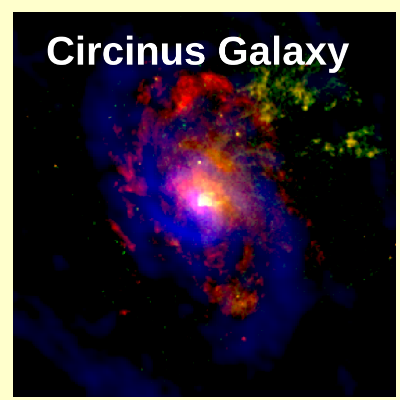


- **> 300 lines**
- **45 molecules**
- **U-lines !**



Spatially resolved chemistry in Circinus





- **Multi-band, beam matched obs at 40 pc resolution**
- **Spatially resolved excitation and abundance**

Costagliola et al., 2015 ; Costagliola et al., in prep.

Extragalactic molecular complexity
Multi-band ALMA observations in obscured AGN

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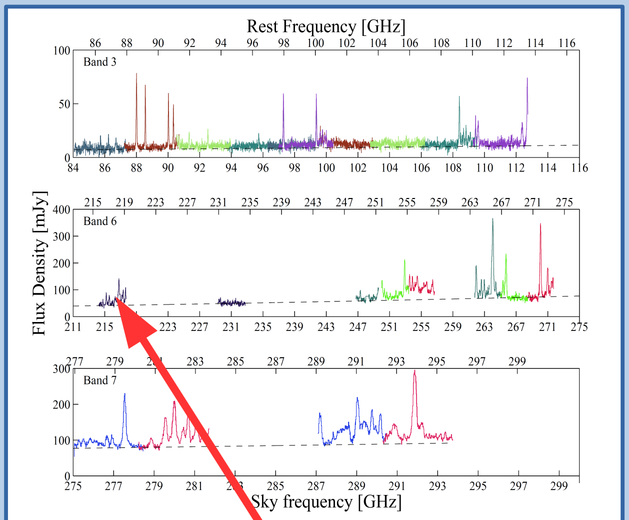

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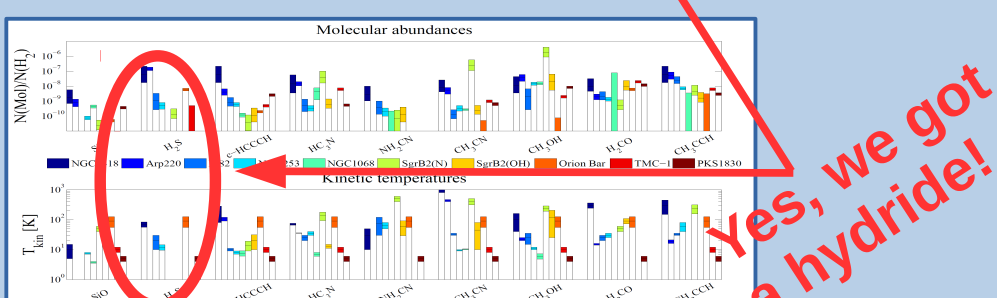

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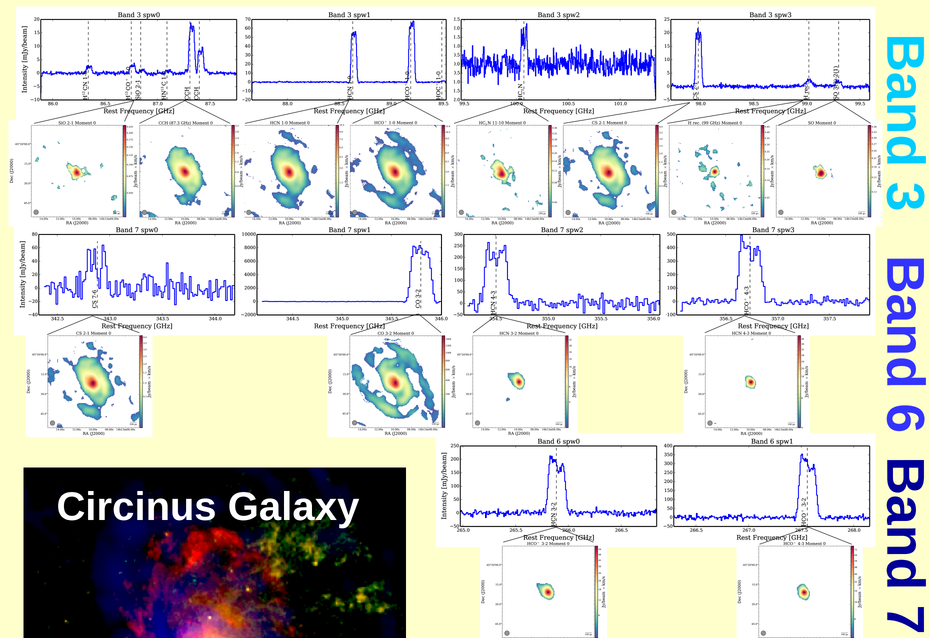

