DISCOVERING NOVEL GAS-PHASE NITROGEN-HETEROCYCLE FORMATION PATHWAYS WITH AN AB INITIO NANOREACTOR

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Nitrogen-containing heterocycles pose an intriguing astrochemical mystery. 45 different varieties have been detected on meteorites with non-terrestrial isotopic abundances, but none have been detected in space despite numerous search attempts. It is unclear if these species are most likely to form through low-temperature gas-phase chemistry, photoprocessing of icy grains, aqueous chemistry in a meteorite parent body, or a combination of processes. Reactions involving radicals have recently shown promise as N-heterocycle formation mechanisms, particularly in low temperature gas-phase chemistry. We have used an ab initio molecular dynamics "nanoreactor" simulation developed for chemical reaction discovery to reveal multiple novel gas-phase N-heterocycle formation pathways from nonintuitive molecular precursors. Many reactants identified in the simulations are similar to known interstellar molecules but have not specifically been studied with rotational spectroscopy, precluding astronomical searches and warranting further experimental and theoretical study. These simulations also reinforce previous experimental and theoretical studies which have shown that smaller N-heterocycles may serve as precursors to larger ones. This type of computational investigation may be a useful tool for furthering our understanding of chemistry in the interstellar medium.