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"Interstellar hydrides with Herschel: from the 20th to the 21th century"

# Designing the mission : spectroscopy



 T.G. Phillips in ESA, From Ground-Based to Space-Borne Sub-mm Astronomy p 221-228 (SEE N91-21986 13-89)

Figure 3. The anticipated spectrum of a 30K, dense interstellar cloud, showing the dust spectrum, heavy and light molecule rotation spectra and atomic fine-structure lines. Fine structure lines : ISO & KAO before Herschel & SOFIA

KAO : DR21





- KAO : [OI] in DR21 (*Poglitsch et al. 1997*)
- ISO : SgrB2, W49 at "high" spectral resolution (FP) (Vastel et al. 2000, Lis et al. 2001) :

 Detection of absorption in [CII] and [OI] 63µm

 Limited velocity resolution → Difficulty in determining the opacity and for disentangling narrow and features ISO : SgrB2



#### [CII] with HIFI & PACS towards W49N



- HIFI : Load chop observations with "ref" position 1.5° OFF the Galactic plane
- PACS : Chopped with 6' OFF. Correction for OFF contamination
- Complex line profiles with prominent absorption from foreground gas
- PACS with low spectral resolution : absorption in the central pixel → can contribute to the [CII] deficit ?

## Determination of the diffuse gas pressure distribution



From FUV : Jenkins & Tripp 2011

From FIR with Herschel : Gerin+2015, Velusamy+2017



Median pressure : log(p) = 3.58 + - 0.175p ~ nT ~ 3800 Kcm<sup>-3</sup> within a factor 1.5 Variation of pressure with Galactic radius : 6900 Kcm<sup>-3</sup> At the mean Galactic radius of 5 kpc Good agreement for the same sources

#### N<sup>+</sup> absorption as a tracer of the WIM



 $N(N^{+}) \simeq 1.5 \ 10^{17} \ cm^{-2} - N(C^{+})/N(N^{+}) \simeq 40$ 

Diffuse ionized gas with n(H<sup>+</sup>) ~ 0.1 – 0.3 cm<sup>-3</sup> and T ~ 8 000 K  $\rightarrow$  Warm Ionized Medium (WIM) C/N ~ 3 – 4 ;  $\rightarrow$  about 10% of the C<sup>+</sup> absorption is associated with the WIM

#### GOT C+ [CII] Distribution in the Milky Way



Goldsmith, Langer, Pineda, Velusamy+

# The CNM/WNM fraction from Herschel GotC+ survey



Pineda, Langer, Velusamy, and Goldsmith: A Herschel [Cu] Galactic Plane Survey

[CII] fine structure line at 158  $\mu m$  is the main coolant of the CNM. The Comparison of HI and [CII] emission enables the separation of the CNM and WNM



#### Pineda+2018 [CII] in M51





Large scale [CII] maps : Star formation rate Feedback effect from massive stars Pabst+2019 [CII] in Orion / L1630

## Preparation for Herschel/HIFI observations : molecules

- 1/ Choosing the species :
- Hydrides from the main elements (C, N, O)
- Hydrides with specific properties (F, Cl)

#### 2/ Choose the targets :

- Use SWAS & ODIN + VLA subset of strong FIR sources with known foreground absorption

#### 3/ Define the observations :

- Expected abundances from models ?
- Constant sensititivity : S/N = 100 on continuum
- Frequencies & line strengths ? Ask spectroscopists



Figure 4.1 "The Astronomer's Periodic Table".