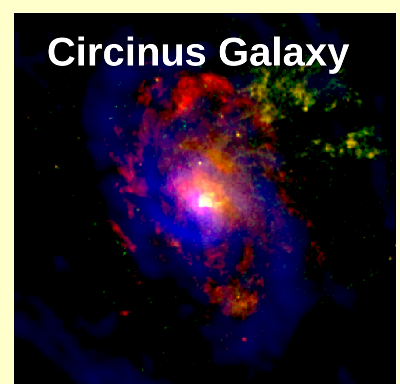

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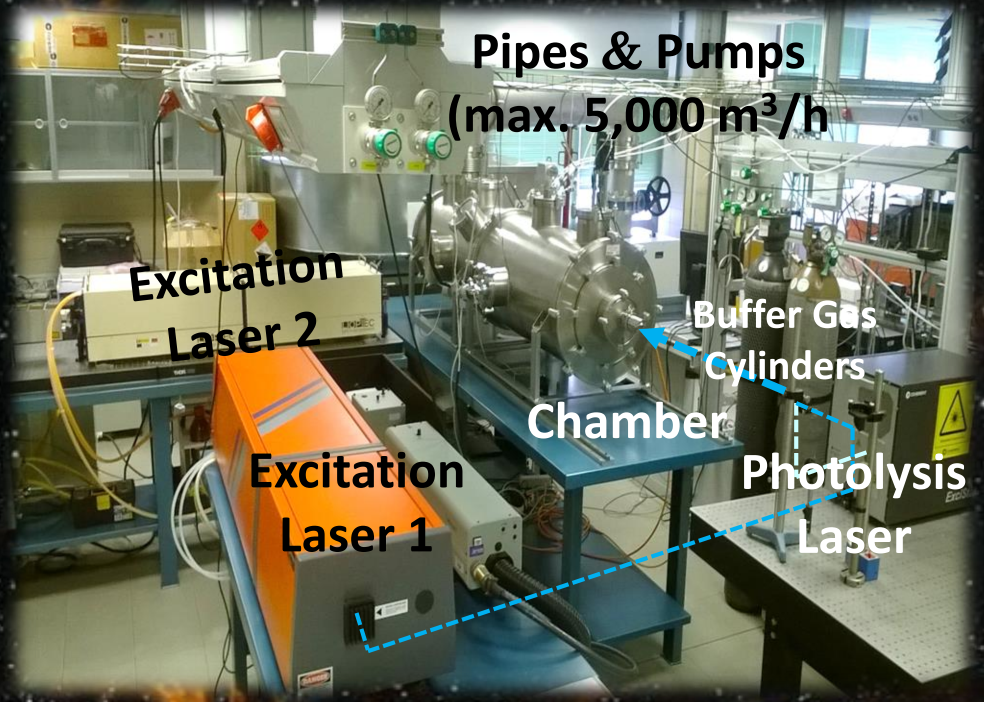
CHALMERS

