Read the paper “Complete Multidimensional Analytic Potential Energy Surface for Cl\(^-\) + CH\(_3\)Cl S\(_2\)2 Nucleophilic Substitution”, *J. Phys. Chem.* **1990**, *94*, 2778-2788, and use the following questions to guide your reading. We will discuss these questions in class on Wednesday, 10/17.

- What was the main question that the researchers were trying to answer? What was the hypothesis of the paper?
- What are the purpose of the $S$ terms in the potential energy function given in equation (2)?
- In developing the bending potentials (eq. 5, 6), why is each term in the expansion a sum from $i = 1$-3?
- What functional form (Morse potential, LJ potential, harmonic (or Taylor series expansion) potential, etc.) is used for the bending potentials?
- What functional form is used for the CIC and CH stretch potentials?
- What do $r_c$ and $g_c$ stand for?
- How did the researchers determine the specific terms in the potential functions and how did they decide when they needed to combine two functions with a “switching potential”?
- What are the functions of the three terms in eq. (33)?
- Why is it important that the switching functions have continuous first derivatives? What does it mean (geometrically) if the first derivative is not continuous?
- In developing the plot in Figure 7, were the H-C-H angles and C-H distances fixed or were they allowed to vary in some way? If so, how were they varied?
- In the PES in Figure 7, what is the shape of the surface near the transition state?
- What were the main conclusions of the paper? Did the researchers answer the questions that they were trying to answer?
- This paper is seventeen years old. How (if at all) might this project have differed if it had been done today?
- Please also make note of any questions that you have when you are reading the paper so that we can also address these in class.