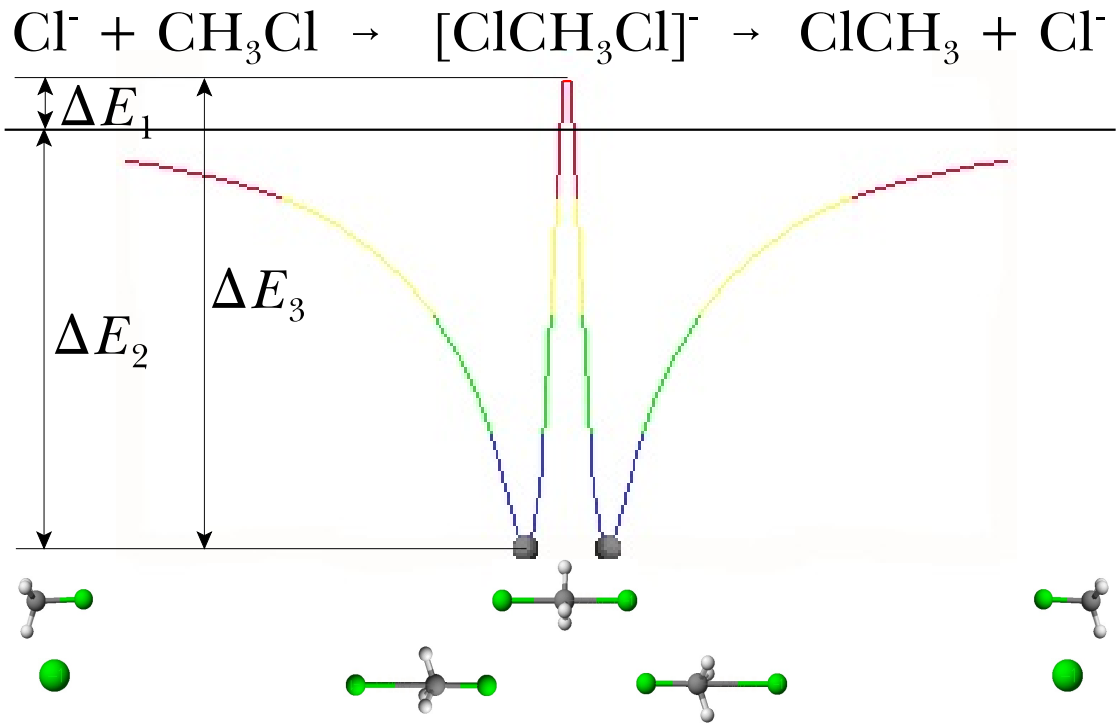
9 Transition States

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



Construct Cl^- using the Chlorine Atom fragment. Calculate the energy at the PM3 level using Job: Energy and be sure the charge is listed as -1, Save as clneg.chk and clneg.cjf. Record the energy from the summary of results window _____ Eh.

Construct CH_3Cl and minimize at the PM3 level. Save the files with appropriate names. Record the energy _____ Eh and use the Inquire icon to determine the C-Cl bond length _____ Å.

Close everything except the main Control Panel.

Construct $ClCH_3Cl^-$. Start with the Carbon Tetravalent fragment. Click the Add Valence icon (1st row, 10th across) and click the C atom. Click each of the axial H atoms with a Chlorine terminal fragment. Click the Clean icon.

Click the Redundant Coordinate Editor icon to open the Redundant Coordinate Editor dialog window. Click the Create a New Coordinate icon and choose Bond for the Coordinate. Click one of the Cl atoms and the C atom. Click Scan Coordinates, 35 steps, 0.1 Å. Set the minimum as 1.5 and the maximum as 5.0. Click OK.

Click Calculate / Gaussian and choose Job: Scan, Relaxed (Redundant Coordinates) and Method: PM3, -1 for charge, Doublet. Save as clch3clneg.chk and clch3clneg.cjf.

Open the output file and summary of results. Click View / Labels to label the atoms with numbers so that the Cl atom can be identified. Click the up/down arrows to observe the steps in the PES above.

Record the energy of the first structure corresponding to the van der Waals complex and record the two C-Cl bond lengths using the Inquire icon: _____ Eh, _____ Å, _____ Å (literature 3.27 Å, 1.83 Å).

Click the up/down arrows until the trigonal bipyramidal transition structure is obtained. Record the two C-Cl bond lengths using the Inquire icon: _____ Eh, _____ Å, _____ Å (literature 2.38 Å).

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.)