The cold path to saturation:
hydrogenation of cyanoacetylene towards ethyl cyanide in dark molecular clouds

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Cyanoacetylene (HC_3N) is a nitrogen-bearing carbon chain that is ubiquitous in the 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 it 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 and CCSD(T)-F12 calculations to obtain the energy profiles of various hydrogenation pathways. Based on activation and reaction energies of the gas phase reactions, the most favourable pathways lead to vinyl cyanide and ethyl cyanide, which have also been detected in the ISM. Additionally we present some first results on the interaction of HC_3N with H_2O ice clusters. The next step is to obtain the energy profiles for the HC_3N hydrogenation on an H_2O ice cluster, and to investigate the kinetics of the reactions. This will indicate whether HC_3N can hydrogenate to form saturated species on ice grains in the ISM.