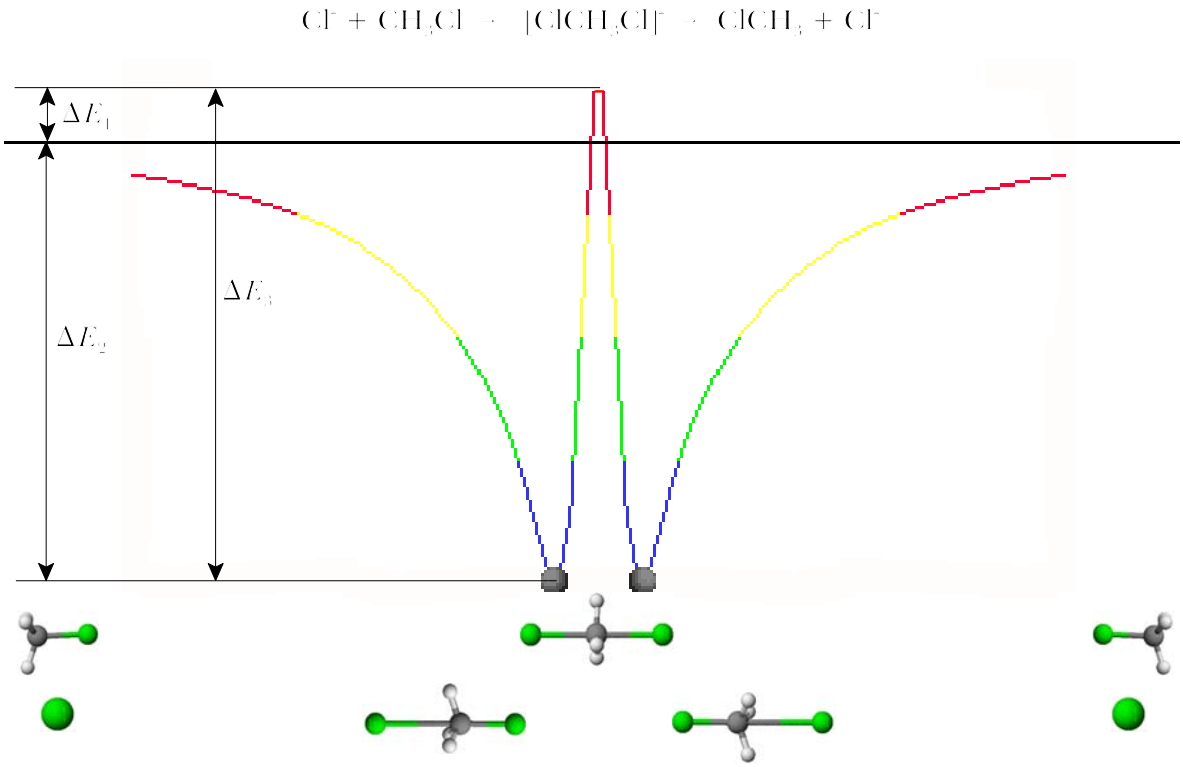
9 Transition States

This laboratory will study the S_N2 reaction between Cl^- and CH_3Cl involving a Walden inversion.



Construct Cl^- using the Text Tool.
Find the $\Delta_f H$ by clicking MOPAC / Compute Properties / Theory: PM3 / Properties: Heat of Formation and click Run.
Save as cl-pm3.c3d. Record $\Delta_f H(Cl^-)$ = _____ kcal mol^{-1}.
Close.

Construct CH_3Cl using the Text Tool and minimize at the PM3 level.
Save as ch3clpm3.c3d. Record $\Delta_f H(CH_3Cl)$ = _____ kcal mol^{-1}.

Save as clch3cl-pm3.c3d.
Construct $ClCH_3Cl^-$ by adding a Cl^- using the Text Tool and connecting the Cl^- and the C atom using the Uncoordinated Bond Tool (7^{th} on left) and calculate $\Delta_f H$.
Minimize at the PM3 level and record $\Delta_f H(ClCH_3Cl^-)$ = _____ kcal mol^{-1}.
Save.

Save as clch3cl-tspm3.c3d.
Click View / Setup / Model Build and uncheck Rectify. Click OK.
Click the C atom and drag it to the center of the H atoms.
Determine the energy of the transition structure by clicking MOPAC / Optimize to Transition State / Theory: PM3 and click Run.
Save and record $\Delta_f H(ClCH_3Cl^-ts)$ = _____ kcal mol^{-1}.

Calculate ΔE_1 = _____ kcal mol^{-1} (literature 3 ± 1 kcal mol^{-1}), ΔE_2 = _____ kcal mol^{-1} (literature -12 ± 2 kcal mol^{-1}), and ΔE_3 = _____ kcal mol^{-1} (literature 13 ±2 kcal mol^{-1}). Note better agreement can be obtained by using a higher level of theory.