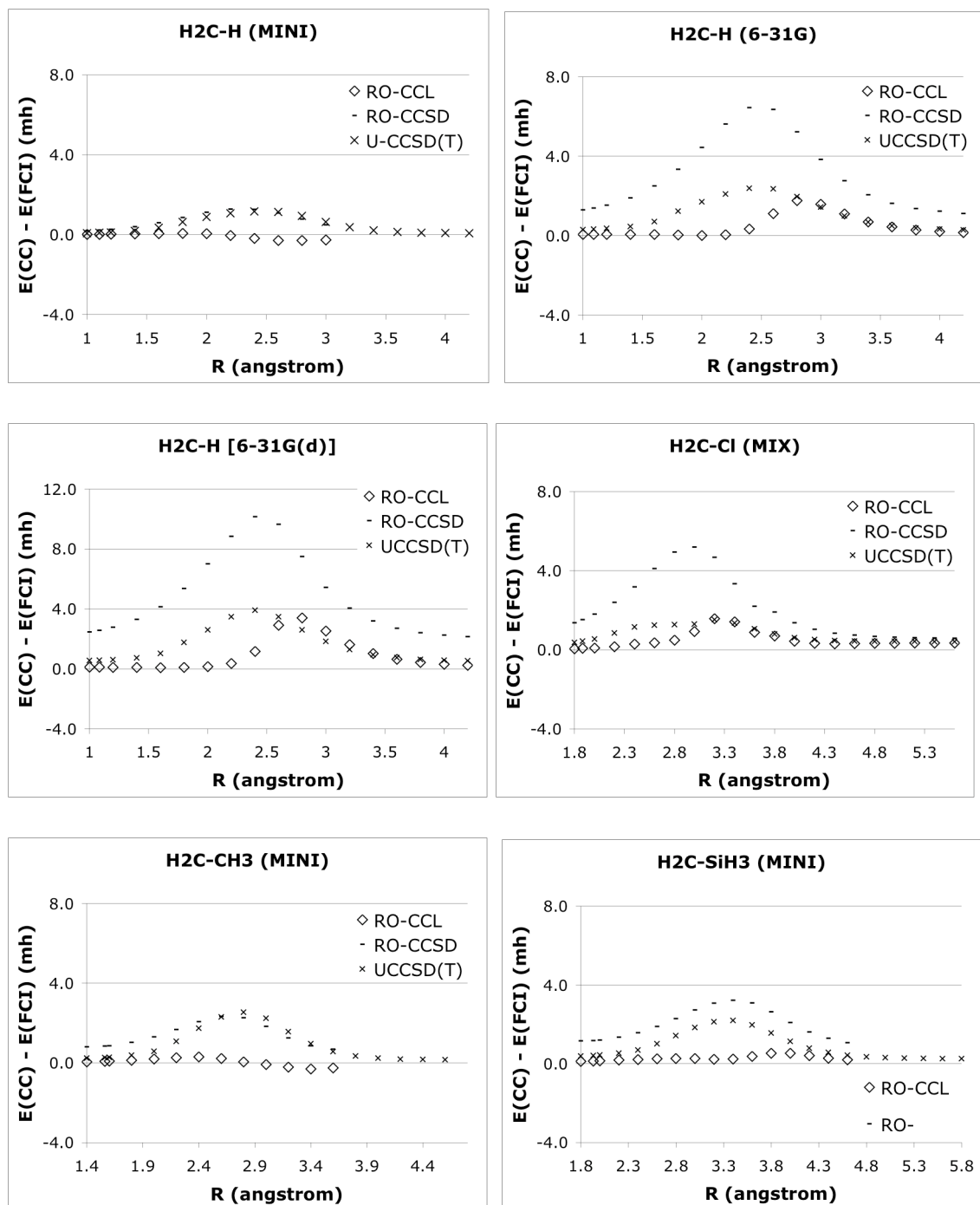
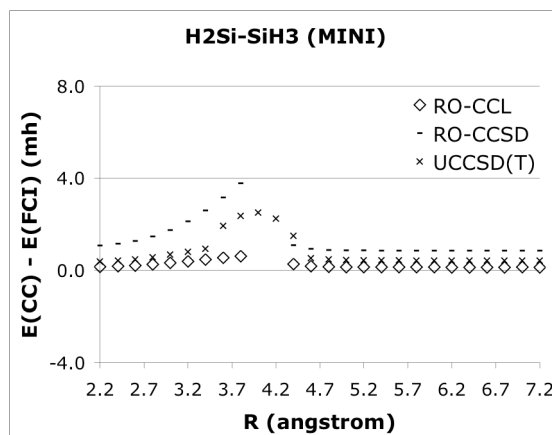
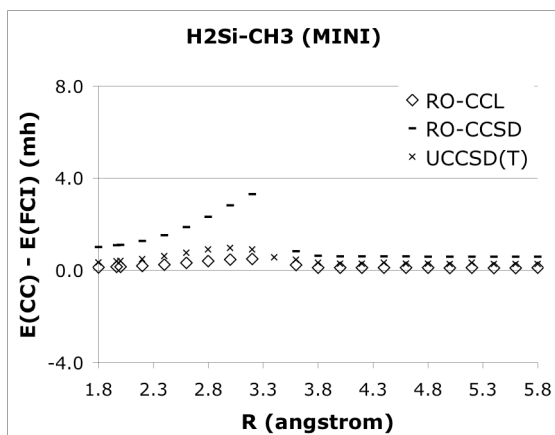
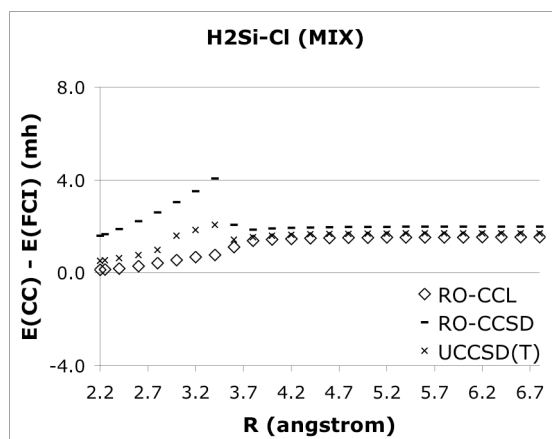
