Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

SUPPORTING INFORMATION

Theoretical investigation of the S_N2 mechanism of X^- [X = SH, PH_2] + CH_3Y [Y = F, Cl, Br, I] reactions in water solution

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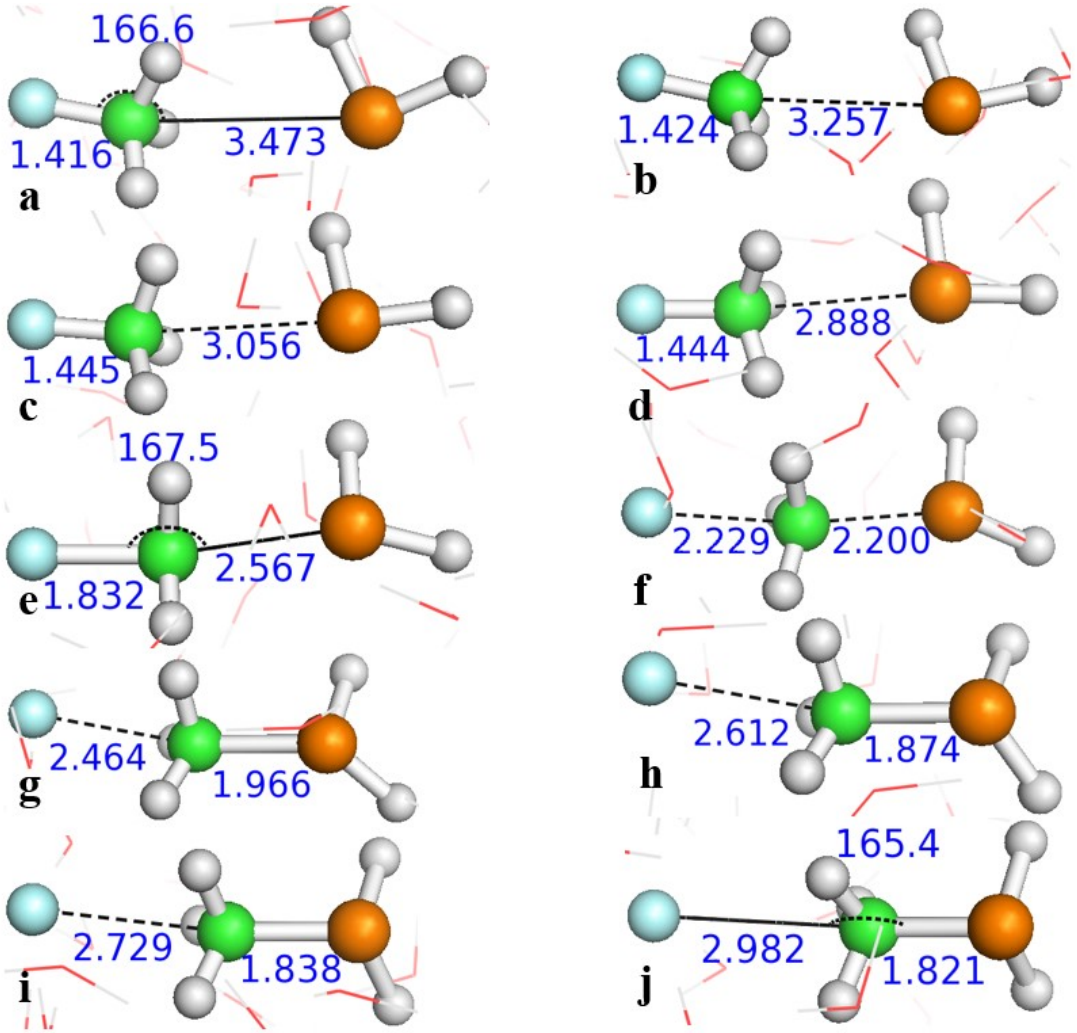

Fig. S1 Structural evolution along the NEB reaction path for the PH_2^- + CH_3F reaction in water solution. No. a is the reactant complex, No. e is the transition state, and No. j is the product complex. The units of the distances and angles are angstroms and degrees, respectively.

