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

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Team H_3^+

Team Herschel

Outline

- Background
 - Cosmic rays
 - Interstellar chemistry
- Observations & Results
 - $-H_3^+$ in the local ISM
 - OH^+ and H_2O^+ 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⁺*, *α*, heavy bare nuclei)

Particle Interactions

Ionization

 $p + H_2 \rightarrow H_2^+ + e^- + p'$

- Spallation and Fusion
 [p, α] + [¹²C, ¹⁴N, ¹⁶O] → [⁶Li,⁷Li,⁹Be,¹⁰B,¹¹B]
- Nuclear Excitation $[p, \alpha] + {}^{12}C \rightarrow {}^{12}C^* \rightarrow {}^{12}C + \gamma_{4.44 \text{ MeV}}$

Rate of Interactions

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

- *G_x*: Interaction specific coefficient
- σ_x : Interaction cross section
- *j(E)dE*: Differential proton spectrum

Interaction Cross Sections



Indriolo & McCall 2013, Chem. Soc. Rev., 42, 7763 (and references therein)

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



Swordy 2001, Space Sci. Rev., 99, 85

The Hydride Toolbox











Ionization and Astrochemistry

- Interstellar chemistry is driven by fast ionmolecule 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</p>
- In diffuse and dense molecular clouds H and H₂ 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



- H₃⁺ 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.,

 $\frac{d}{dt}n(\mathbf{H}_{3}^{+}) = n(\mathbf{H}_{2})n(\mathbf{H}_{2}^{+})k(\mathbf{H}_{2}|\mathbf{H}_{2}^{+}) - n(\mathbf{H}_{3}^{+})n(e)k(\mathbf{H}_{3}^{+}|e) - n(\mathbf{H}_{3}^{+})n(CO)k(\mathbf{H}_{3}^{+}|CO)$

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
 - $CR + H_2 \rightarrow H_2^+ + e^- + CR'$
 - $H_2^+ + H_2 \rightarrow H_3^+ + H$
- Destruction
 - $H_3^+ + e^- \rightarrow H + H + H$

- Dense Clouds - $H_3^+ + CO \rightarrow HCO^+ + H_2$
 - $H_3^+ + O \rightarrow OH^+ + H_2$
- Atomic Clouds $- H_2^+ + H \rightarrow H_2 + H^+$ $- H_2^+ + e^- \rightarrow H + H$

Ionization Rate from H₃⁺

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

CR + H₂ H₃⁺ + e⁻

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



 $k(H_3^+|e^-)$ measured in laboratory (2×10⁻⁷ cm³ s⁻¹) McCall et al. 2004, Phys. Rev. A, 70, 052716

 x_{e} approximated by $x(C^{+})$ (1.5×10⁻⁴) Sofia et al. 2004, ApJ, 605, 272

 $n_{\rm H}$ estimated from molecular observations (100 cm⁻³) e.g., Sonnentrucker et al. 2007, ApJS, 168, 58

 $N(H_2)$ measured or estimated (10²⁰-10²¹ cm⁻²) Rachford et al. 2002, ApJ, 577, 221

determine $N(H_3^+)$ from NIR observations



Targeted Transitions



Energy level diagram for the ground vibrational state of H₃⁺

- Transitions of the v₂ ← 0 band of H₃⁺ 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)^I: 3.715479 μm
 - Q(1,1): 3.928625 μm
 - *Q(1,0)*: 3.953000 μm

H₃⁺ Data: Finally All Processed!!!



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The Hydride Toolbox

Distribution of ζ_2



Mean log(ζ_2): -15.33 (4.7×10⁻¹⁶ s⁻¹); Standard deviation: 0.23

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Oxygen Chemistry



- $CR + H \rightarrow H^+ + e^- + CR'$
- $H^+ + O \rightarrow O^+ + H$
- $O^+ + H_2 \rightarrow OH^+ + H$
- $OH^+ + H_2 \rightarrow H_2O^+ + H$

• $H_2O^+ + H_2 \rightarrow H_3O^+ + H_2$

- $O^+ + H \rightarrow H^+ + O$

• OH⁺ + $e^- \rightarrow$ products

• $H_2O^+ + e^- \rightarrow \text{products}$

• $H_3O^+ + e^- \rightarrow \text{products}$

- $H^+ + e^- \rightarrow H + hv$
- $H^+ + PAH \rightarrow PAH^+ + H$

Observing OH⁺ and H_2O^+

- OH⁺ rotational transitions out of the ground state: 909, 972, & 1033 GHz
- H₂O⁺ 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



OH⁺ Transitions



H₂O⁺ Transitions



The Hydride Toolbox

Herschel Observations

- 20 Galactic sight lines surveyed in multiple *Herschel* programs in both OH⁺ and H₂O⁺
- Observations probe gas up to 11 kpc distant
- Roughly 100 separate components where ionization rate can be determined



Example OH⁺ and H₂O⁺ Spectra

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



Example OH⁺ and H₂O⁺ Spectra



Indriolo et al. 2015, ApJ, 800, 40

- Overall, OH⁺ and H₂O⁺ 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 H₂O⁺

- 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



H₂ Fraction toward G034.3+00.15

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

v _{LSR} (km/s)	<i>N</i> (OH ⁺) (10 ¹³ cm ⁻²)	<i>N</i> (H ₂ O ⁺) (10 ¹³ cm ⁻²)	<i>f</i> (H ₂)
[-12, 7]	2.5	0.26	0.03
[7, 18]	3.0	0.67	0.06
[18, 36]	2.7	0.31	0.03
[36, 44]	1.7	0.21	0.03
[44, 52]	3.7	0.93	0.07
[52, 70]	4.2	1.2	0.08

Distribution of *f*(H₂)



- 92 components with OH⁺ and H₂O⁺ 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

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

V _{LSR} (km/s)	<i>N</i> (OH⁺) (10 ¹³ cm ⁻²)	<i>N</i> (H ₂ O ⁺) (10 ¹³ cm ⁻²)	<i>f</i> (H ₂)	N(H) (10 ²¹ cm ⁻²)	ζ _H (10 ⁻¹⁶ s ⁻¹)
[-12, 7]	2.5	0.26	0.03	1.3	2.1
[7, 18]	3.0	0.67	0.06	2.1	2.8
[18, 36]	2.7	0.31	0.03	>3.6	<0.9
[36, 44]	1.7	0.21	0.03	2.4	0.9
[44, 52]	3.7	0.93	0.07	3.6	2.2
[52, 70]	4.2	1.2	0.08	>5.2	<2.0

ε=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 $\zeta_{\rm H}$



- Gas associated with background sources is shown in red
- ζ_H>10⁻¹⁵ s⁻¹ is from gas in Galactic center region
- Log-normal distributions
 - Mean log(ζ_H) = -15.75 (1.8×10⁻¹⁶ s⁻¹); σ = 0.29
 - H_3^+ : log(ζ_H) = -15.52 (3.0×10⁻¹⁶ s⁻¹); σ = 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 H₂O⁺

- ULIRG Arp 220 & Seyfert NGC 4418

 González-Alfonso et al. 2013 A&A 550, A25
- 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 H¹³CO⁺, N₂H⁺, C¹⁸O, and DCO⁺ in dense, starless cores
- Clouds have been observed in gamma rays with *FERMI*-LAT
- Use to constrain both the low and high energy portions of the cosmic ray spectrum