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

Maryvonne Gerin
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: [OI] in DR21 (Poglitsch et al. 1997)
  - Detection of absorption in [CII] and [OI] 63µm
  - Limited velocity resolution → Difficulty in determining the opacity and for disentangling narrow and features
[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

Median pressure: \( \log(p) = 3.58 \pm 0.175 \)
\( p \sim n T \sim 3800 \text{ Kcm}^{-3} \)
within a factor 1.5

Variation of pressure with Galactic radius: 6900 Kcm\(^{-3}\)
At the mean Galactic radius of 5 kpc
Good agreement for the same sources
N⁺ absorption as a tracer of the WIM

$N(N^+) \sim 1.5 \times 10^{17} \text{ cm}^{-2}$, $N(C^+)/N(N^+) \sim 40$

Diffuse ionized gas with $n(H^+) \sim 0.1 - 0.3 \text{ cm}^{-3}$ and $T \sim 8000 \text{ K}$ → Warm Ionized Medium (WIM)

$C/N \sim 3 - 4$; → about 10% of the $C^+$ absorption is associated with the WIM

Persson+ 2014
GOT C+ [CII] Distribution in the Milky Way

Goldsmith, Langer, Pineda, Velusamy+
The CNM/WNM fraction from Herschel GotC+ survey

[CII] fine structure line at 158 µm 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

Pabst+2019
[CII] in Orion / L1630

Large scale [CII] maps:
Star formation rate
Feedback effect from massive stars
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 sensitivity**: $S/N = 100$ on continuum
- Frequencies & line strengths? Ask spectroscopists
### Table 1  Main astrophysical hydrides

<table>
<thead>
<tr>
<th>Formula</th>
<th>Name</th>
<th>Spectral domain</th>
<th>Ref.</th>
</tr>
</thead>
<tbody>
<tr>
<td>H₂</td>
<td>Molecular Hydrogen</td>
<td>UV-Visible, IR, FIR</td>
<td>Carruthers (1970b)</td>
</tr>
<tr>
<td>H₃⁺</td>
<td>Protonated molecular hydrogen</td>
<td>IR</td>
<td>Geballe &amp; Oka (1996)</td>
</tr>
<tr>
<td>CH</td>
<td>Methylidyne</td>
<td>UV-Visible, (sub)mm, cm</td>
<td>Swings &amp; Rosenfeld (1937)</td>
</tr>
<tr>
<td>CH₂</td>
<td>Methylene</td>
<td>IR</td>
<td>Holli, Jewell &amp; Lovas (1995)</td>
</tr>
<tr>
<td>CH₃</td>
<td>Methyl</td>
<td>IR</td>
<td>Feuchtgruber et al. (2000)</td>
</tr>
<tr>
<td>CH₄</td>
<td>Methane</td>
<td>IR</td>
<td>Lacy et al. (1991)</td>
</tr>
<tr>
<td>CH⁺⁺</td>
<td>Methyldieny</td>
<td>UV-Visible, FIR, (sub)mm</td>
<td>Douglas &amp; Herzberg (1941)</td>
</tr>
<tr>
<td>CH₃⁺</td>
<td>Methylidium</td>
<td>IR, (sub)mm</td>
<td>Roueff et al. (2013)</td>
</tr>
<tr>
<td>NH</td>
<td>Imidogen</td>
<td>UV-Visible, (sub)mm</td>
<td>Meyer &amp; Roth (1991)</td>
</tr>
<tr>
<td>NH₂⁺</td>
<td>Ammonogen</td>
<td>(sub)mm</td>
<td>van Dishoeck et al. (1993)</td>
</tr>
<tr>
<td>NH₃</td>
<td>Ammonia</td>
<td>(sub)mm, cm</td>
<td>Cheung et al. (1968)</td>
</tr>
<tr>
<td>NH₄⁺</td>
<td>Ammonium</td>
<td>(sub)mm</td>
<td>Cernicharo et al. (2013)</td>
</tr>
<tr>
<td>OH</td>
<td>Hydroxy radical</td>
<td>UV-Visible, FIR, cm</td>
<td>Weinreb et al. (1963)</td>
</tr>
<tr>
<td>H₂O</td>
<td>Water</td>
<td>IR, (sub)mm, cm</td>
<td>Cheung et al. (1969)</td>
</tr>
<tr>
<td>OH⁺⁺</td>
<td>Hydroxyl</td>
<td>UV-Visible, (sub)mm</td>
<td>Wyrowski et al. (2010)</td>
</tr>
<tr>
<td>H₂O⁺⁺</td>
<td>Oxidanium</td>
<td>UV-Visible, (sub)mm</td>
<td>Ossenkop et al. (2010)</td>
</tr>
<tr>
<td>H₂O⁺⁺</td>
<td>Hydronium</td>
<td>FIR, (sub)mm</td>
<td>Phillips, van Dishoeck &amp; Keene (1992)</td>
</tr>
<tr>
<td>HF</td>
<td>Hydrogen fluoride</td>
<td>FIR</td>
<td>Neufeld et al. (1997)</td>
</tr>
<tr>
<td>SH</td>
<td>Mercapto radical</td>
<td>UV-visible, FIR</td>
<td>Neufeld et al. (2012)</td>
</tr>
<tr>
<td>H₂S</td>
<td>Hydrogen sulfide</td>
<td>(sub)mm</td>
<td>Thaddeus et al. (1972)</td>
</tr>
<tr>
<td>SH⁺⁺</td>
<td>Sulfanum</td>
<td>(sub)mm</td>
<td>Benz et al. (2010); Menten et al. (2011)</td>
</tr>
<tr>
<td>HCl</td>
<td>Hydrogen chloride</td>
<td>UV-visible, (sub)mm</td>
<td>Blake, Keene &amp; Phillips (1985)</td>
</tr>
<tr>
<td>HCl⁺⁺</td>
<td>Chloronium</td>
<td>UV-visible, FIR</td>
<td>De Luca et al. (2012)</td>
</tr>
<tr>
<td>H₂Cl⁺⁺</td>
<td>Chloronium</td>
<td>(sub)mm</td>
<td>Lis et al. (2010a)</td>
</tr>
<tr>
<td>ArH⁺⁺</td>
<td>Argonium</td>
<td>(sub)mm</td>
<td>Barlow et al. (2013)</td>
</tr>
</tbody>
</table>