The Astronomer's Periodic Table ; B. Mc Call

#### Table 1 Main astrophysical hydrides<sup>a)</sup>

Formula	Name	Spectral domain <sup>b)</sup>	Ref.	
H <sub>2</sub>	Molecular Hydrogen	UV-Visible, IR, FIR	Carruthers (1970b)	
$H_3^+$	Protonated molecular hydrogen	IR	Geballe & Oka (1996)	
CH	Methylidyne	UV-Visible, (sub)mm, cm	Swings & Rosenfeld (1937)	
CH <sub>2</sub>	Methylene	FIR, (sub)mm	Hollis, Jewell & Lovas (1995)	
CH <sub>3</sub>	Methyl	IR	Feuchtgruber et al. (2000)	
CH <sub>4</sub>	Methane	IR	Lacy et al. (1991)	
$CH^+$	Methylidynium	UV-Visible, FIR, (sub)mm	Douglas & Herzberg (1941)	
$CH_3^+$	Methylium	IR, (sub)mm	Roueff et al. (2013) <sup>c</sup>	
NH	Imidogen	UV-Visible, (sub)mm	Meyer & Roth (1991)	
NH <sub>2</sub>	Amidogen	(sub)mm	van Dishoeck et al. (1993)	
NH <sub>3</sub>	Ammonia	(sub)mm, cm	Cheung et al. (1968)	
$NH_4^+$	Ammonium	(sub)mm	Cernicharo et al. (2013) <sup>d)</sup>	
OH	Hydroxyl radical	UV-Visible, FIR, cm	Weinreb et al. (1963)	
$H_2O$	Water	FIR, (sub)mm, cm	Cheung et al. (1969)	
$OH^+$	Hydroxylium	UV-Visible, (sub)mm	Wyrowski et al. (2010)	
$H_2O^+$	Oxidaniumyl	UV-Visible, (sub)mm	Ossenkopf et al. (2010)	
$H_3O^+$	Hydronium	FIR, (sub)mm	Phillips, van Dishoeck & Keene (1992)	
HF	Hydrogen fluoride	FIR	Neufeld et al. (1997)	
SH	Mercapto radical	UV-visible, FIR	Neufeld et al. (2012)	
$H_2S$	Hydrogen sulfide	(sub)mm	Thaddeus et al. (1972)	
SH <sup>+</sup>	Sulfanylium	(sub)mm	Benz et al. (2010); Menten et al. (2011)	
HCl	Hydrogen chloride	UV-visible, (sub)mm	Blake, Keene & Phillips (1985)	
HCl <sup>+</sup>	Chloroniumyl	FIR	De Luca et al. (2012)	
$H_2Cl^+$	Chloronium	(sub)mm	Lis et al. (2010a)	
ArH <sup>+</sup>	Argonium	(sub)mm	Barlow et al. (2013)	

<sup>a)</sup>Adapted from The Astrochymist (www.astrochymist.org); <sup>b)</sup> The corresponding wavelength ranges are : UV-Visible 100 – 1000nm, IR :  $1 - 20 \ \mu m$ , FIR 20 – 300  $\mu m$ ; (sub)mm 0.3 – 4 mm; cm 1 - 20 cm; <sup>c)</sup> A tentative detection of the isotopologue CH<sub>2</sub>D<sup>+</sup> is reported; <sup>d)</sup> The detection of the isotopologue NH<sub>3</sub>D<sup>+</sup> is reported.

Element	Ionization Potential	Endothermicity (Kelvin equivalent = $\Delta E/k_B$ ) for			Driver
	(eV)	$X + H_2 \rightarrow XH + H$	$X^+ + H_2 \rightarrow XH^+ + H$	$X + H_3^+ \rightarrow XH^+ + H_2$	
Не	24.587	No reaction	Exothermic, but primary channel is to He + H + H <sup>+</sup>	29000	
С	11.260	11000	4300 🗹		Warm gas
N	14.534	15000	230	10000	Cosmic rays
0	13.618	920 🗹	V	$\checkmark$	Warm gas or cosmic rays
F	17.423	$\checkmark$		10000	None needed
Ne	21.564	No reaction	Exothermic, but primary channel is to Ne + H + H <sup>+</sup>	27000	
Si	8.152	17000	15000		Warm gas
Р	10.487	19000	13000		Warm gas
S	10.360	10000	10000 🗹		Warm gas
Cl	12.968	515			UV with hv > 12.97 eV
Ar	15.760	No reaction		6400	Cosmic rays

