

Surface Chemistry of CN Radicals on Interstellar Ices: A Route to Molecular Complexity

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Nitriles are fundamental intermediates in prebiotic chemistry and are thought to have played a pivotal role in the chemical evolution that led to the origin of life in the Universe. In this contribution we present our latest DFT simulations on the surface reactivity of CN radicals, specifically amorphous water and carbon monoxide ices [1, 2].

Our results show that CN radicals, once adsorbed onto dust grain surfaces, exhibit high reactivity under cold interstellar conditions and can follow multiple reaction pathways that contribute to increasing molecular complexity budget of N-bearing species. We identify viable mechanisms for the formation of several astrochemically relevant species, including HCN, HNC, CH₃CN, CH₃NC, HOCN, HCOCN, CH₃C(OH)NH (acetimidic acid), and a potential connection to CH₃CONH₂ (acetamide). The way CN radicals interact with the ice surface plays a crucial role in the emergence of many of these products, highlighting the active chemical role that interstellar ice matrices can have towards molecular complexity.

Finally, we have also investigated the hydrogenation pathways of HCN and HNC, demonstrating how these nitriles can be converted into methanimine and methylamine through reactions with both atomic and molecular hydrogen. We further examine the implications of these pathways for the formation of their deuterated analogues. Our findings are discussed in the context of existing literature, providing new insights into the role of grain-surface chemistry in shaping molecular complexity during astrochemical evolution.

References

- [1] J. Enrique-Romero & T. Lamberts, *J. Phys. Chem. Lett.* 2024, 15, 30, 7799–7805.
- [2] J. Enrique-Romero & T. Lamberts, *A&A*, 2025, 699, A235