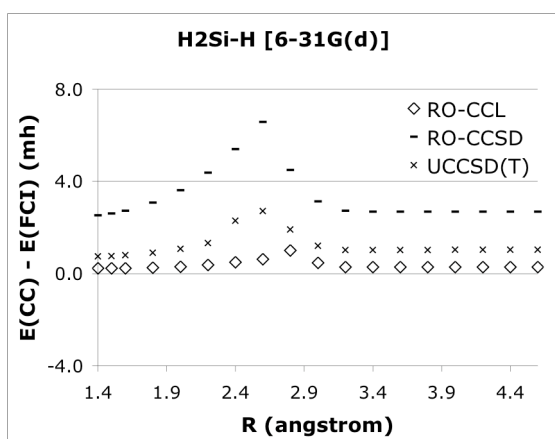
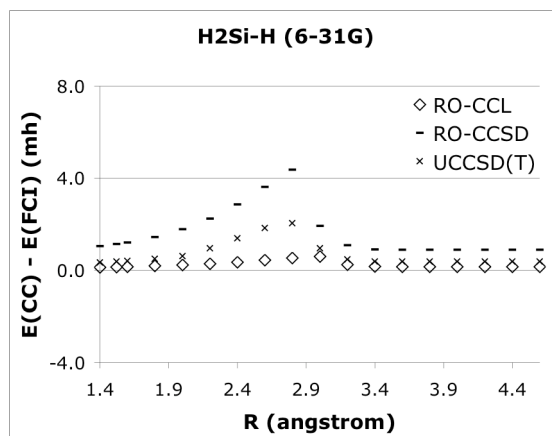
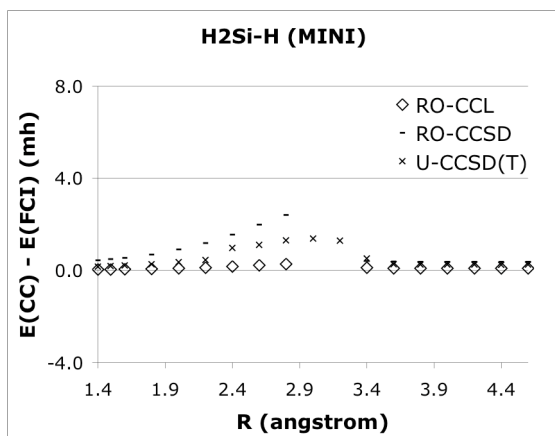