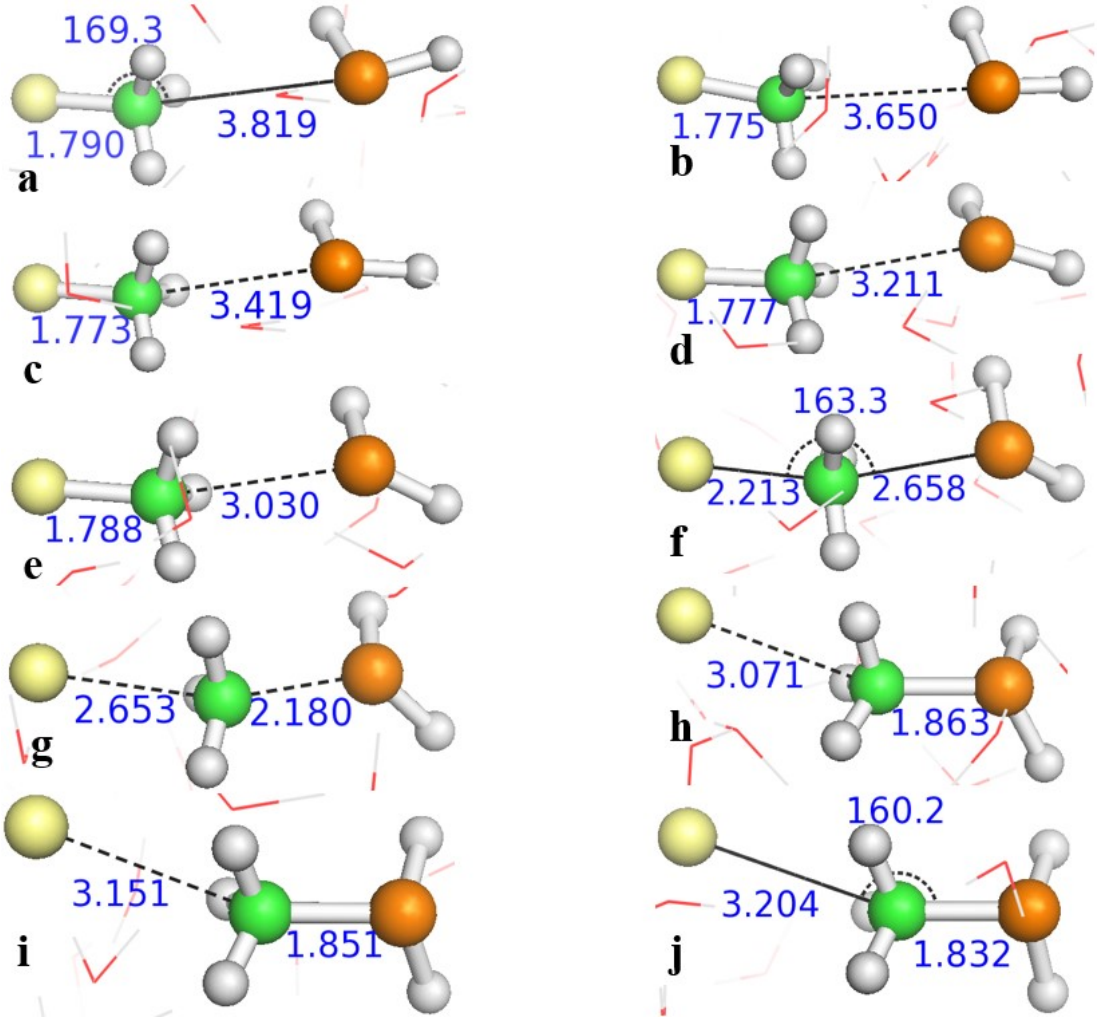

Fig. S2 Structural evolution along the NEB reaction path for the PH_2^- + CH_3Cl reaction in water solution. No. a is the reactant complex, No. f is the transition state, and No. j is the product complex. The units of the distances and angles are angstroms and degrees, respectively.

