Dissociative Recombination of Cold $\text{H}_3^+$ and its Interstellar Implications

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H₃⁺: Cornerstone of Interstellar Chemistry
Observing Interstellar H$_3^+$

- Equilateral triangle
- “No” rotational spectrum
- “No” electronic spectrum
- Vibrational spectrum is only probe
- Absorption spectroscopy against background or embedded star
Interstellar Cloud Classification*

Dense molecular clouds:
- $H \rightarrow H_2$
- $C \rightarrow CO$
- $n(H_2) \sim 10^4$–$10^6$ cm$^{-3}$
- $T \sim 20$ K

Diffuse clouds:
- $H \leftrightarrow H_2$
- $C \rightarrow C^+$
- $n(H_2) \sim 10^1$–$10^3$ cm$^{-3}$
  - [$\sim 10^{-18}$ atm]
- $T \sim 50$ K

Diffuse atomic clouds
- $H_2 << 10\%$

Diffuse molecular clouds
- $H_2 > 10\%$ (self-shielded)

* Snow & McCall, ARAA, 2006 (in prep)

Barnard 68 (courtesy João Alves, ESO)

Photo: Jose Fernandez Garcia
$N(\text{H}_3^+) = 1 - 5 \times 10^{14} \text{ cm}^{-2}$

McCall, Geballe, Hinkle, & Oka
**Dense Cloud H$_3^+$ Chemistry**

**Formation**

\[
\begin{align*}
H_2 & \xrightarrow{\text{cosmic ray}} H_2^+ + e^- \\
H_2 + H_2^+ & \rightarrow H_3^+ + H
\end{align*}
\]

Rate = $\zeta [H_2]$  

**Deformation**

\[
\begin{align*}
H_3^+ + CO & \rightarrow HCO^+ + H_2
\end{align*}
\]

Rate = $k [H_3^+] [CO]$  

**Steady State**

\[
\begin{align*}
\text{Density Independent!}
\end{align*}
\]

\[
\frac{(3 \times 10^{-17} \text{ s}^{-1})}{(2 \times 10^{-9} \text{ cm}^3 \text{ s}^{-1})} \times (6700) = 10^{-4} \text{ cm}^{-3}
\]

McCall, Geballe, Hinkle, & Oka  
H$_3^+$ as a Probe of Dense Clouds

- Given $n$(H$_3^+$) from model, and $N$(H$_3^+$) from infrared observations:
  - path length $L = N/n \sim 3 \times 10^{18}$ cm $\sim$ 1 pc
  - density $\langle n(H_2) \rangle = N(H_2)/L \sim 6 \times 10^4$ cm$^{-3}$
  - temperature $T \sim 30$ K

- Unique probe of clouds
- Consistent with expectations
  - confirms dense cloud chemistry

Diagram:
- Energy levels
  - $J$: 0, 1, 2
  - $E$(Kelvin): 0, 100, 200, 300, 400
  - Emission transitions
    - $J=0 \rightarrow J=1$ (forbidden)
    - $J=1 \rightarrow J=2$
  - $T$ = 32.9 K
Diffuse Molecular Cloud $\text{H}_3^+$ Chemistry

**Formation**

$$
\begin{align*}
\text{H}_2 & \xrightarrow{\text{cosmic ray}} \text{H}_2^+ + \text{e}^- \\
\text{H}_2 + \text{H}_2^+ & \rightarrow \text{H}_3^+ + \text{H}
\end{align*}
$$

**Rate**

$$
\text{Rate} = \zeta [\text{H}_2]
$$

**Destruction**

$$
\begin{align*}
\text{H}_3^+ + \text{e}^- & \rightarrow \text{H} + \text{H}_2 \text{ or } 3\text{H}
\end{align*}
$$

**Rate**

$$
\text{Rate} = k_e [\text{H}_3^+] [\text{e}^-]
$$

**Steady State**

$$
[\text{H}_3^+] = \frac{\zeta [\text{H}_2]}{k_e [\text{e}^-]} = \frac{(3 \times 10^{-17} \text{ s}^{-1})}{(5 \times 10^{-7} \text{ cm}^3 \text{ s}^{-1})} \times (2400)
$$

$$
[\text{H}_3^+] = 10^{-7} \text{ cm}^{-3}
$$

Density Independent!

$10^3$ times smaller than dense clouds!
Lots of $\text{H}_3^+$ in Diffuse Clouds!

$\text{H}_3^+$ Column Density ($10^{14}\text{ cm}^{-2}$)

$\text{N}(\text{H}_3^+) \sim \text{dense clouds}$

$n(\text{H}_3^+) \sim 1000\text{ times less}$

$\therefore L \sim 1000\text{ times longer ?!!}$

McCall, et al.
Big Problem with the Chemistry!

- ~2 orders of magnitude!!

Steady State: \[ [H_3^+] = \frac{\zeta [H_2]}{k_e [e^-]} \]

To increase the value of \([H_3^+]\), we need:

- Smaller electron fraction \([e^-]/[H_2]\)
- Smaller recombination rate constant \(k_e\)
- Higher ionization rate \(\zeta\)
**H$_3^+$ toward ζ Persei**

**[e$^-$/[H$_2$]] not to blame**

**N(C$^+$) from HST**

**N(H$_2$) from Copernicus**

---

**Table:**

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<tr>
<th>HD</th>
<th>NAME</th>
<th>$t$ $^{TT}$</th>
<th>$b$ $^{TT}$</th>
<th>S. T.</th>
<th>$E$(B-V)</th>
<th>r [pc]</th>
<th>$log$ N(H$_2$) [cm$^{-2}$]</th>
<th>$log$ N(H$_2$) [cm$^{-2}$]</th>
<th>$log$ N(HI + N$_2$) [cm$^{-2}$]</th>
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<tr>
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<tr>
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<td>1164</td>
<td>20.36</td>
<td>20.90</td>
<td>21.09</td>
</tr>
</tbody>
</table>

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Big Problem with the Chemistry!

