Chemistry of MOLECULAR IONS in protostellar shocks

Linda Podio
AstroFlt Fellow - Arcetri

B. Lefloch, C. Ceccarelli (IPAG - France), C. Codella (Oss. Arcetri - Italy), R. Bachiller (OAN - Spain)
& the CHESS + ASAI team
Molecular Ions in the ISM

Molecular ions detected in pre-stellar cores, protostars, star forming regions

\[ \text{e.g., HCO}^+, \text{N}_2\text{H}^+, \text{HOCO}^+, \text{SO}^+, \text{HCS}^+ \]


What about shocks ??

HCO$^+$ detected in several outflows

*butterfly morphology $\rightarrow$ outflow cavities*

N$_2$H$^+$ detected only very recently in L1157-B1 (*Yamaguchi*+ 2012, *Codella*+ 2013)

HOCO$^+$ ????


around the low-mass star L1527 (*Sakai*+ 2008)

BUT never detected in a shock !

SO$^+$ ????

detected in translucent and cold clouds, in active sfr (*Turner* 1994, 1996)

shock models predict X(SO$^+$) enhanced by orders of magnitude in shocks

BUT never detected in a shock !

HCS$^+$ only very tentative detection in L1157-B1 (*BPG97*)


*Hogerheijde*+ 1998, *Tafalla*+ 2010

*Tappe*+ 2012

Neufeld & Dalgarno 1989
IRAM-30m – Herschel/HIFI survey of L1157-B1 bow-shock

A census of molecular ions down to a sensitivity of ~1 mk / km/s at 3mm

**IRAM-30m**
- 3 mm (80–116 GHz)
- 2 mm (128–173 GHz)
- 1.3 mm (200–320 GHz)
- 0.8 mm (328–350 GHz)
  - HPBW ~ 7” - 33”

**Herschel/HIFI**
- Band 1 (488–628 GHz)
  - HPBW ~ 39”

**IRAM-30m obs → IRAM Large Program ASAI**  [http://www.oan.es/asai/](http://www.oan.es/asai/)


**B1 bow-shock**

**L1157 outflow**

*Bachiller+ 2001*

*Codella+ 2009*
Molecular ions in L1157-B1 bow-shock

Already reported by BP97
Bachiller+ 2001
Codella+ 2010
Yamahuchi+ 2012

First detection in a shock!!
Codella+ 2013
Podio+ 2014

HCO⁺
H¹³CO⁺
HCS⁺

N₂H⁺
HOCO⁺
SO⁺

Lines are blueshifted: \( |V-V_{sys}| \sim 0.5 - 3 \text{ km/s} \)

Lines are broad: FWHM \sim 3 - 7 \text{ km/s}

→ origin in the shock/outflow cavities
Analysis of line fluxes

with a radiative transfer code in LVG approximation

--- we estimate gas physical conditions & ions fractional abundances

As found for CO lines (*Lefloch+ 2012*) → different velocity components $I(V) = I(0) \exp(- V/V_0)$

- $g_1$: $V_0 = 12.5$ km/s, jet impact region on the cavity (~ 5” – 10”), $T \sim 210$ K
  - $V_0 = 4.4$ km/s, outflow cavity (~ 20”), $T \sim 60 – 80$ K
- $g_2$: $V_0 = 2.5$ km/s, B2 older cavity, $T \sim 35$ K