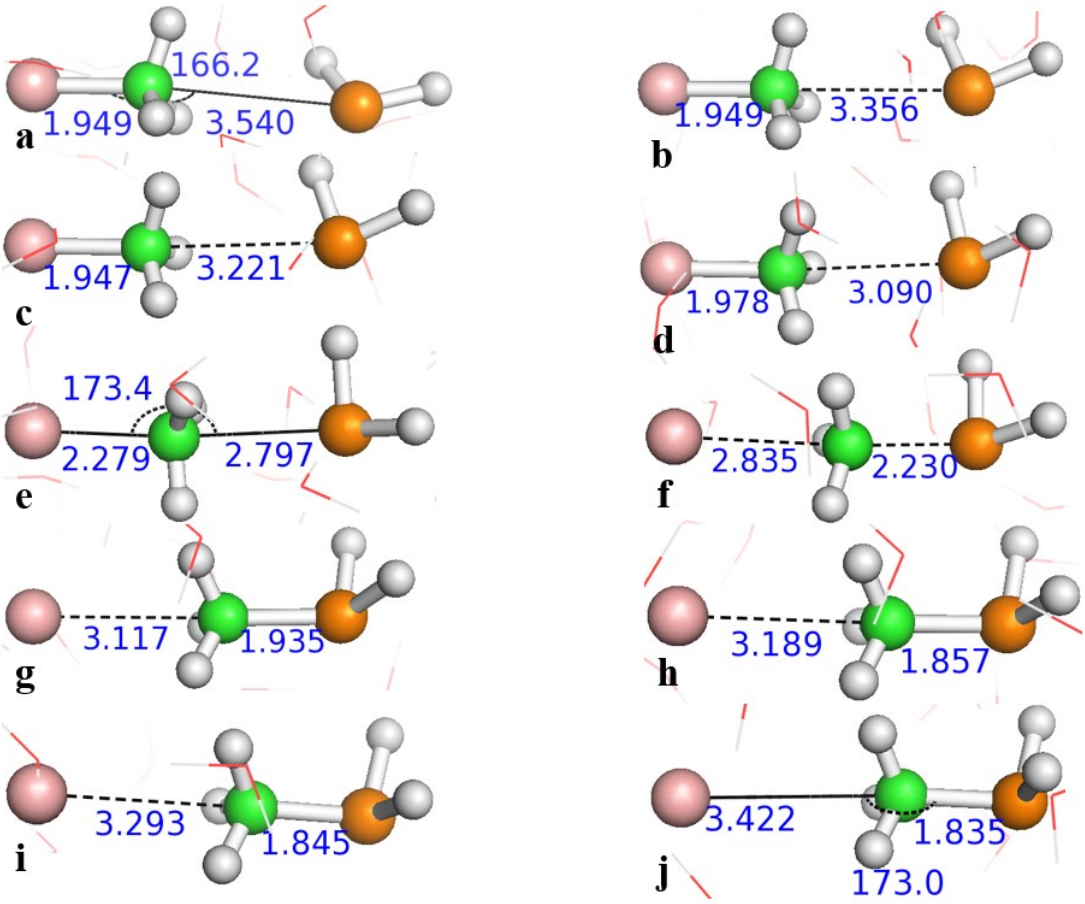

Fig. S3 Structural evolution along the NEB reaction path for the PH_2^- + CH_3Br in water solution. No. a is the reactant complex, No. e is the transition state, and No. j is the product complex. The units of the distances and angles are angstroms and degrees, respectively.