Steady State: \[ [H_3^+] = \frac{\zeta}{k_e} \frac{[H_2]}{[e^-]} \]

To increase the value of \([H_3^+]\), we need:

- Smaller electron fraction \([e^-]/[H_2]\)
- Smaller recombination rate constant \(k_e\)
- Higher ionization rate \(\zeta\)
H$_3^+$ Dissociative Recombination

- Laboratory values of $k_e$ have varied by 4 orders of magnitude!
- Theory unreliable (until recently)...
- Problem (?): not measuring H$_3^+$ in ground states
Storage Ring Measurements

CRYRING

- Very simple experiment
- Complete vibrational relaxation
- Control $H_3^+$ – $e^-$ impact energy
- Rotationally hot ions produced
- “No” rotational cooling in ring
Supersonic Expansion Ion Source

- Similar to sources for laboratory spectroscopy in many groups
- Pulsed nozzle design
- Supersonic expansion leads to rapid cooling
- Discharge from ring electrode downstream
- Spectroscopy used to characterize ions
- Skimmer employed to minimize arcing to ring
**H$_3^+$ Energy Level Structure**

- **Probe of temperature**
- **Not detected**

The diagram illustrates energy levels for H$_3^+$ ions, with transitions labeled as $R(1,0)$, $R(1,1)^u$, and $R(2,2)$, along with energy values of 33 K and 151 K.
Spectroscopy of H$_3^+$ Source

- Confirmed that H$_3^+$ produced is rotationally cold, as in interstellar medium

Infrared Cavity Ringdown Laser Absorption Spectroscopy

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McCall, et al.
Nature 422, 500 (2003)
CRYRING Results

- Chris Greene: new theory
- Andreas Wolf: TSR results

- Considerable amount of structure (resonances) in the cross-section
- $k_e = 2.6 \times 10^{-7} \text{ cm}^3 \text{s}^{-1}$
- Factor of two smaller

McCall, et al.
Steady State: \[ [H_3^+] = \frac{\zeta}{k_e} \frac{[H_2]}{[e^-]} \]

To increase the value of \([H_3^+]\), we need:

- Smaller electron fraction \([e^-]/[H_2]\)
- Smaller recombination rate constant \(k_e\)
- Higher ionization rate \(\zeta\)
Implications for ζ Persei

\[
\frac{N(H_3^+)}{L} = [H_3^+] = \frac{\zeta}{k_e} \frac{N(H_2)}{N(e^-)}
\]

\[
\zeta L = \left(2.6 \times 10^7 \text{ cm}^3 \text{ s}^{-1}\right) \left(8 \times 10^{13} \text{ cm}^{-2}\right) \left(3.8 \times 10^{-4}\right)
\]

\[
\zeta L = 8000 \text{ cm s}^{-1} \quad \text{(solid)}
\]

Adopt

ζ = 3 × 10^{-17} s^{-1}

L = 85 pc

⟨n⟩ = 6 cm^{-3}

Adopt

L = 2.1 pc

ζ = 1.2 × 10^{-15} s^{-1}

(40x higher!)
What Does This Mean?

• Enhanced ionization rate in ζ Persei
• Widespread H$_3^+$ in diffuse clouds
  – perhaps widespread ionization enhancement?
• Dense cloud H$_3^+$ is "normal"
  – enhanced ionization rate only in diffuse clouds
  – low energy cosmic-ray flux?
  – cosmic-ray self-confinement?
  – no constraints, aside from chemistry!!
• New chemical models necessary
  – Harvey Liszt
  – Franck Le Petit
CONFINEMENT-DRIVEN SPATIAL VARIATIONS IN THE COSMIC-RAY FLUX

Paolo Padoan¹ and John Scalo²

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ABSTRACT

Low-energy cosmic rays (CRs) are confined by self-generated MHD waves in the mostly neutral interstellar medium. We show that the CR transport equation can be expressed as a continuity equation for the CR number density involving an effective convection velocity. Assuming a balance between wave growth and ion-neutral damping, this equation gives a steady state condition $n_{\text{cr}} \propto n_{\text{i}}^{3/2}$ up to a critical density for free streaming. This relation naturally accounts for the heretofore unexplained difference in CR ionization rates derived for dense diffuse clouds (McCall et al.) and dark clouds, and predicts large spatial variations in the CR heating rate and pressure.
Future Work

• More experiments!
  – Improved spectroscopy of ion source
    • Higher resolution & higher sensitivity
    • Better characterization of ro-vib distribution
  – Testing of new (piezo) ion source
  – Single quantum-state CRYRING measurements
    • produce pure para-H$_3^+$ using para-H$_2$

• More observational data!
  – Search for H$_3^+$ in more diffuse cloud sightlines
    • Confirm generality of result in classical diffuse clouds
  – Observations of H$_3^+$ in "translucent" sightlines
    • C$^+$ → C → CO
Rich Diffuse Cloud Chemistry

• From 1930s through the mid-1990s, only diatomic molecules thought to be abundant in diffuse clouds

• Recently, many polyatomics observed:
  – $\text{H}_3^+$ in infrared
  – $\text{HCO}^+$, $\text{C}_2\text{H}$, $\text{C}_3\text{H}_2$, etc. in radio (Lucas & Liszt)
  – $\text{C}_3$ in near-UV (Maier, et al.)

• Diffuse Interstellar Bands!
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