QUANTUM CHEMICAL STUDIES OF LOW-ENERGY PATHWAYS TO ORGANIC MOLECULES ON INTERSTELLAR ICY GRAIN MANTLES. D. E. Woon and L. Chen, Department of Chemistry, University of Illinois at Urbana-Champaign, Box 92-6 CLSL, 600 S. Mathews Ave., Urbana, IL 61801; email: de-woon@illinois.edu.

Abstract. Quantum chemical density functional theory cluster calculations were used to characterize low-energy pathways on interstellar icy grain mantles that lead to the formation of organic species of interest to astrobiology. One set of calculations involved ammonia (NH$_3$) reactions with the carbonyl species formaldehyde, acetaldehyde, and acetone. It was found that in large ice clusters NH$_3$ reacts spontaneously with all three species to form protonated hydroxyl amine species, and a second NH$_3$ can remove the extra proton with little or no barrier. Another set of calculations investigated low-energy deposition of various cations on ice clusters and found that a sequence of barrierless processes can occur that offer alternative pathways to well known interstellar molecules. For example, the HCO$^+$ and CH$_3^+$ cations will react with H$_2$O in ice with no barrier to produce protonated formic acid (HCOOH$_2^+$) and protonated methanol (CH$_2$OH$_2^+$), respectively. These intermediates then spontaneously lose their protons to the ice to yield the neutrals. Also, OH$^+$ can react with CO adsorbed on ice to yield HOCO$^+$, then lose the extra proton to form CO$_2$, all without barriers. All of these ion-ice reactions can occur at ultracold interstellar temperatures with no energetic processing. They yield carbon-containing species that can contribute to the formation of biological precursor molecules.