Cosmic Ray-Driven Radiation Chemistry in Astrochemical Models

Christopher N. Shingledecker1,2,3
Jessica Tennis1, Romane Le Gal1, & Eric Herbst1,5

1. Department of Chemistry, University of Virginia, Charlottesville, VA 22904, USA
2. Max-Planck-Institut für extraterrestrische Physik, D-85748 Garching, Germany
3. Institute for Theoretical Chemistry, University of Stuttgart, Pfaffenwaldring 55, 70569 Stuttgart, Germany
4. Harvard-Smithsonian Center for Astrophysics, 60 Garden Street, Cambridge, MA 02138, USA
5. Department of Astronomy, University of Virginia, Charlottesville, VA 22904, USA

Abstract
Cosmic rays are widely known to have significant physiochemical impact on interstellar sources. In addition, laboratory astrophysics experiments have indicated that cosmic ray interactions with dust grain ice mantles could lead to astrochemically relevant species, including complex organic and prebiotic molecules [1].

In spite of the growing body of experimental work on interstellar radiation chemistry, incorporating cosmic ray-driven reactions and processes into astrochemical models has proven challenging, in part because of a lack of relevant data for many species now included in chemical networks. Recently [2], we have developed a general method of estimating radiochemical yields (G-values), rate coefficients, and decomposition pathways for species that have not been studied in detail in the laboratory in this context. Here, we will describe the derivation and application of our method, as well as point to much needed areas for future development in astrochemical radiation chemistry modeling.

Suprathermal Species

Example Network
\[ A \rightarrow A^+ + e^- + B^+ + C \]
\[ A + B^+ \rightarrow \text{Products} \]

The Fate of Suprathermal Species in Our Network

Possibility 1: Quenching
\[ \phi = \frac{2N_{B^+}}{\pi \alpha^2} \]
Formation of B^+

Possibility 2: Reaction
\[ k_p = \frac{v^*}{n_{B^+} \delta} \]

Results in Cold Core Models

Methyl Formate (HCOOCH3)

(a) Gas Phase

(b) Ice Surface

(c) Ice Bulk

Abundances of methyl formate in the gas (a), ice surface (b), and ice bulk (c) calculated both with (solid line) and without (dotted line) cosmic ray-driven solid-phase radiation chemistry [3]

Formations of Superthermal Precursors

H2CO + H2 + \text{e}^- \rightarrow \text{HCO}^+ + \text{H} + \text{H} \]
\[ \text{CH}_3\text{OH} + \text{CH}_2\text{OH} + \text{e}^- \rightarrow \text{CH}_3\text{O}^+ + \text{H} + \text{H} \]

Formation of Ethanol (CH3CH2OH)

Gas Phase

(a) Formations of Superthermal Precursors

HCO + CH2OH \rightarrow \text{HCOOCH3} \]

Ethanol in the gas (a), (b) and (c) calculated both with (solid line) and without (dotted line) cosmic ray-driven solid-phase radiation chemistry [3]

(b) Ice Surface

(c) Ice Bulk

Abundances of ethanol in the gas (a), ice surface (b), and ice bulk (c) calculated both with (solid line) and without (dotted line) cosmic ray-driven solid-phase radiation chemistry [3]

Formations of Ethanol

CH2 + CH2O + \text{e}^- \rightarrow \text{CH}_3\text{OH} + \text{H} \]

Reference