<table>
<thead>
<tr>
<th>Species</th>
<th>Cmp</th>
<th>$T_{\text{kin}}$ K</th>
<th>$n_{\text{H}_2}$ cm$^{-3}$</th>
<th>$N_{\text{species}}$ cm$^{-2}$</th>
<th>$X = N_{\text{species}}/N_{\text{H}_2}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>CO$^a$</td>
<td>$g_1$</td>
<td>210</td>
<td>$\geq 10^6$</td>
<td>9 $10^{15}$</td>
<td>10$^{-4}$</td>
</tr>
<tr>
<td></td>
<td>$g_2$</td>
<td>60–80</td>
<td>$\geq 10^5$</td>
<td>9 $10^{16}$</td>
<td>10$^{-4}$</td>
</tr>
<tr>
<td></td>
<td>$g_3$</td>
<td>20</td>
<td>$\geq 10^5$</td>
<td>1 $10^{17}$</td>
<td>10$^{-4}$</td>
</tr>
<tr>
<td>HCO$^+$</td>
<td>$g_1$</td>
<td>210$^b$</td>
<td>$10^6$-$10^7b$</td>
<td>1–3 $10^{12}$</td>
<td>1–3 $10^{-8}$</td>
</tr>
<tr>
<td></td>
<td>$g_2$</td>
<td>60</td>
<td>$10^5$</td>
<td>6 $10^{12}$</td>
<td>7 $10^{-9}$</td>
</tr>
<tr>
<td>N$_2$H$^+$</td>
<td>$g_2/g_3$</td>
<td>20–70$^c$</td>
<td>-</td>
<td>0.4–8 $10^{12}$</td>
<td>0.4–8 $10^{-9}$</td>
</tr>
<tr>
<td>HOCO$^+$</td>
<td>$g_2/g_3$</td>
<td>35</td>
<td>$10^4$</td>
<td>1 $10^{12}$</td>
<td>1 $10^{-9}$</td>
</tr>
<tr>
<td>SO$^+\text{d}$</td>
<td>$g_2/g_3$</td>
<td>25$^d$</td>
<td>-</td>
<td>7 $10^{11}$</td>
<td>8 $10^{-10}$</td>
</tr>
<tr>
<td>HCS$^+$</td>
<td>$g_2$</td>
<td>80</td>
<td>$8 \times 10^5$</td>
<td>6 $10^{11}$</td>
<td>7 $10^{-10}$</td>
</tr>
<tr>
<td></td>
<td>$g_3$</td>
<td>20$^e$</td>
<td>$10^5e$</td>
<td>3 $10^{11}$</td>
<td>3 $10^{-10}$</td>
</tr>
</tbody>
</table>

$HCO^+$ & N$_2$H$^+$ NOT significantly enhanced wrt on-source values by BP97!

(*X_{\text{outflow}}/X_{\text{source}} \leq 5*)

NO HCO$^+$ enhancement in outflows seen also by Hogerheijde+ 1998 Tafalla+ 2010
Origin of molecular ions with ASTROCHEM

Molecular ions are enhanced in shocks?

ASTROCHEM

http://smaret.github.io/astrochem/

Computes the chemical evolution of a gas at a given temperature, $T$, and density, $n(H_2)$

It reads a network of chemical reactions, builds a system of kinetic rates equations, and solves it.

It considers gas-phase processes and simple gas-grain interaction due to freeze-out, and desorption (thermal, cosmic rays, and photo-desorption).

We use the OSU chemical network http://www.physics.ohio-state.edu/eric/research.html

We assume: $A_v = 10$ mag, grain size = 0.1 um, and initial abundances by Wakelam+ (2006)

<table>
<thead>
<tr>
<th>Species</th>
<th>$X = \frac{N_{\text{species}}}{N_{H_2}}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>He</td>
<td>0.14</td>
</tr>
<tr>
<td>N</td>
<td>$7.40 \times 10^{-5}$</td>
</tr>
<tr>
<td>O</td>
<td>$3.52 \times 10^{-4}$</td>
</tr>
<tr>
<td>C$^+$</td>
<td>$1.46 \times 10^{-4}$</td>
</tr>
<tr>
<td>S$^+$</td>
<td>$1.60 \times 10^{-7}$</td>
</tr>
<tr>
<td>Si$^+$</td>
<td>$1.60 \times 10^{-8}$</td>
</tr>
<tr>
<td>Fe$^+$</td>
<td>$6.00 \times 10^{-9}$</td>
</tr>
<tr>
<td>Na$^+$</td>
<td>$4.00 \times 10^{-9}$</td>
</tr>
<tr>
<td>Mg$^+$</td>
<td>$1.40 \times 10^{-8}$</td>
</tr>
</tbody>
</table>
Origin of molecular ions with ASTROCHEM