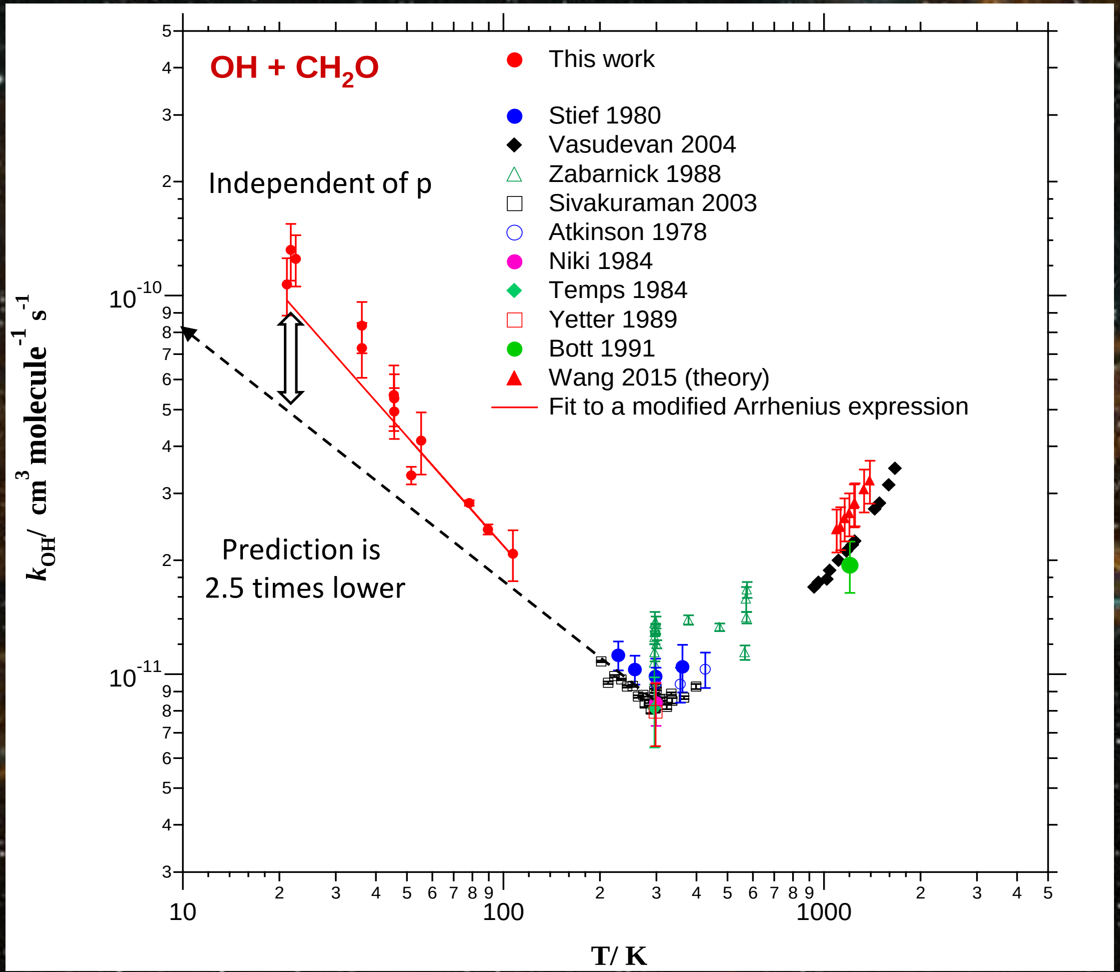
Costagliola et al., 2015 ; Costagliola et al., in prep.

Chemistry of Hydroxyl (OH) Radicals in the ISM Molecular Clouds: Gas-phase Reaction with H_2CO between 22 and 107 K



CRESU

French acronym for *Cinétique de Réaction en Ecoulement Supersonique Uniforme* or *Reaction Kinetics in a Uniform Supersonic Flow*



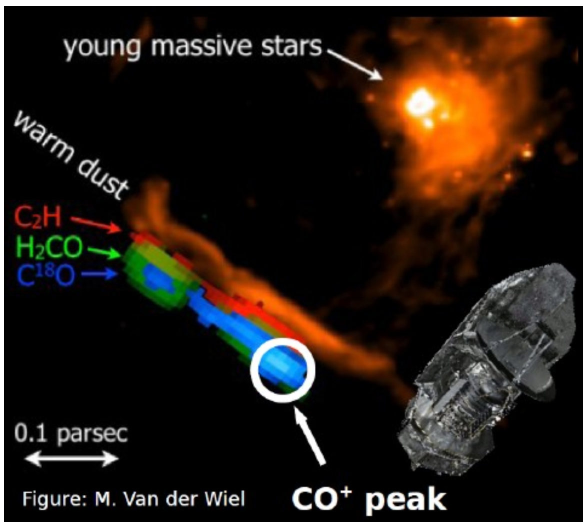
Herschel /HIFI spectral line survey of the Orion Bar

