# Toward Unraveling Cyanopolyyne Chemistry on Interstellar Ices: From HC3N to Ethyl Cyanide and Propylamine

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Cyanoacetylene ($HC_3N$) is a nitrogen-bearing carbon chain that is ubiquitous in the interstellar medium (ISM). Once it is formed in the gas phase, it is thought to freeze out on the icy grain mantles in dense molecular clouds. Atop the ice it could react with a number of available chemical species, but little is known about the surface reactivity of $HC_3N$, in part because of experimental difficulties. In this work we present a computational investigation of the hydrogenation of $HC_3N$ under interstellar conditions. We have performed DFT, CCSD(T)-F12 and CASPT2 calculations to obtain the energy profiles of various hydrogenation pathways. Based on activation and reaction energies of the gas phase reactions, we found two likely reaction pathways. The first pathway leads to the formation of vinyl cyanide ($C_2H_3CN$) and ethyl cyanide ($C_2H_5CN$), which have both been detected in the ISM. The second pathway leads to the fully saturated species propylamine ($C_3H_9N$). These results might indicate how general carbon chains can hydrogenate in the ISM and how functional groups, such as the cyano-group can hydrogenate under cold conditions. Future work will include how surface molecules possibly influence the presented reactions.