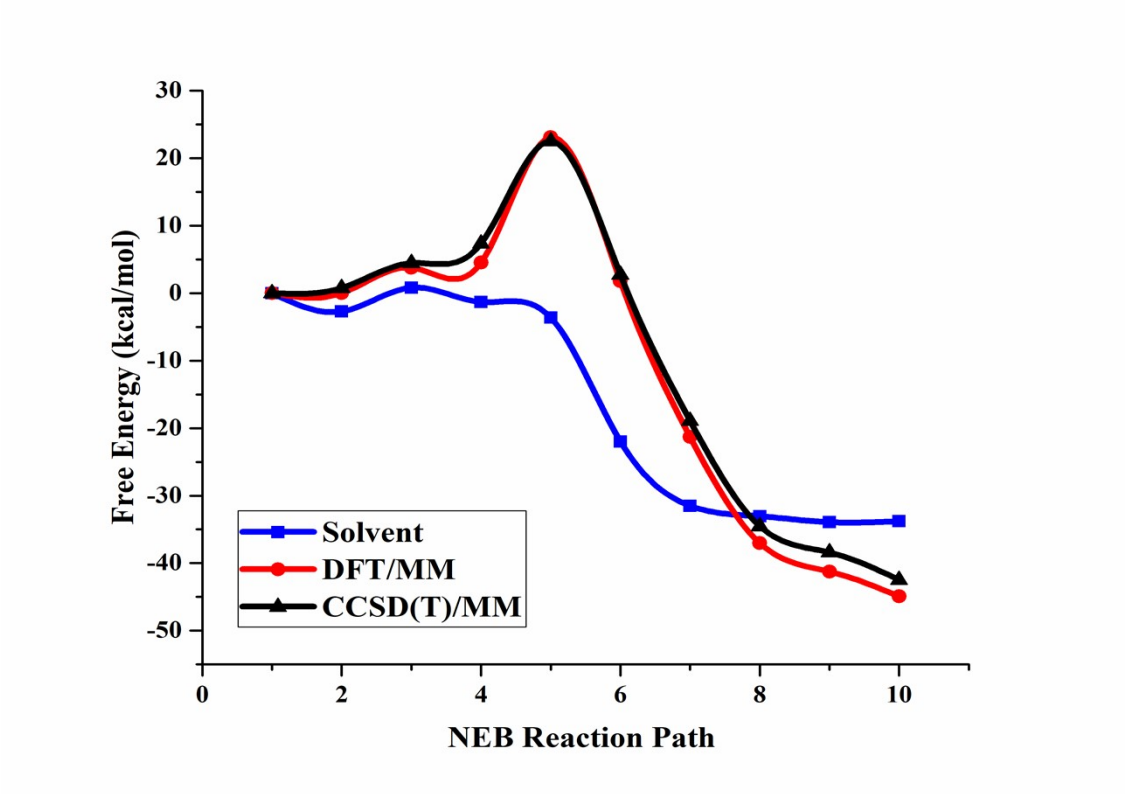

Fig. S4 The potentials of mean force calculated at DFT/MM and CCSD(T)/MM levels of theory and solvent energy contribution with the reactant complex as the energy reference point for the $PH_2^- + CH_3F$ reaction in water solution.

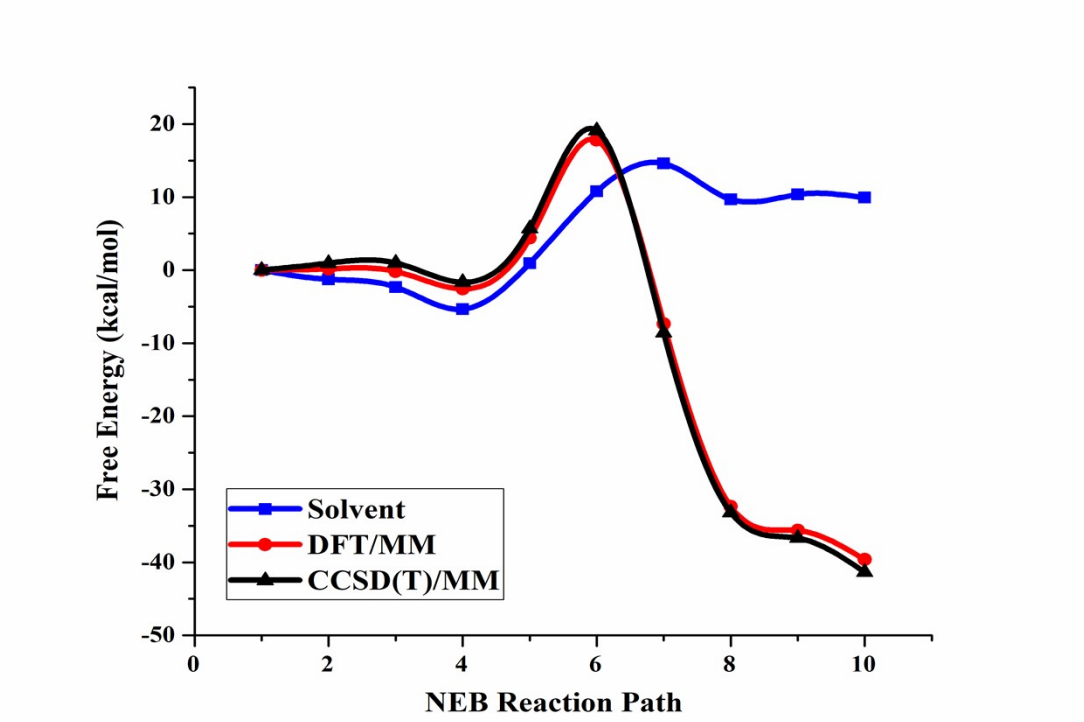

Fig. S5 The potentials of mean force calculated at DFT/MM and CCSD(T)/MM levels of theory and solvent energy contribution with the reactant complex as the energy reference point for the $PH_2^- + CH_3Cl$ reaction in water solution.

