Molecular Ions as Tracers of the Cosmic-Ray Ionization Rate and Molecular Hydrogen Fraction

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Team $\text{H}_3^+$

Team Herschel

Dec. 14, 2016
Outline

• Background
  – Cosmic rays
  – Interstellar chemistry

• Observations & Results
  – $\text{H}_3^+$ in the local ISM
  – OH$^+$ and H$_2$O$^+$ in the Milky Way disk

• Future Work
Cosmic Rays

- Discovered in 1912 by Victor Hess during balloon-borne experiments that showed radiation *increasing* at higher altitudes
- Dubbed cosmic rays by Millikan (1926)
Cosmic Rays

We can draw some fairly reliable conclusions of a general sort as to the origin of these very penetrating and very high frequency rays. The most penetrating rays that we have known anything about thus far, the gamma rays of radium and thorium, are produced only by nuclear transformations within atoms. In other words, they are produced by the change of one atom over into another atom, or by the creation of a new type of atom. It is scarcely possible, then, to avoid the conclusion that these still more penetrating rays which we have here been studying are produced similarly by nuclear transformations of some sort. But these transformations must be enormously more energetic than are those taking place in any radioactive changes that we know anything about. For, according to our present knowledge, the frequency of any emitted ray is proportional to the energy of the subatomic change giving birth to it. We can scarcely avoid the conclusion, then, that nuclear changes having an energy value perhaps fifty times as great as the energy changes involved in observed radioactive processes are taking place all through space, and that signals of these changes are being sent to us in these high frequency rays.

Millikan 1926, PNAS, 12, 48
Cosmic Rays

• Discovered in 1912 by Victor Hess during balloon-borne experiments that showed radiation increasing at higher altitudes
• Dubbed cosmic rays by Millikan (1926)
• Now known to be highly energetic charged particles ($p$, $e^-$, $e^+$, $\alpha$, heavy bare nuclei)
Particle Interactions

- Ionization
  \[ p + H_2 \rightarrow H_2^+ + e^- + p' \]

- Spallation and Fusion
  \[ [p, \alpha] + [{}^{12}\text{C}, {}^{14}\text{N}, {}^{16}\text{O}] \rightarrow [{}^6\text{Li}, {}^7\text{Li}, {}^9\text{Be}, {}^{10}\text{B}, {}^{11}\text{B}] \]

- Nuclear Excitation
  \[ [p, \alpha] + {}^{12}\text{C} \rightarrow {}^{12}\text{C}^* \rightarrow {}^{12}\text{C} + \gamma_{4.44\text{ MeV}} \]

- Inelastic Collisions
  \[ p + H \rightarrow p' + H + \pi^0 \]
  \[ \gamma + \gamma \]
Rate of Interactions

\[ R_x = 4\pi G_x \int j(E)\sigma_x(E)dE \]

- \( G_x \): Interaction specific coefficient
- \( \sigma_x \): Interaction cross section
- \( j(E)dE \): Differential proton spectrum
Interaction Cross Sections

Indriolo & McCall 2013, Chem. Soc. Rev., 42, 7763 (and references therein)
Cosmic-Ray Energy Distribution

- Power law in energy \( (\phi \sim E^{-2.7}) \) spanning 12 decades in \( E \), and 30 decades in flux
- Poorly constrained below 1 GeV

Cosmic-Ray Energy Distribution

+ AMS Collaboration (2002)
Cosmic-Ray Energy Distribution

Dec. 14, 2016
The Hydride Toolbox
Cosmic-Ray Energy Distribution

[Graph showing the energy distribution of cosmic rays with different data points and lines representing various studies.]

ASMS Collaboration (2002)
Mori (1997)
Spitzer & Tomasko (1968)
Cosmic-Ray Energy Distribution

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Cosmic-Ray Energy Distribution
Ionization and Astrochemistry

• Interstellar chemistry is driven by fast ion-molecule reactions
• Requires source of ionization
  – UV photons with $E > 13.6$ eV are absorbed by atomic H in H II regions
  – species with FIP > 13.6 eV are primarily neutral
  – species with FIP < 13.6 eV are singly ionized
• In diffuse and dense molecular clouds H and H$_2$ are ionized by cosmic rays
• $\zeta_2 = 2.3\zeta_p; \zeta_H = 1.5\zeta_p$; Glassgold & Langer 1974 ApJ, 193, 73
Ion-Molecule Reactions

- $\text{H}_3^+$ acts as a universal proton donor
- Molecular ions linked to CR ionization
Ionization Rate from Molecules