*Adapted from The Astrochymist (www.astrochymist.org); b) The corresponding wavelength ranges are: UV-Visible 100 – 1000 nm, IR: 1 – 20 μm, FIR 20 – 300 μm; (sub)mm 0.3 – 4 mm; cm 1 – 20 cm; c) A tentative detection of the isotopologue CH₂D⁺ is reported; d) The detection of the isotopologue NH₂D⁺ is reported.*
<table>
<thead>
<tr>
<th>Element</th>
<th>Ionization Potential (eV)</th>
<th>Endothermicity (Kelvin equivalent $= \Delta E/k_B$) for</th>
<th>Driver</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>$X + H_2 \rightarrow XH + H$</td>
<td>$X^+ + H_2 \rightarrow XH^+ + H$</td>
<td>$X + H_3^+ \rightarrow XH^+ + H_2$</td>
</tr>
<tr>
<td>He</td>
<td>24.587</td>
<td>No reaction</td>
<td>29000</td>
</tr>
<tr>
<td>C</td>
<td>11.260</td>
<td>11k00</td>
<td>Exothermic, but primary channel is to He + H + H$^+$</td>
</tr>
<tr>
<td>N</td>
<td>14.534</td>
<td>15k00</td>
<td>230</td>
</tr>
<tr>
<td>O</td>
<td>13.618</td>
<td>9k20</td>
<td>4300</td>
</tr>
<tr>
<td>F</td>
<td>17.423</td>
<td></td>
<td>10k00</td>
</tr>
<tr>
<td>Ne</td>
<td>21.564</td>
<td>No reaction</td>
<td>27k00</td>
</tr>
<tr>
<td>Si</td>
<td>8.152</td>
<td>17k00</td>
<td>15k00</td>
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<tr>
<td>P</td>
<td>10.487</td>
<td>19k00</td>
<td>13k00</td>
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<td>S</td>
<td>10.360</td>
<td>10k00</td>
<td>10k00</td>
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<tr>
<td>Cl</td>
<td>12.968</td>
<td>515</td>
<td></td>
</tr>
<tr>
<td>Ar</td>
<td>15.760</td>
<td>No reaction</td>
<td>6k400</td>
</tr>
</tbody>
</table>

*Gerin, Neufeld & Goicoechea ARAA 2016*
**PRISMAS**
PRobing InterStellar Molecules with Absorption line Studies