Gerin, Neufeld & Goicoechea ARAA 2016







SOFIA new detection

Other telescopes *No detection yet* 

**ALMA** 

Warm And Dense ISM

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HeH<sup>+</sup>
He
                                                           CH, <sup>13</sup>CH, CH<sup>+</sup>, <sup>13</sup>CH<sup>+</sup>, CH<sub>2</sub>, CH<sub>3</sub>, CH<sub>3</sub><sup>+</sup>, CH<sub>2</sub>D<sup>+</sup>, CH<sub>4</sub>, C, C<sup>+</sup>
NH, <sup>15</sup>NH NH<sub>2</sub>, NH<sub>3</sub> (o & p), <sup>15</sup>NH<sub>3</sub>, ND, NH<sub>2</sub>D, ND<sub>2</sub>H, ND<sub>3</sub>, NH<sub>3</sub>D<sup>+</sup>, NH<sup>+</sup>, N<sup>+</sup>
OH<sup>+</sup>, H<sub>2</sub>O<sup>'+</sup> (o & p), H<sub>3</sub>O<sup>+</sup>, H<sub>2</sub>O (o & p), H<sub>2</sub><sup>18</sup>O, HDO, D<sub>2</sub>O, OD
С
Ν
0
 F
                                                            HF, DF
C
                                                            HCl, HCl<sup>+</sup>, H<sub>2</sub>Cl<sup>+</sup>
                                                            SH, H_2S, SH^+
S
Ar
                                                            ArH<sup>+</sup>
                                                                                                                                                                                                                              ISO
                                                                                                                                                                                                                              Herschel new detection
                                                                                                                                                                                                                              Herschel observations
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#### Molecular absorption profiles : from SWAS & ODIN to Herschel & SOFIA



*Plume+ 2004* 



*Gerin,Neufeld, Goicoechea ARAA 2016* 

## PCA analysis of hydride absorption spectra



Separation of different families :

- "HI" : ions like CH<sup>+</sup>, OH<sup>+</sup> &  $H_2O^{+}$  Gas with a low fraction of hydrogen in  $H_2$
- CH & H<sub>2</sub>O for diffuse molecular gas : trace the H<sub>2</sub> column density
- H<sub>2</sub>S & NH<sub>3</sub> molecular gas with lower filling factor (higher density). Similar behavior as CN & HNC

Gerin, Neufeld & Goicoechea 2016 ARAA

# Tracing the H<sub>2</sub> fraction

Local value  $f(H_2) = 2n(H_2)/(n(HI)+2n(H_2))$   $\not\equiv$ Integrated value  $f(H_2) = 2N(H_2)/(N(HI)+2N(H_2))$ 

- Global tracers = molecules with a nearly constant abundance relative to H<sub>2</sub> (well mixed) : CH, HF, OH, H<sub>2</sub>O, HCO<sup>+</sup>, CCH,...
  - Provide the integrated H<sub>2</sub> column along the line of sight for each velocity feature
  - Abundance uncertainty  $\leq$  factor of 2
  - Characteristic scales probed are ~ few pc for local sight-lines, up to ~ 100pc for Galactic Plane sources
  - Averaging effect along the line of sight  $\rightarrow$  better accuracy for long sightlines
- Local H<sub>2</sub> tracers = species with enhanced abundance in a special range of H<sub>2</sub> fraction :
  - molecular ions formed and destroyed by H<sub>2</sub> reach a peak abundance at a given f(H<sub>2</sub>) (which may depend on the conditions) (e.g. OH<sup>+</sup>, H<sub>2</sub>O<sup>+</sup>, ArH<sup>+</sup>)
  - Trace only the gas close to this optimum f(H<sub>2</sub>)
  - The local H<sub>2</sub> fraction may therefore be different from the global value



# CH , HF & $H_2O$

- HF : formed exothermically in the F +  $H_2$ reaction  $\rightarrow$  HF tracks  $H_2$
- CH is shown from observations and models to track  $H_2$  with a. constant abundance CH/ $H_2$ = 3.6 10<sup>-8</sup>

N(HF) / N(CH) ~ 0.4 → HF/H<sub>2</sub>~ 0.6 – 2.4x10<sup>-8</sup> H<sub>2</sub>O/HF ~2 → H2O/H2 ~ 2.5x10<sup>-8</sup>

Consistent with chemical models & direct measurement towards stars

Good understanding of the chemistry Molecular probes of the H/H<sub>2</sub> transition



# Other Molecules tracing H<sub>2</sub>



- Species with strong absorption lines at lower frequencies (~ 100GHz) where the sky is more transparent : HCO<sup>+</sup>, CCH, HOC+, CF+
- Nearly constant abundances over a decade in N(H2) with a real dispersion (0.2 dex or a factor 1.6)
- Includes the regime of CO-dark H2 with N(H2) ~ 5x10<sup>20</sup> cm<sup>-2</sup>
- Choice of species to cover a range in N(H2) : HF is the most sensitive probe in the THz domain HCO<sup>+</sup> is the most sensitive probe in the mm domain HCO<sup>+</sup> n-H O & OH (THz) probe the same range