HCO$^+$ & N$_2$H$^+$ are reproduced by gas-phase chemistry in the CLOUD

HCO$^+$ & N$_2$H$^+$ → PROBE PRE-SHOCK ABUNDANCES!

HOCO$^+$, SO$^+$, HCS$^+$ abundances are 1-3 orders of magnitude larger than predicted in the CLOUD, and even more after compression in the shock ...
Origin of molecular ions with ASTROCHEM

Molecular ions are enhanced in shocks?

\[ \text{CO}_2 + \text{H}_3^+ \rightarrow \text{HOCO}^+ + \text{H}_2 \]
\[ \text{S}^+ + \text{OH} \rightarrow \text{SO}^+ + \text{H} \]
\[ \text{CS} + (\text{HCO}^+, \text{H}_3^+, \text{H}_3\text{O}^+) \rightarrow \text{HCS}^+ + \ldots. \]

\text{HOCO}^+, \text{SO}^+, \text{HCS}^+ \text{ may be enhanced}
due to the release of \text{CO}_2 \text{ and } \text{S-bearing molecules from dust grains mantles via evaporation or sputtering in shocks (Neufeld & Dalgarno 1989, Minh+ 1988, 1991, Deguchi+ 2006, Sakai+ 2008)}
Step 2: evolution from SS for enhanced gas to reproduce $X($HOCO$^+)$

- $X($CO$_2)$ ≥ 2e-5 = 100$^*$ $X($CO$_2$)$_{gas}$ in sfr consistent with solid CO$_2$ on ices (e.g., van Dishoeck+ 2004)
- HOCO$^+$ is a probe of CO$_2$
  - No permanent electric dipole, not obs at mm

- $X($S$)$ ≥ 2e-6, $X($H$_2$S$)$ ≥ 2e-7 consistent with $X($H$_2$S$)$ estimated by BPG97 in B1

- $X($S$)$
- $X($H$_2$S$)$
- $X($OCS$)$
- $X($HOCO$^+$)

$X($OCS$)$ ≥ 2e-6, i.e. OCS should be the main sulphur carrier!

(e.g. Codella+ 2005; Wakelam+ 2004, 2005)
Conclusions

First census of molecular ions in the L1157-B1 shock down to ~1 mK / 1 km/s at 3mm: HCO$^+$, H$^{13}$CO$^+$, HCS$^+$ and for the first time in a shock N$_2$H$^+$ (Codella+ 2013), HOCO$^+$ and SO$^+$

HCO$^+$ & N$_2$H$^+$ → probe PRE-SHOCK ABUNDANCES
we need Zeta = 1-3e-16 s$^{-1}$

HOCO$^+$, SO$^+$, HCS$^+$ → effective SHOCK TRACERS

HOCO$^+$ is enhanced due to CO$_2$ release from grains mantles → X(CO$_2$) ≥ 2e-5
SO$^+$ is enhanced due to release of S, H$_2$S and its subsequent ionization → X(S) ≥ 2e-6, X(H$_2$S) ≥ 2e-7
HCS$^+$ is enhanced due to release of OCS → X(OCS) ≥ 2e-6

HCS$^+$ abundance is larger than predicted in the cloud by two orders of magnitude not enhanced enough by S or H$_2$S release in the shock
OCS should be the main S carrier on dust grains!

FUTURE: 2.5” resolution IRAM-PdBI observations of SO$^+$ (PI: L. Podio, C. Codella) + IRAM-PdBI obs of OCS (PI: F. Fontani)