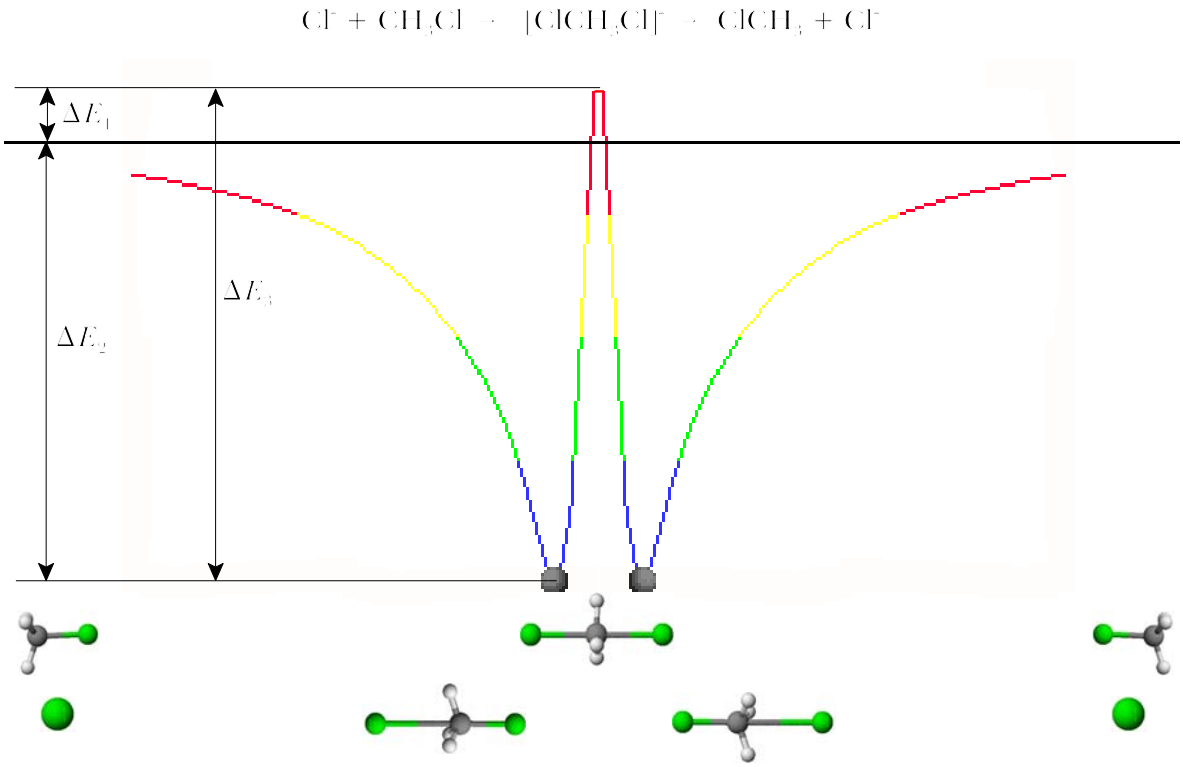
9 Transition States

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



Construct Cl^-. Double click the Drawing Tool, choose Cl, and draw a Cl atom in the workspace. Click the Select Tool and select the Cl atom. Click Build / Set Charge and enter -1. Click OK.

Click Setup / Semiempirical / PM3. Click Options and enter -1 for Total Charge and 1 for Spin Multiplicity. Click OK twice.

Find the $\Delta_f H$ by clicking Compute / Single Point and record $\Delta_f H(Cl^-)$ = _____ kcal mol^{-1}.

Save as cl-pm3.HIN.

Close.

Construct CH_3Cl and minimize at the PM3 level. Record $\Delta_f H(CH_3Cl)$ = _____ kcal mol^{-1}.

Save as ch3clpm3.HIN.

Save as clch3cl-pm3.HIN.

Construct $ClCH_3Cl^-$ by attaching a Cl^- to the C atom. Click Build / Allow Arbitrary Valences and draw a Cl atom connected to the C atom on the H side using a long bond. Select the C atom and set the charge as -1.

Minimize at the PM3 level using a charge of -1 and Spin Multiplicity of 1 in the PM3 setup. Record $\Delta_f H(ClCH_3Cl^-)$ = _____ kcal mol^{-1}.

Save.

Save as clch3cl-tspm3.HIN.

Click Select to confirm that Multiple Selections and Atoms are checked. Select the C atom and the three H atoms. Click Select / Name Selection / Other and enter "flat" or some other name. Click OK. Right click in the workspace.

Click Setup / Restraints and Add 4-flat. Click Restrained Value / Other and enter 180 and Force Constant / Other and enter 500.

Minimize at the PM3 level 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.