



**Joint Seminar Series of the
CENTRE FOR RESEARCH IN MOLECULAR MODELING,
MERCK FROSST and the
DEPARTMENT OF CHEMISTRY AND BIOCHEMISTRY**

March 2nd, 2007, 2:30 pm - Concordia University SP-S110

On the Formation of Glycine in the Interstellar Medium

Dr. Denise M. Koch

**Département de chimie, Ecole Normale Supérieure, Paris
CERMM and Department of Chemistry & Biochemistry, Concordia University**

In recent years, there has been increasing evidence suggesting that amino acids were originally formed in the Interstellar Medium (ISM) and transported to prebiotic Earth in meteorites and comets. In this presentation, theoretical investigations of possible ion-molecule and neutral routes to the formation of the simplest amino acid glycine under ISM conditions will be reported. The various possible ion-molecule routes investigated so far by electronic structure calculations do not seem to lead to favorable glycine formation in the gas phase. Thus, a neutral Strecker synthesis route to glycine formation has been explored at the surface of cold icy grain mantles in the ISM. In particular, the penultimate step of the Strecker synthesis, which is the reaction between methanimine (CH_2NH) and hydrogen cyanide isomers (HCN or HNC) to produce aminoacetonitrile ($\text{H}_2\text{C(NH)CN}$), and which immediately precedes glycine formation via hydrolysis, will be discussed in detail. Electronic structure calculations indicate that, in the presence of a few water molecules, aminoacetonitrile formation can proceed with a very low barrier of approximately 1 kcal/mol with the HNC (hydrogen isocyanide) isomer, but with a much higher and prohibitive barrier with the HCN (hydrogen cyanide) isomer. A separate study shows that HNC isomerization is slow and that HNC from the ISM adsorbed at the surface of ice grain mantles is likely to survive long enough to react with methanimine to form the aminoacetonitrile precursor. These results support the theory for the origin of life on Earth that glycine may have been formed in the ISM and transported to the prebiotic Earth.

Denise Koch received her undergraduate degree in Chemistry from Concordia University, in 2000. She then pursued graduate studies in Theoretical/Computational Chemistry with Prof. Gilles Peslherbe at Concordia University, where she received a PhD in 2006 for the study of the structure, thermodynamics and spectroscopy of seeded water clusters. She spent one year as a Chateaubriand and NSERC postdoctoral fellow in the group of Dr. James T. Hynes at Ecole Normale Supérieure in Paris, where she studied various reaction pathways of amino acid formation in the interstellar medium, and drug-DNA intercalation. She is presently an NSERC postdoctoral fellow with Prof. Ann English at Concordia, investigating the mechanisms of NO uptake by thiol groups in large proteins such as Calbindin and Hemoglobin.