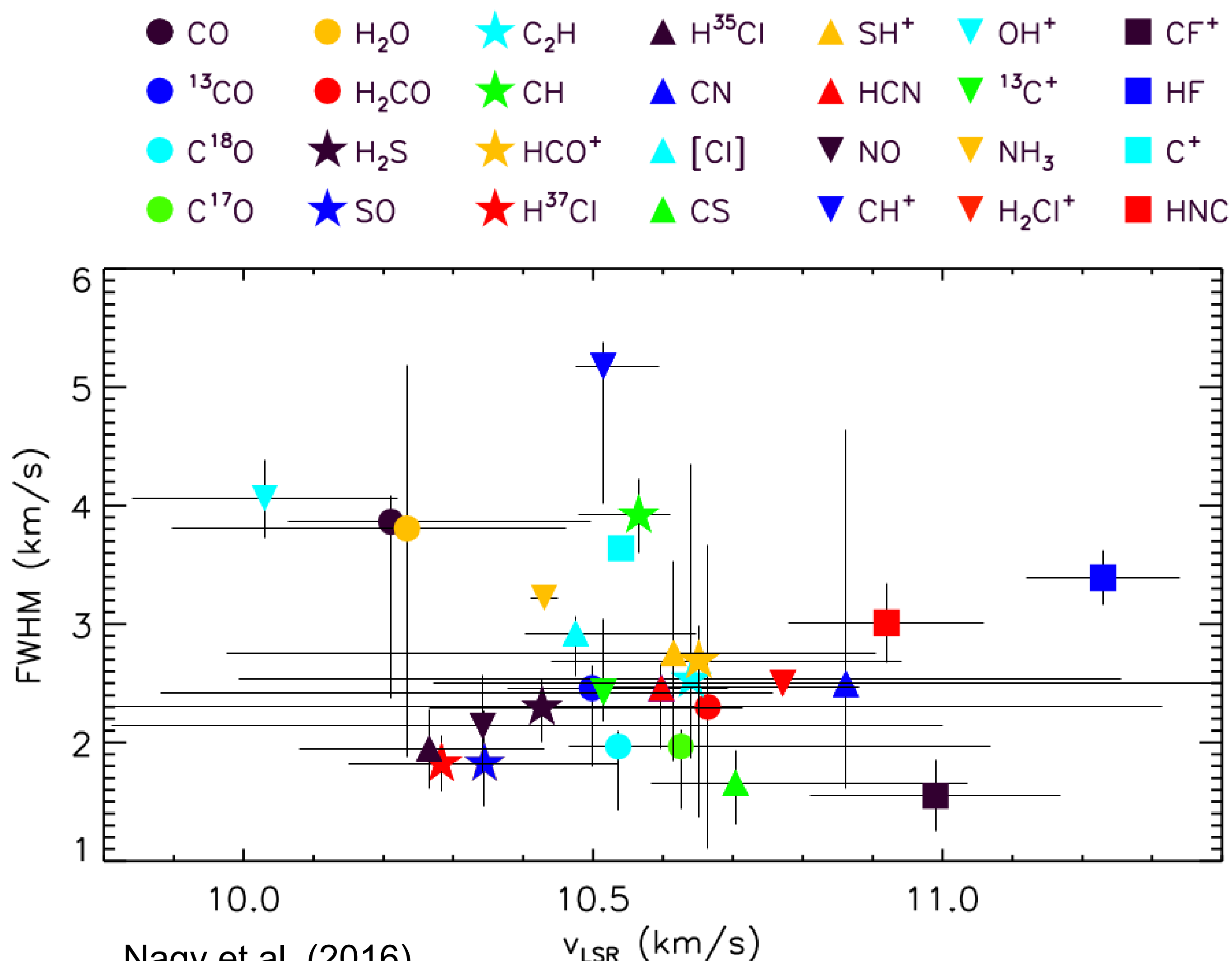
Temperature and density differentiation near the PDR surface

Z. Nagy[1,2], Y. Choi[3,4], V. Ossenkopf-Okada[2], F.F.S. van der Tak[4], E. A. Bergin[5], M. Gerin[6], C. Joblin[7], M. Röllig[2], R. Simon[2], J. Stutzki[2]

[1]University of Toledo, [2]University of Cologne, [3]Kyung Hee University, [4]University of Groningen & SRON, [5]University of Michigan, [6]LERMA, Observatoire de Paris and ENS, [7]Université de Toulouse