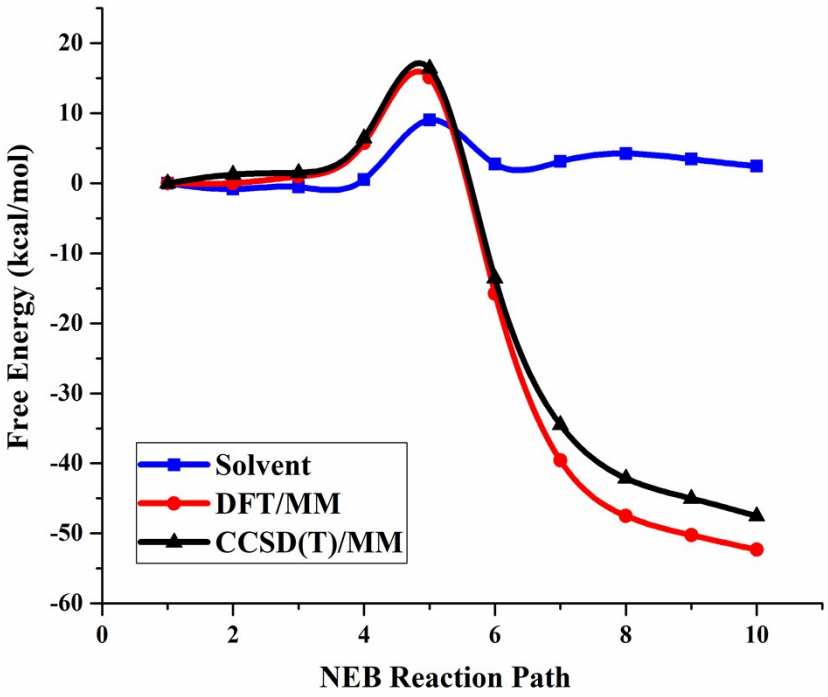

Fig. S6 The potentials of mean force calculated at DFT/MM and CCSD(T)/MM levels of theory and solvent energy contribution with the reactant complex as the energy reference point for the $PH_2^- + CH_3Br$ reaction in water solution.

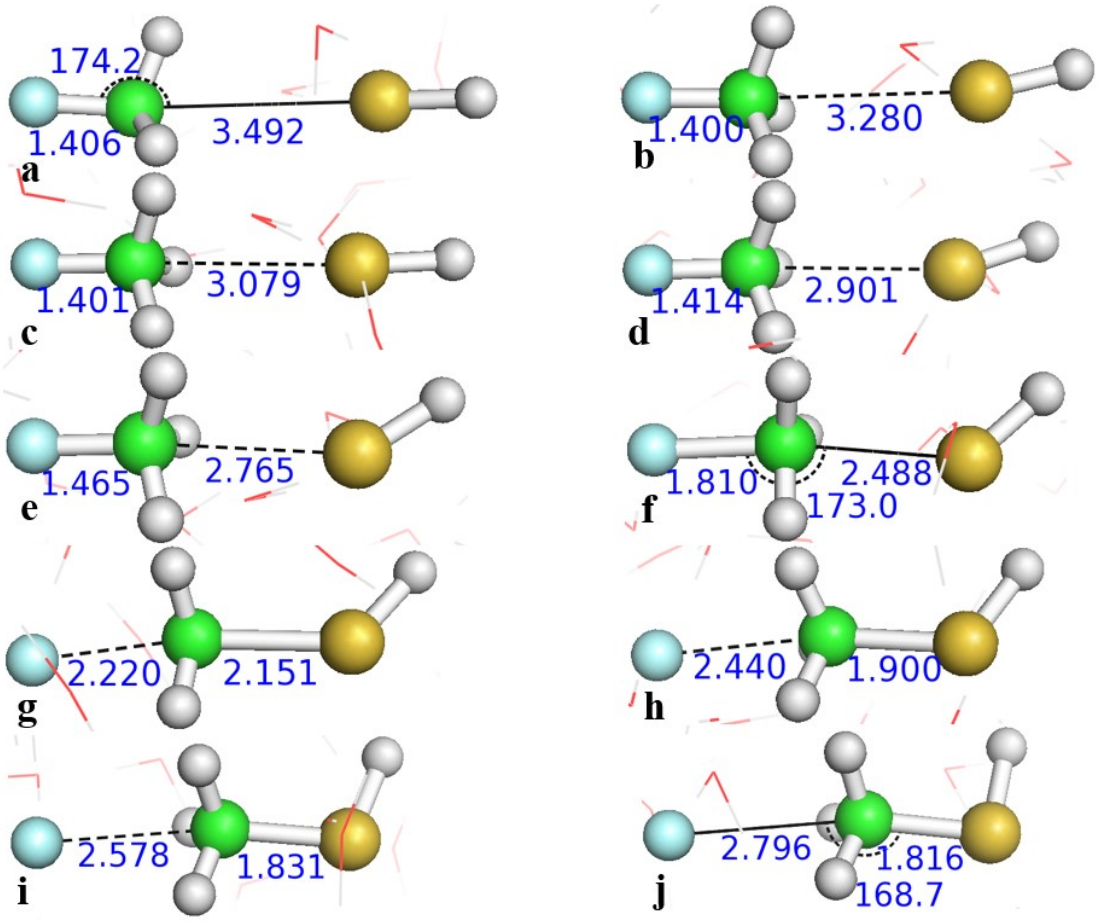

Fig. S7 Structural evolution along the NEB reaction path for the SH^- + CH_3F reaction in water solution. No. a is the reactant complex, No. f is the transition state, and No. j is the product complex. The units of the distances and angles are angstroms and degrees, respectively.