Theoretical Study of $\text{H}_2\text{C}-\text{X} = {}^3\text{H}_2\text{C} + \text{X}$ and $\text{H}_2\text{Si}-\text{X} = {}^1\text{H}_2\text{Si} + \text{X}$

($\text{X}=\text{H}, \text{Cl}, \text{CH}_3,$ and SiH_3) Bond Breaking Reactions

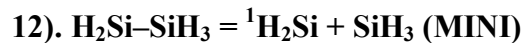
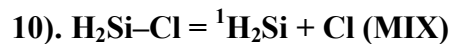
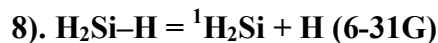
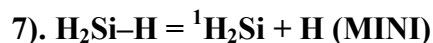
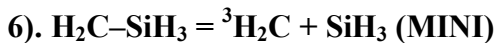
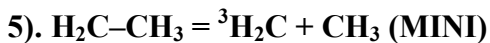
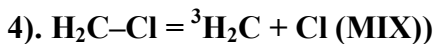
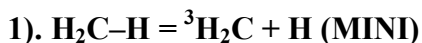
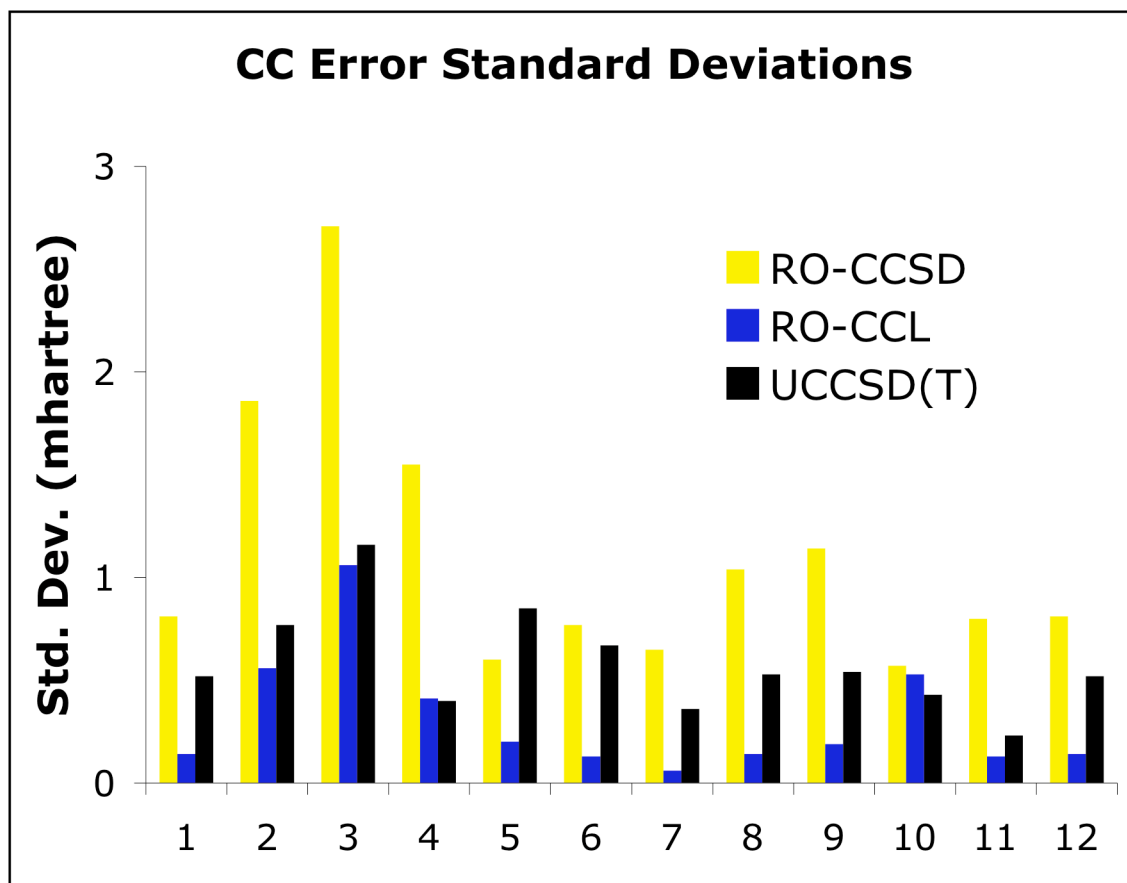
Figure 1: RO-CCSD, RO-CCL, and U-CCSD(T) errors in mhartree. R is the studied bond distance in angstrom.





* MIX stands for the MINI basis set on the C/Si-Cl bond and 6-311G on the H atoms.

Figure 2. Standard deviation (in mhartree) of the errors of the RO-CCSD, RO-CCL, and UCCSD(T) methods.



Conclusions:

The RO-CCL potential energy surfaces agree with the FCI ones within 2 mhartree error for most of the studied bond breaking reactions of open shell species. The largest error is 3.4 mhartree for the $\text{H}_2\text{C}-\text{H} = {}^3\text{H}_2\text{C} + \text{H}$ bond breaking reaction with a 6-31G(d) basis set being used. RO-CCL can be used to predict reasonably accurate potential energy surfaces that are needed to calculate reaction rate constants.

The RO-CCL potential energy surfaces match the FCI ones better than the U-CCSD(T) ones. Also the characteristic CC energy error humps appear at longer bond distances on the RO-CCL PES.