HIFI spectral scan in the Orion Bar

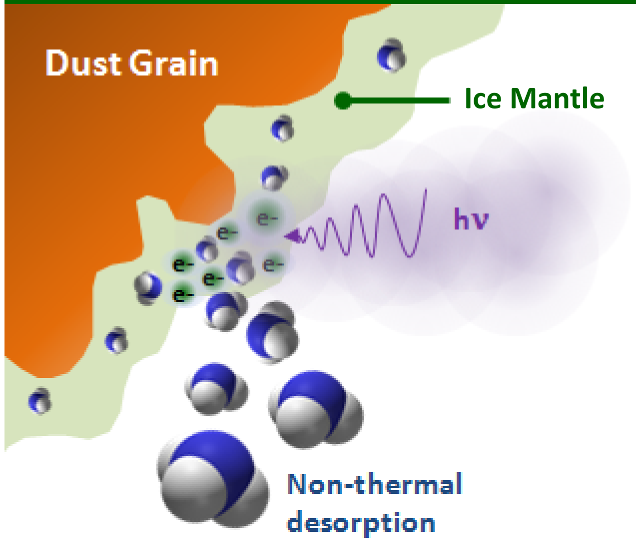


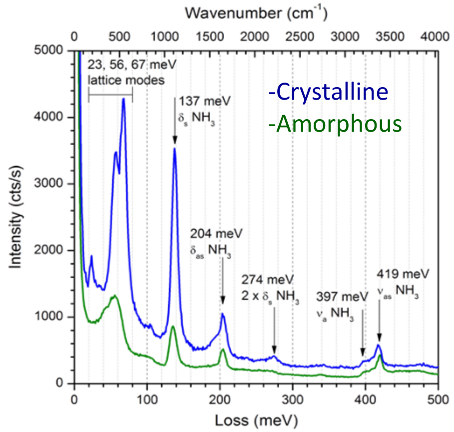


Nagy et al. (2016)

Low energy electron induced processes in pure ammonia ice

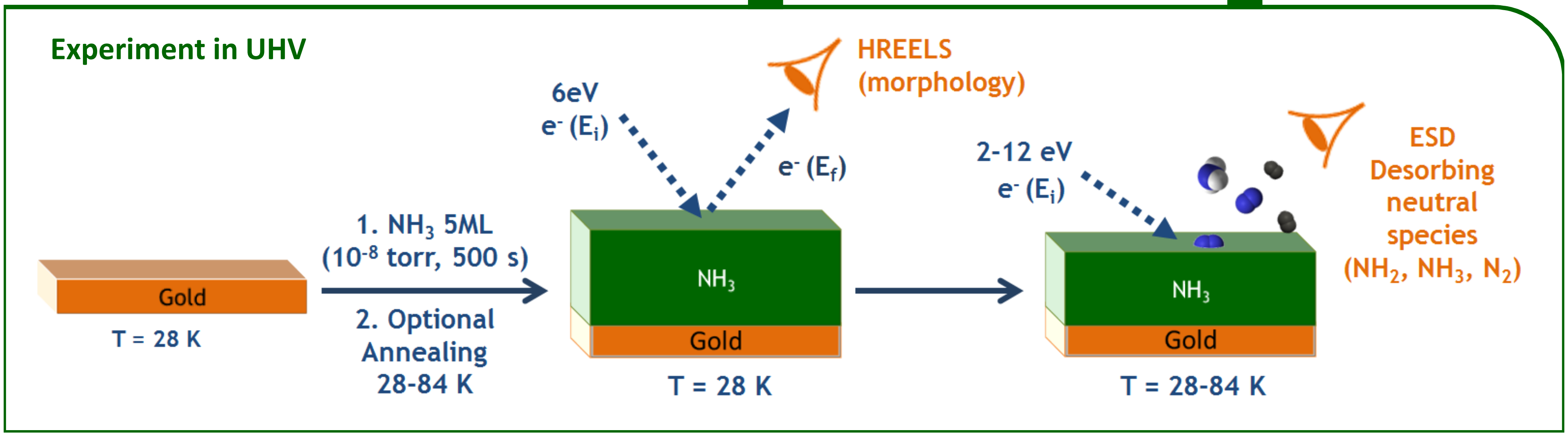
Leo Albert Sala, Lionel Amiaud, Céline Dablemont, Anne Lafosse