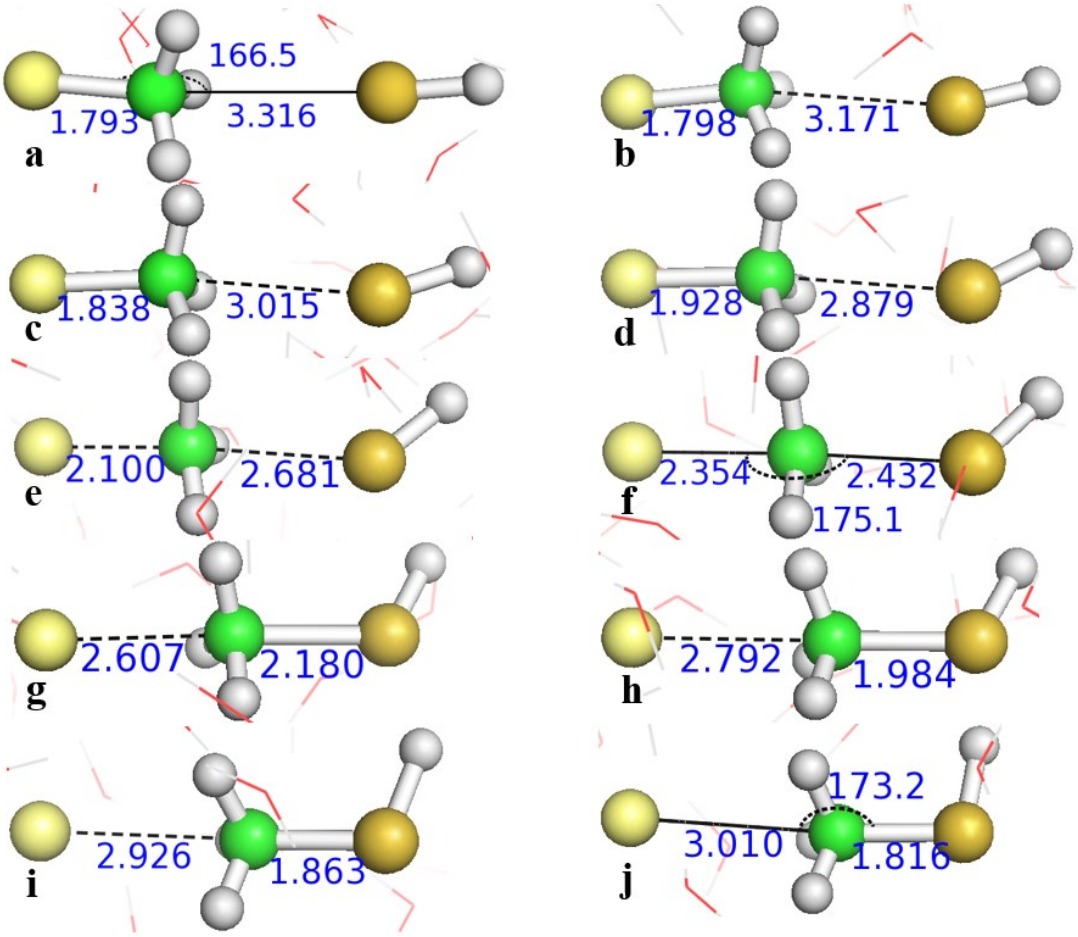

Fig. S8 Structural evolution along the NEB reaction path for the SH^- + CH_3Cl reaction in water solution. No. a is the reactant complex, No. f is the transition state, and No. j is the product complex. The units of the distances and angles are angstroms and degrees, respectively.