**Warm And Dense ISM**
Herschel observations
SOFIA new detection
ALMA
Other telescopes
No detection yet

<table>
<thead>
<tr>
<th>Element</th>
<th>Molecules</th>
</tr>
</thead>
<tbody>
<tr>
<td>He</td>
<td>HeH⁺, (^{13}\text{CH}, \text{CH}^+, \text{CH}_{2}, \text{CH}_3, \text{CH}_2\text{D}^+, \text{CH}_4, \text{C}, \text{C}^+)</td>
</tr>
<tr>
<td>C</td>
<td>(^{15}\text{NH}, \text{NH}_2, \text{NH}_3) (o &amp; p), (^{15}\text{NH}_3, \text{ND}, \text{NH}_2\text{D}, \text{ND}_2\text{H}, \text{ND}_3, \text{NH}_3\text{D}^+, \text{NH}^+, \text{N}^+)</td>
</tr>
<tr>
<td>N</td>
<td>(^{18}\text{O}, \text{HDO}, \text{D}_2\text{O}, \text{OD})</td>
</tr>
<tr>
<td>O</td>
<td>(^{18}\text{O}, \text{HDO}, \text{D}_2\text{O}, \text{OD})</td>
</tr>
<tr>
<td>F</td>
<td>(^{18}\text{O}, \text{HDO}, \text{D}_2\text{O}, \text{OD})</td>
</tr>
<tr>
<td>Cl</td>
<td>(^{18}\text{O}, \text{HDO}, \text{D}_2\text{O}, \text{OD})</td>
</tr>
<tr>
<td>S</td>
<td>(^{18}\text{O}, \text{HDO}, \text{D}_2\text{O}, \text{OD})</td>
</tr>
<tr>
<td>Ar</td>
<td>ArH⁺</td>
</tr>
</tbody>
</table>
Molecular absorption profiles: from SWAS & ODIN to Herschel & SOFIA

Plume+ 2004

W31C

Gerin, Neufeld, Goicoechea
ARAA 2016
PCA analysis of hydride absorption spectra

Separation of different families:
- "HI" : ions like CH⁺, OH⁺ & H₂O⁺. Gas with a low fraction of hydrogen in H₂
- CH & H₂O for diffuse molecular gas: trace the H₂ column density
- H₂S & NH₃ molecular gas with lower filling factor (higher density). Similar behavior as CN & HNC

Gerin, Neufeld & Goicoechea 2016 ARAA
Tracing the H$_2$ fraction

- **Global tracers** = molecules with a nearly constant abundance relative to H$_2$ (well mixed) : CH, HF, OH, H$_2$O, HCO$^+$, CCH,...
  - Provide the integrated H$_2$ column along the line of sight for each velocity feature
  - Abundance uncertainty ≤ 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 → better accuracy for long sightlines

- **Local H$_2$ tracers** = species with enhanced abundance in a special range of H$_2$ fraction :
  - Molecular ions formed and destroyed by H$_2$ reach a peak abundance at a given f(H$_2$) (which may depend on the conditions) (e.g. OH$^+$, H$_2$O$^+$, ArH$^+$)
  - Trace only the gas close to this optimum f(H$_2$)
  - The local H$_2$ fraction may therefore be different from the global value

\[
\text{Local value} \quad f(H_2) = \frac{2n(H_2)}{n(H_1)+2n(H_2)}
\]

\[
\text{Integrated value} \quad f(H_2) = \frac{2N(H_2)}{N(H_1)+2N(H_2)}
\]
CH, HF & H₂O

- HF: formed exothermically in the F + H₂ reaction → HF tracks H₂
- CH is shown from observations and models to track H₂ with a constant abundance CH/H₂ = 3.6 x 10⁻⁸

N(HF) / N(CH) ~ 0.4 → HF/H₂ ~ 0.6 – 2.4 x 10⁻⁸
H₂O/HF ~ 2 → H₂O/H₂ ~ 2.5 x 10⁻⁸

Consistent with chemical models & direct measurement towards stars

Good understanding of the chemistry
Molecular probes of the H/H₂ transition

Other Molecules tracing $\text{H}_2$

- Species with strong absorption lines at lower frequencies ($\sim 100\text{GHz}$) where the sky is more transparent: $\text{HCO}^+$, $\text{CCH}$, $\text{HOC}^+$, $\text{CF}^+$
- Nearly constant abundances over a decade in $N(\text{H}_2)$ with a real dispersion (0.2 dex or a factor 1.6)
- Includes the regime of CO-dark H$_2$ with $N(\text{H}_2) \sim 5 \times 10^{20}$ cm$^{-2}$
- Choice of species to cover a range in $N(\text{H}_2)$:
  - $\text{HF}$ is the most sensitive probe in the THz domain
  - $\text{HCO}^+$ is the most sensitive probe in the mm domain
  - $\text{HCO}^+$, $p$-$\text{H}_2\text{O}$ & OH (THz) probe the same range of $\text{H}_2$ columns
  - $\text{CH}$ & $\text{CCH}$ allow to reach higher $\text{H}_2$ columns where $\text{HCO}^+$ is saturated

$\text{Gerin+2018}$
Determination of the Cosmic Ray ionization rate

Molecular ions formed by CR-induced ionization of

- $\text{H}_2 : \text{H}_3^+$
- $\text{H} : \text{OH}^+, \text{H}_2\text{O}^+, \text{H}_3\text{O}^+$
- $\text{Ar} : \text{ArH}^+$

New probes of CRIR; Higher value in diffuse gas than in dense & cold clouds

$\zeta(\text{H}) = (2.3 +/- 0.6) \times 10^{-16} \text{ s}^{-1} (\text{H}_2)$; $\zeta(\text{H})/n_{50} = (4.6 +/- 0.5) \times 10^{-16} \text{s}^{-1} (\text{H clouds})$

*Neufeld & Wolfire 2017, Le Petit+2016*
The surprise of $\text{H}_3\text{O}^+$

$\text{H}_3\text{O}^+$ absorption in metastable states: Hot $\text{H}_3\text{O}^+$!