- Rate of change for abundance of any species can be written as a differential equation accounting for formation and destruction mechanisms, e.g.,

\[
\frac{d}{dt} n(H_3^+) = n(H_2)n(H_2^+)k(H_2 | H_2^+) - n(H_3^+)n(e)k(H_3^+ | e) - n(H_3^+)n(CO)k(H_3^+ | CO)
\]

formation destruction

- More terms can be added to account for alternate formation and destruction pathways

- Formation rates of species closely linked to cosmic-ray ionization will be influenced by ionization rate
Hydrogen Chemistry

- **Formation**
  - $\text{CR} + \text{H}_2 \rightarrow \text{H}_2^+ + e^- + \text{CR}'$
  - $\text{H}_2^+ + \text{H}_2 \rightarrow \text{H}_3^+ + \text{H}$

- **Destruction**
  - $\text{H}_3^+ + e^- \rightarrow \text{H} + \text{H} + \text{H}$

- **Dense Clouds**
  - $\text{H}_3^+ + \text{CO} \rightarrow \text{HCO}^+ + \text{H}_2$
  - $\text{H}_3^+ + \text{O} \rightarrow \text{OH}^+ + \text{H}_2$

- **Atomic Clouds**
  - $\text{H}_2^+ + \text{H} \rightarrow \text{H}_2 + \text{H}^+$
  - $\text{H}_2^+ + e^- \rightarrow \text{H} + \text{H}$
Ionization Rate from $\text{H}_3^+$

$$\zeta_2 n(\text{H}_2) = k(\text{H}_3^+ | e^-) n(\text{H}_3^+) n_e$$

$$\zeta_2 = k(\text{H}_3^+ | e^-) x_e n_H \frac{N(\text{H}_3^+)}{N(\text{H}_2)}$$

$\zeta_2 n(\text{H}_2)$ measured in laboratory ($2 \times 10^{-7}$ cm$^3$ s$^{-1}$)

$x_e$ approximated by $x(\text{C}^+)$ ($1.5 \times 10^{-4}$)

$n_H$ estimated from molecular observations (100 cm$^{-3}$)
e.g., Sonnentrucker et al. 2007, ApJS, 168, 58

$N(\text{H}_2)$ measured or estimated ($10^{20}$-10$^{21}$ cm$^{-2}$)

determine $N(\text{H}_3^+)$ from NIR observations
Targeted Transitions

- Transitions of the $\nu_2 \leftarrow 0$ band of $\text{H}_3^+$ are available in the infrared.
- Given average diffuse cloud temperatures (70 K) only the (J,K)=(1,0) & (1,1) levels are significantly populated.
- Observable transitions are:
  - $R(1,1)^u$: 3.668083 µm
  - $R(1,0)$: 3.668516 µm
  - $R(1,1)^l$: 3.715479 µm
  - $Q(1,1)$: 3.928625 µm
  - $Q(1,0)$: 3.953000 µm

Energy level diagram for the ground vibrational state of $\text{H}_3^+$
H$_3^+$ Data: Finally All Processed!!!
Distribution of $\zeta_2$

Mean log($\zeta_2$): -15.33 ($4.7 \times 10^{-16}$ s$^{-1}$); Standard deviation: 0.23
Mean $\log(\zeta_2)$: -15.33 ($4.7 \times 10^{-16} \, \text{s}^{-1}$); Standard deviation: 0.23
Oxygen Chemistry

CR + H → H⁺ + e⁻ + CR'
H⁺ + O → O⁺ + H
O⁺ + H₂ → OH⁺ + H
OH⁺ + H₂ → H₂O⁺ + H
H₂O⁺ + H₂ → H₃O⁺ + H

OH⁺ + e⁻ → products
H₂O⁺ + e⁻ → products
H₃O⁺ + e⁻ → products
O⁺ + H → H⁺ + O
H⁺ + e⁻ → H + hν
H⁺ + PAH → PAH⁺ + H
Observing OH$^+$ and H$_2$O$^+$

- OH$^+$ rotational transitions out of the ground state: 909, 972, & 1033 GHz
- H$_2$O$^+$ rotational transitions out of ground state(s): 607, 631, 1115, & 1139 GHz

Earth’s atmosphere is opaque at relevant frequencies

*Herschel Space Observatory*

HIFI – Heterodyne Instrument for the Far Infrared
H$_2$O$^+$ Transitions

para

$F=1/2$
$F=3/2$

$J=1/2$
$J=3/2$

ortho

$F=3/2$
$F=1/2$
$F=3/2$
$F=5/2$

$J=1/2$
$J=3/2$
$J=3/2$
$J=1/2$

$N_{K_aK_c}$

$1_{10}$
$1_{11}$

631.7 GHz
607.2 GHz
1115.2 GHz

Dec. 14, 2016

The Hydride Toolbox
Herschel Observations

- 20 Galactic sight lines surveyed in multiple *Herschel* programs in both OH$^+$ and H$_2$O$^+$
- Observations probe gas up to 11 kpc distant
- Roughly 100 separate components where ionization rate can be determined