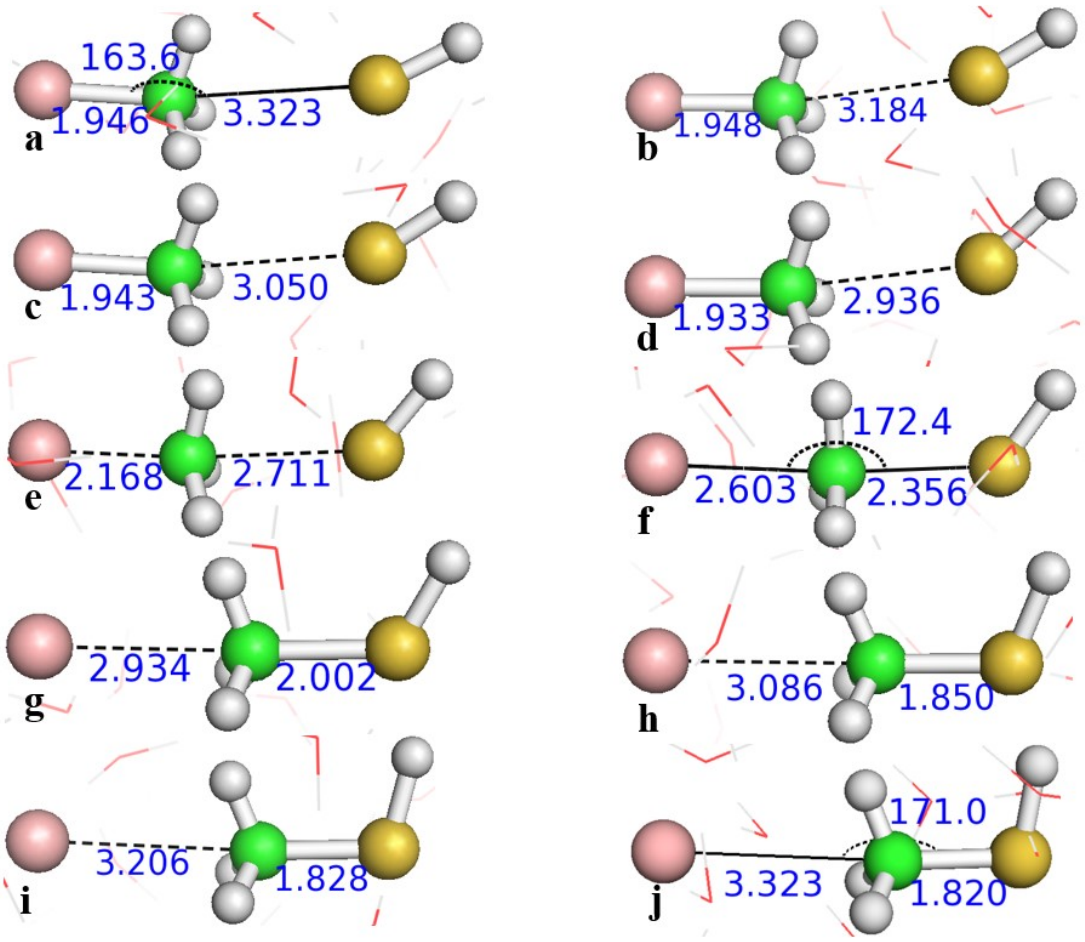

Fig. S9 Structural evolution along the NEB reaction path for the SH^- + CH_3Br reaction in water solution. No. a is the reactant complex, No. f is the transition state, and No. j is the product complex. The units of the distances and angles are angstroms and degrees, respectively.

