Abstract Submitted
for the MAR13 Meeting of
The American Physical Society

**Investigating the Singlet-Triplet Gap in Tetramethyleneethane using Quantum Monte Carlo Techniques**[1] ZACHARY POZUN, Department of Chemistry, University of Pittsburgh, JAN HERMANN, Department of Physical and Macromolecular Chemistry, Faculty of Science, Charles University in Prague, KENNETH JORDAN, Department of Chemistry, University of Pittsburgh — Tetramethyleneethane (TME) is an organic molecule composed of two allyl subunits that is the simplest disjoint diradical. The ground state according to experimental and theoretical evidence is a singlet state with $^1$A symmetry. [2] Due to the near degeneracy of the frontier orbitals, however, this state is inherently two-configurational. As the molecule is twisted through torsional angles about the central C-C bond, we compute the singlet-triplet gap using quantum Monte Carlo (QMC). In its diffusion Monte Carlo (DMC) variant, QMC is an exact method for solving the Schrödinger equation within the bounds of the fixed-node approximation. [3] DMC calculations using a multi-configurational trial wave function produce the correct ordering of the singlet and triplet states. We also investigate an alternate approach, full configuration interaction quantum Monte Carlo (FCIQMC). We compare the FCIQMC singlet-triplet energy gap as a function of torsional angle with the different theoretical methods.

[1] Support through NSF Award number 1225384

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Date submitted: 09 Nov 2012

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