 $HCO^+$ ,  $p-H_2O$  & OH (THz) probe the same range of  $H_2$  columns

CH & CCH allow to reach higher  $H_2$  columns where  $HCO^+$  is saturated





# Determination of the Cosmic Ray ionization rate



New probes of CRIR ; Higher value in diffuse gas than in dense & cold clouds  $\zeta(H) = (2.3+/-0.6) \times 10^{-16} \text{ s}^{-1} (H_2)$ ;  $\zeta(H)/n_{50} = (4.6+/-0.5) \times 10^{-16} \text{ s}^{-1} (H \text{ clouds})$ 

Neufeld & Wolfire 2017, Le Petit+2016





 $H_3O^+$  absorption in metastable states : Hot  $H_3O^+$  !

Different behavior from other ions & neutrals : Chemical pumping of the metastable stables at the molecule formation & slow relaxation

Lis +2014







- U line in HIFI & PACS spectra → Identified as ArH<sup>+</sup>
- Specific chemistry : ArH<sup>+</sup> abundance maximum when  $f(H_2) \simeq 10^{-4}$  to  $10^{-3}$
- ArH<sup>+</sup> abundance relative to H ~ 10<sup>-10</sup> to 10<sup>-9</sup>
- Now detected at high redshift

Barlow et al. 2013, Schilke et al. 2014

Cl chemistry in the ISM : an illustration of the collaboration between spectroscopy, models & observations



HCl in the ISM discovered in 1985 (Blake et al 1985) Herschel/HIFI discovery of  $H_2Cl^+$  (Lis et al. 2010) and HCl<sup>+</sup> (De Luca et al. 2012).





### Two Reactive ions : CH<sup>+</sup> and SH<sup>+</sup>



Endothermic formation pathway (C<sup>+</sup> + H<sub>2</sub>  $\rightarrow$  CH<sup>+</sup> + H  $\Delta$ E 4300K) : use the energy of ion-neutral velocity drift for enhancing the formation in diffuse gas

Diagnostic of turbulence properties

Godard+2012,2014

#### The surprise of detecting extended CH<sup>+</sup> emission







CH<sup>+</sup> in PDRs : Efficient formation with vibrationally excited H<sub>2</sub> Other possibility : irradiated Shocks

> Agundez+2010, Parikka+2017

25

# Tracers of UV irradiated molecular cloud surfaces



### $CH^+ J=1-0$ emission scales with $G_0$ in OMC-1



# Detecting the full CO spectral line energy distribution



Orion Bar : Good fit with constant pressure PDR model, with detailed accounting of the heating processes

The maximum pressure scales with G0



Joblin+2018

# A new hydride : HeH<sup>+</sup> in NGC 7027

- Evidence for efficient radiative association
- HeH+ is the starting point of chemistry in the Early universe (with a somewhat different chemical network)



 $\mathrm{He}^{+} + \mathrm{H} \rightarrow \mathrm{HeH}^{+} + h\nu$ 

 $\mathrm{HeH}^{+} + e^{-} \rightarrow \mathrm{He} + \mathrm{H}$ 

 $HeH^+ + H \mathop{\rightarrow} H_2^+ + He$ 

Güsten+19

## Hydrides at High redshift : use ALMA & NOEMA



#### Muller+2017, Falgarone+2017

# A lot of Challenges for Models :

- ISM Chemistry : Cl ; C<sup>+</sup>/C/CO transition ; CH<sup>+</sup> & SH<sup>+</sup>
- PDR physics : explaining the CO SLED and the relationship between G0 and Pressure
- Understanding Feedback processes for galaxy evolution
- Understanding the intricacy of ISM phases : toward GUSTO
- Cosmic Rays origin and propagation

# General remarks

- Early preparation :
  - Laboratory work (spectroscopy, molecular processes, dust properties ..
  - Theory (collisional cross sections, reactivity ; ..)
  - Source Models : PDR, MHD, radiative transfer
  - Use archives + ground based observations
- Many surprises :
  - do not trust models at 100%
  - Systematic approach in observations (limit in S/N ; broad spectral coverage) as in guaranteed time allows to open the discovery space
- Legacy for the future : unique wavelength coverage & range of spectral resolution

#### ESA Voyage2050 FIR workshop : Paris June 14th

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