BI-CO MATHEMATICS COLLOQUIUM

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"The Flask on the Hard Drive: How to Be a Chemist and Not Get Your Hands Dirty"

Monday, September 10, 2007

Talk at 4:15 p.m.– KINSC H109
Tea at 4:00 p.m. – Math Lounge, KINSC H208

Abstract: "We are perhaps not far removed from the time when we shall be able to submit the bulk of chemical phenomena to calculation." J. L. Gay-Lussac, 1888

Though computational chemistry has existed in theory since the advent of quantum mechanics, it is only within the last few decades with the rapid progress of computers that the practice has come into its own. A major use of computational chemistry is the geometric optimization of a molecular system, used to map its potential energy surface (PES), the potential energy of a system as a function of the relative position of nuclei. Additionally, natural bond orbital (NBO) theory will be discussed in connection with experimental and theoretical results showing significant stabilization in only one conformation of the CH3OCO radical during C-O bond stretching.

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