Example OH$^+$ and H$_2$O$^+$ Spectra

- Absorption toward the W51 star-forming region
- Spread in velocity due to differential rotation of the Galaxy
- Green profile shows “true” distribution in line-of-sight gas velocity

Example OH$^+$ and H$_2$O$^+$ Spectra

• Overall, OH$^+$ and H$_2$O$^+$ spectra have similar velocity profiles
• Absorption occurs at expected velocities for each Galactic quadrant
• Adopting a rotation curve allows us to estimate kinematic distances

Analysis of OH$^+$ and H$_2$O$^+$

- Break spectra down into what appear to be separate velocity components
- Determine column densities for those components
- Calculate parameters of interest: molecular fraction & cosmic-ray ionization rate
## H$_2$ Fraction toward G034.3+00.15

The fraction of H$_2$ can be calculated using the expression:

$$f_{H_2} = \frac{2x_e k(H_2O^+|e^-)/k(OH^+|H_2)}{N(OH^+)/N(H_2O^+) - k(H_2O^+|H_2)/k(OH^+|H_2)}$$

### Table

<table>
<thead>
<tr>
<th>$v_{LSR}$ (km/s)</th>
<th>$N$(OH$^+$) ($10^{13}$ cm$^{-2}$)</th>
<th>$N$(H$_2$O$^+$) ($10^{13}$ cm$^{-2}$)</th>
<th>$f$(H$_2$)</th>
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Distribution of $f(\text{H}_2)$

- 92 components with OH$^+$ and H$_2$O$^+$ absorption
- Shaded bars: total sample
- Red bars: within 5 km/s of background source velocity
- In the foreground cloud sample we find a mean molecular hydrogen fraction of 0.042 with standard deviation 0.018

Ionization Rate toward G034.3+00.15

\[
\epsilon \zeta_H = \frac{N(OH^+)}{N(H)} n_H \left[ \frac{f_{H_2}}{2} k(OH^+|H_2) + x_e k(OH^+|e^-) \right]
\]

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$\epsilon=0.07$ from Indriolo et al. 2012, ApJ, 758, 83; simultaneous analysis of $H_3^+$, OH$^+$, and $H_2O^+$ in a diffuse cloud

$N(H)$ from Winkel et al. 2016 (submitted to A&A); 21 cm survey of H II regions with JVLA & Effelsberg
Distribution of $\zeta_H$

- Gas associated with background sources is shown in red
- $\zeta_H > 10^{-15}$ s$^{-1}$ is from gas in Galactic center region
- Log-normal distributions
  - Mean $\log(\zeta_H) = -15.75$ ($1.8 \times 10^{-16}$ s$^{-1}$); $\sigma = 0.29$
  - $H_3^+$: $\log(\zeta_H) = -15.52$ ($3.0 \times 10^{-16}$ s$^{-1}$); $\sigma = 0.23$
- Two-sample K-S test cannot rule out same distribution

Ionization Rate & Molecular Hydrogen Fraction vs. Galactocentric Radius

- Black are foreground clouds, and red are background sources
- Molecular hydrogen fraction shows no correlation
- Possible gradient in ionization rate with distance from GC
Extragalactic OH$^+$ and H$_2$O$^+$

- ULIRG Arp 220 & Seyfert NGC 4418
- Local starburst galaxies (e.g., M82, Cen A)
  - Van der Tak et al. 2016 A&A 593, A43
- z=0.89 absorber PKS 1830-211
  - Muller et al. 2016 A&A 595, A128
- z~2.3 absorbers
  - ALMA observations underway
Summary

• Observations of molecular ions are useful in inferring the cosmic-ray ionization rate
• Mean ionization rate in the diffuse ISM is a few times $10^{-16}$ s$^{-1}$, with a distribution spread across about 1 order of magnitude
• ALMA provides the sensitivity to extend similar analysis to high redshift galaxies
Future Directions: Dense Clouds

- IRAM 30m maps of \( \text{H}^{13}\text{CO}^+ \), \( \text{N}_2\text{H}^+ \), \( \text{C}^{18}\text{O} \), and \( \text{DCO}^+ \) in dense, starless cores
- Clouds have been observed in gamma rays with \textit{FERMI}-LAT
- Use to constrain both the low and high energy portions of the cosmic ray spectrum