QUANTUM CHEMICAL STUDIES OF LOW-ENERGY PATHWAYS TO ORGANIC SPECIES ON INTERSTELLAR ICY GRAIN MANTLES

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Quantum chemical density functional theory cluster calculations were used to investigate low-energy pathways on icy grain mantles that lead to the formation of organic molecules of relevance to astrobiology. After providing an update on a series of calculations on reactions between NH_3 and carbonyl species (formaldehyde, acetaldehyde, and acetone), we will present results about a new family of reactions, the low-energy deposition of various cations on ice clusters. It was found that a sequence of barrierless processes can occur that offer alternative pathways to well-known, abundant astromolecules. For example, the HCO^+ and CH_3^+ cations will react with H_2O in ice with no barrier to produce, respectively, protonated formic acid ($HCOOH_2^+$) and protonated methanol ($CH_3OH_2^+$). These intermediates then spontaneously lose their protons to the ice to yield formic acid and methanol. An incoming ion can also react with other species already adsorbed on ice. An example of this is the reaction of OH^+ with CO to yield $HOCO^+$, which subsequently loses its proton to yield CO_2. The calculations indicate that all of these ion-ice reactions can occur at ultracold temperatures with no energetic processing.