Next-generation cosmic ice models for the JWST Era

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The key role of grain-surface processes for accurately simulating interstellar chemistry has long been known [1]; however, the importance of modelling processes occurring within dust grain ice mantles has only been fully realized in the last decade or so [2,3]. This new appreciation for solid-phase chemistry has been largely motivated by an extensive body of laboratory astrochemical studies, which have conclusively demonstrated the rich array of complex molecules that can form at very low temperatures [4-6]. More recently, data from the newly-launched James Webb Space Telescope has already revealed that even in regions previously thought to have been COM-poor, there exists a hidden reservoir of COMs within cosmic ice, which are unlikely to have been formed primarily via gas-phase reactions [7]. Substantial progress in treating cosmic ice chemistry is likely needed before simulations will be able to reliably replicate such observational results, and in this talk, I review some of our recent work along these lines, as well as present preliminary results from two projects that represent promising breakthroughs in how grain-surface chemistry is simulated in astrochemical models.

References

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[1] T. I. Hasegawa, E. Herbst, C. M. Leung, Models of gas-grain chemistry in dense interstellar clouds with complex organic molecules. *The Astrophysical Journal Supplement Series*. **82**, 167–195 (1992).

[2] R. T. Garrod, A Three-phase Chemical Model of Hot Cores: The Formation of Glycine. *The Astrophysical Journal*. **765**, 60 (2013).

[3] C. N. Shingledecker, T. Lamberts, J. C. Laas, A. Vasyunin, E. Herbst, J. Kästner, P. Caselli, Efficient Production of S8 in Interstellar Ices: The Effects of Cosmic-Ray-driven Radiation Chemistry and Nondiffusive Bulk Reactions. *ApJ*. **888**, 52 (2020).

[4] R. I. Kaiser, K. Roessler, Theoretical and Laboratory Studies on the Interaction of Cosmic-Ray Particles with Interstellar Ices. I. Synthesis of Polycyclic Aromatic Hydrocarbons by a Cosmic-Ray-Induced Multicenter Mechanism. *The Astrophysical Journal*. **475**, 144–154 (1997).

[5] P. D. Holtom, C. J. Bennett, Y. Osamura, N. J. Mason, R. I. Kaiser, A combined experimental and theoretical study on the formation of the amino acid glycine (NH2CH2COOH) and its isomer (CH3NHCOOH) in extraterrestrial ices. *The Astrophysical Journal*. **626**, 940 (2005).

[6] R. L. Hudson, M. H. Moore, J. P. Dworkin, M. P. Martin, Z. D. Pozun, Amino Acids from Ion-Irradiated Nitrile-Containing Ices. *Astrobiology*. **8**, 771–779 (2008).

[7] Y.-L. Yang, J. D. Green, K. M. Pontoppidan, J. B. Bergner, L. I. Cleeves, N. J. E. II, R. T. Garrod, M. Jin, C. H. Kim, J. Kim, J.-E. Lee, N. Sakai, C. N. Shingledecker, B. Shope, J. J. Tobin, E. F. van Dishoeck, CORINOS. I. JWST/MIRI Spectroscopy and Imaging of a Class 0 Protostar IRAS 15398–3359. *ApJL*. **941**, L13 (2022).