Control of Ice Morphology

Desorption of N_2, NH_2, and NH_3



Scaling the Collisional Rate Coefficients of C_6H^-

Kyle M. Walker

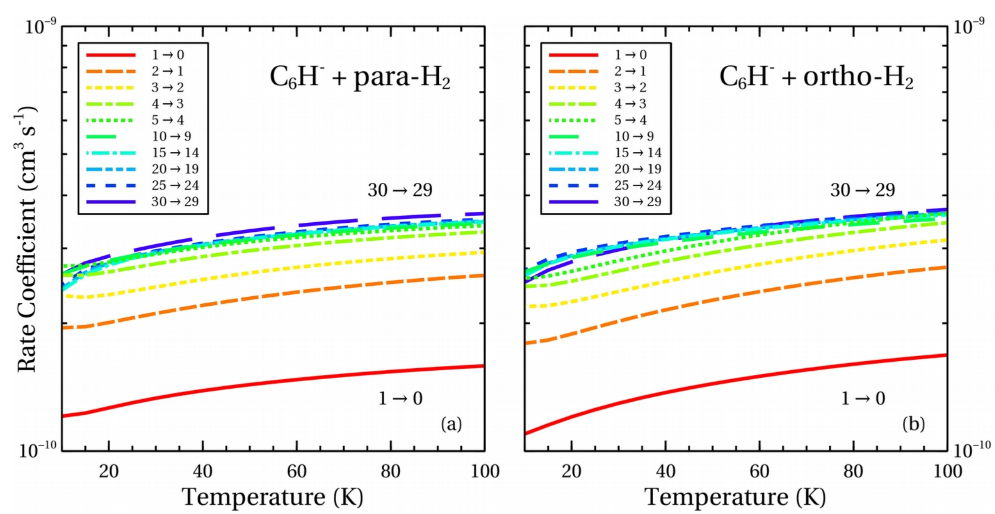
LOMC UMR 6294, CNRS - Universite du Havre, France

Fabien Dumouchel, François Lique, Richard Dawes

- Anions in the ISM: molecular clouds, circumstellar envelopes
- Collisional rate coefficients needed to model non-thermal emission
- C_6H^- potential energy surface & scattering calculations
- Use hydride relationship to scale anion rate coefficients

HF ➡ HCl

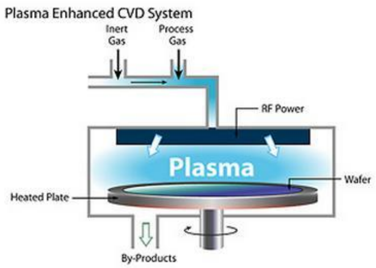
C_6H^- ➡ C_xH^-



Theoretical ab-initio calculations of photoabsorption spectra of XH_2^+ (X= C, O, Si) molecular ions: comparison with experimental data

Alessandra Puglisi[1], Nicolas Sisourat[1], Jean-Paul Mosnier[2], Eugene T. Kennedy[2], Paul van Kampen[2], Denis Cubaynes[3,4], Ségolène Guilbaud[3], Jean-Marc Bizau[3,4], Stéphane Carniato[1]

1. Sorbonne Universités, UPMC Univ. Paris 06, CNRS, Laboratoire de Chimie Physique Matière et Rayonnement, F-75005, Paris,France
2. National Centre of Plasma Science and Technology, School of Physical Sciences, Dublin City University, Glasnevin, Dublin 9, Ireland
3. Institut des Sciences Moléculaires d'Orsay, CNRS, Université Paris-Sud and Université Paris-Saclay, F-91405 Orsay, France
4.Synchrotron SOLEIL, L'Orme des Merisiers, Saint-Aubin, BP 48, F-91192 Gif-sur-Yvette Cedex, France



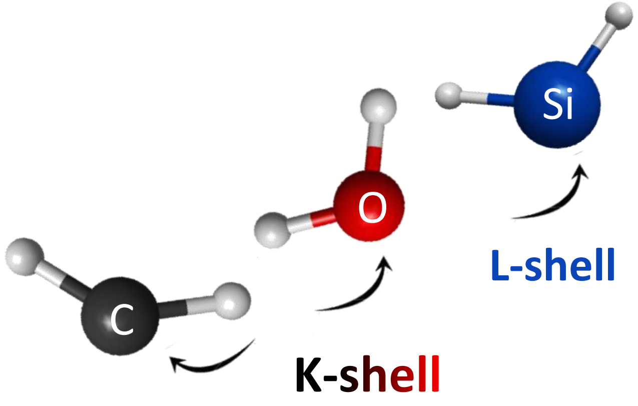
X-Ray spectroscopy provides a powerful tool to study *astrophysical* and *laboratory* plasma

Synchrotron facilities and theoretical/computational approaches are developed to probe the chemical composition of the plasma

Centaure A view par *Chandra*
Source:

Most results have already been obtained on ***atomic ions*** and ***molecules***

Hydride Molecular ions



Hydride Toolbox conference
12-15 December 2016
Paris