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

$L\text{i}s$ $+2014$
The surprise of ArH⁺

• U line in HIFI & PACS spectra → Identified as ArH⁺
• Specific chemistry: ArH⁺ abundance maximum when \( f(\text{H}_2) \sim 10^{-4} \) to \( 10^{-3} \)
• ArH⁺ abundance relative to H ~ \( 10^{-10} \) to \( 10^{-9} \)
• 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 $\text{H}_2\text{Cl}^+$ (Lis et al. 2010) and HCl$^+$ (De Luca et al. 2012).

De Luca+2012
Two Reactive ions: $\text{CH}^+$ and $\text{SH}^+$

Endothermic formation pathway ($\text{C}^+ + \text{H}_2 \rightarrow \text{CH}^+ + \text{H} \Delta E \ 4300\text{K}$): 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$^+$ emission

CH$^+$ in PDRs: Efficient formation with vibrationally excited H$_2$
Other possibility: irradiated Shocks

Agundez+2010,
Parikka+2017
Tracers of UV irradiated molecular cloud surfaces

CH$^+$ and C$^+$ emission show similar spatial distributions.

The reaction with vib excited H$_2$ is efficient at large scales!
CH$^+$ $J=1$-$0$ emission scales with $G_0$ in OMC-1

**Observations**

- Correlation = 0.89

**Isobaric PDR model grid**

- $P_{th}/G_0 = [10^3-10^5]$

- Correlation = 0.94

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**G$_0$ (FUV field)**

**CH$^+$ $J=1$-$0$ (Contours)**

**Meudon PDR code**

**Goicoechea+15,19**

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Author: Goicoechea & Le Bourlot 2007; Bron et al. 2014

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**Top panel**: Predicted gas temperature ($\text{G}_\text{H} = 7.5 \times 10^8 \text{ K cm}^{-3}$, CH$^+$ peak at the edge of the PDR, be-

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**5.1. PDR modeling**

- The CH$^+$ mapped area (isobaric PDR illuminated by the mean FUV radiation flux in the fore the C$^+$ line intensities follow the same spatial distribution.

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**Fig. 8.** Narrow-line CH$^+$ emission is very extended and HCO$^+$ abundances peak at the edge of the PDR, be-

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**Fig. 7.** Only if the gas temperature is higher than the CO $1$ $\to$ $0$ line intensity correlation plots extracted from maps convolved to a uniform angular resolution of 27

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**KS 1–0 line intensity correlation plots**

- Correlation, in logarithmic scale, is $1.4\pm0.1$. This value is $1.0\pm0.1$.

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**Fig. 11.** In this wide parameter space of illumination con-

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**Intensities**

- $v_J^0$ values, the stationary isobaric PDR model does capture

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**J$^J_1–0$ emission scales**

- $G_0 = [10^3-10^5]$

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**PACS we detect CH$^+$ and the CH$^+$ $1–0$ integrated intensity map in black con-

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**Correlation along OMC-1 reflect the tight connection between**

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**Fig. 12.** Data points are $\text{KS}$ $1–0$ line

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**Hill & Hollenbach 1978; Bertoldi 1989; Burton 1990). Only if the gas temperature is**

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**Goicoechea+19, submitted.**

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**Excited shocked gas from BN**

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**Herschel**

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**Strong UV field from the Trapezium stars; and locally by thermally-

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**Herschel**

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**Photoevaporative PDR models (Bron et al. 2018).**
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 $G_0$

_Joblin+2018_
A new hydride: HeH$^+$ 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)

\[
\text{He}^+ + \text{H} \rightarrow \text{HeH}^+ + h\nu
\]

\[
\text{HeH}^+ + e^- \rightarrow \text{He} + \text{H}
\]

\[
\text{HeH}^+ + \text{H} \rightarrow \text{H}_2^+ + \text{He}
\]
Hydrides at High redshift: use ALMA & NOEMA

Muller+2017, Falgarone+2017
A lot of Challenges for Models:

- ISM Chemistry: Cl; C⁺/C/CO transition; CH⁺ & SH⁺
- 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**

*Contact Martina Wiedner (martina.wiedner@obspm.fr) & me*