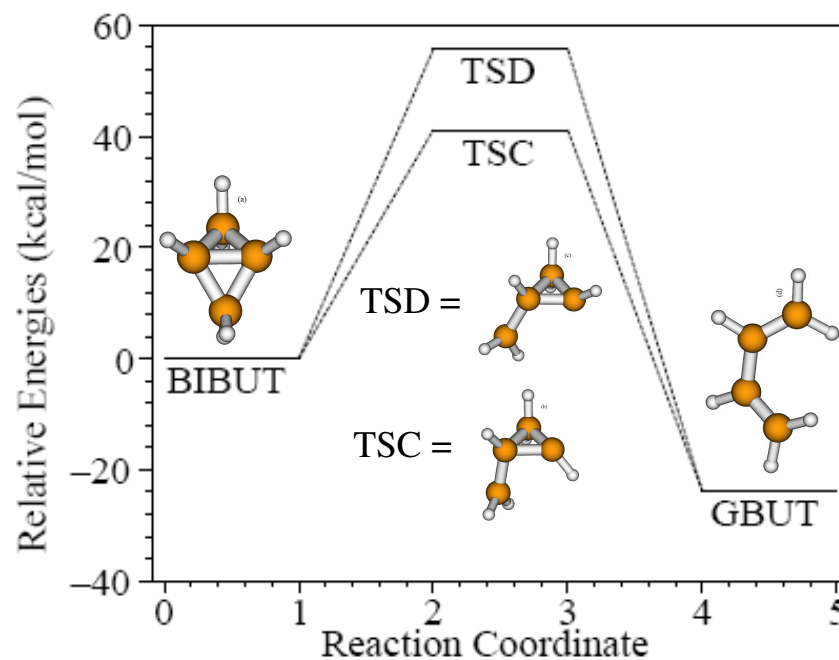


Single- and Multi-reference Correlation Effects from the Direct Calculation of the Two-electron Reduced Density Matrix from the Anti-Hermitian Contracted Schrödinger Equation (ACSE)

What is the ACSE?

$$\int \Psi^* H \Psi d^3d^4\dots dN = E^2 D$$

Schrödinger Equation is Projected Onto the Space of Two Electrons (and then the anti-Hermitian part is selected!)



Conversion of 1,3-Bicyclobutane to *gauche*-1,3-Butadiene via the ACSE

D. A. Mazziotti, *Phys. Rev. Lett.* **97**, 143002 (2006);

D. A. Mazziotti, *Phys. Rev. A* **76**, 052502 (2007);

D. A. Mazziotti, *J. Phys. Chem. A* (submitted).