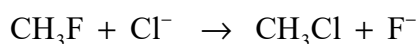


Homework 3: transition states and ground state properties

1. Compare proton hyperfine couplings computed for the UB3LYP/cc-pVDZ optimised structure of neutral phenyl radical (benzene without one hydrogen) using RB3LYP/cc-pVDZ, UB3LYP/cc-pVDZ and UB3LYP/EPR-II methods. Comment on the results and compare them to experimental data.
2. Use the redundant coordinate editor in GaussView to set up a potential energy scan with respect to the C–H bond stretch in methane (between 1 and 4 Angstroms). Run the scan using RHF, UHF, RMP2, UMP2, RCCSD, UCCSD, RB3LYP and UB3LYP methods in a cc-pVDZ basis set. Read the logs with GaussView and use its scan visualisation functionality to plot the molecular energy against the C–H bond length. Comment on what you see.

3. Try locating the reaction intermediate saddle point for the nucleophilic substitution reaction:



using M06/cc-pVTZ method. Set `opt=ts` to switch off Hessian eigenvalue control and cause Gaussian to converge to a saddle point. The starting point for the optimisation should be your best guess for the transition state structure of the $\text{S}_{\text{N}}2$ mechanism. Run the vibrational frequency calculation (use `freq` keyword) to demonstrate that the transition state is a saddle point.

4. Optimise the geometry of cyclobutane and run a vibrational analysis job (use `freq` keyword). Visualise the resulting normal mode vibrations in GaussView.
5. Set up a potential energy scan with respect to the C=C bond stretch in ethylene using MP2/cc-pVDZ method with and without counterpoise BSSE correction. Observe the difference in the bond breaking energy profile.