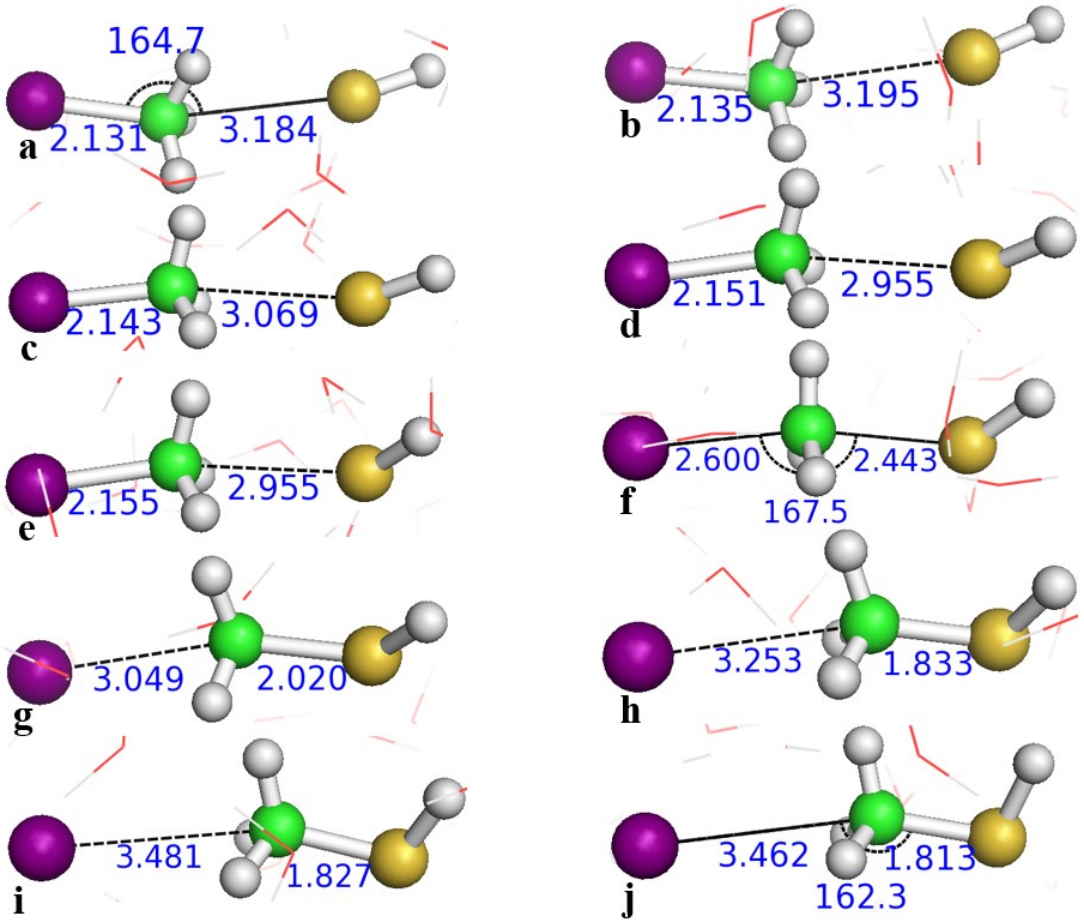

Fig. S10 Structural evolution of the NEB reaction path for the $SH^- + CH_3I$ reaction in water solution. No. a is the reactant complex, No. f is the transition state, and No. j is the product complex. The units of the distances and angles are angstroms and degrees, respectively.

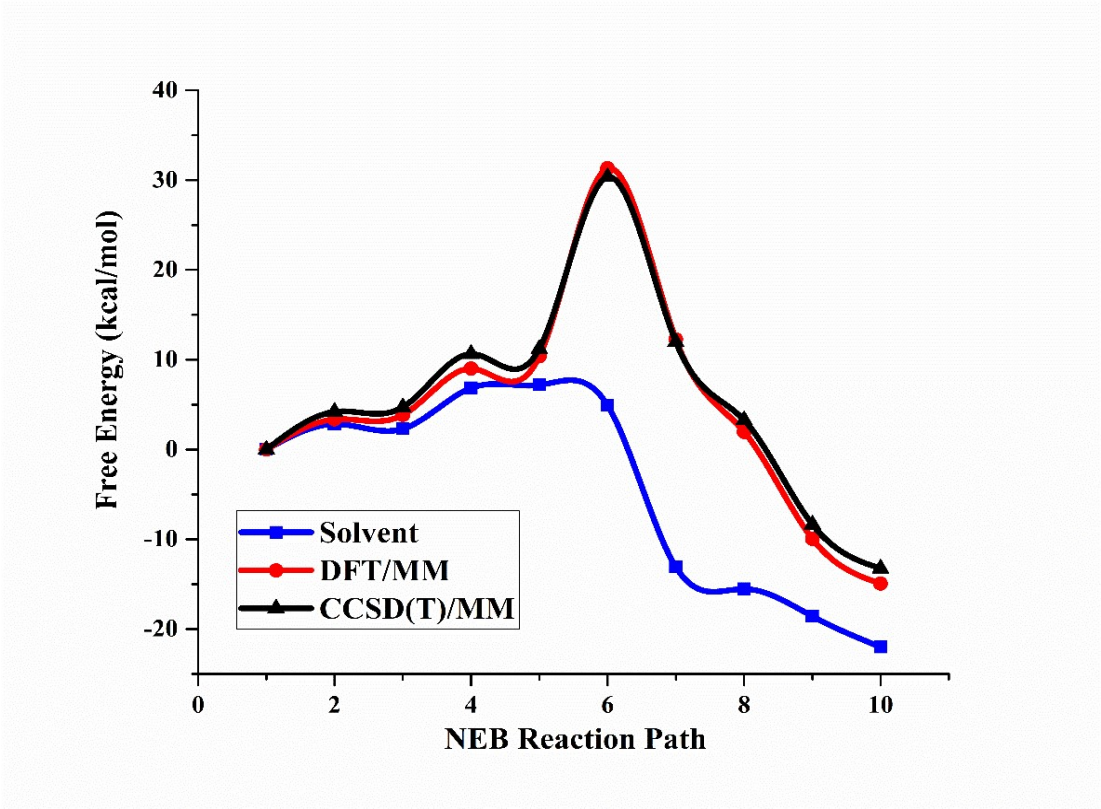

Fig. S11 The potentials of mean force calculated at DFT/MM and CCSD(T)/MM levels of theory and solvent energy contribution with the reactant complex as the energy reference point for the $SH^- + CH_3F$ reaction in water solution.

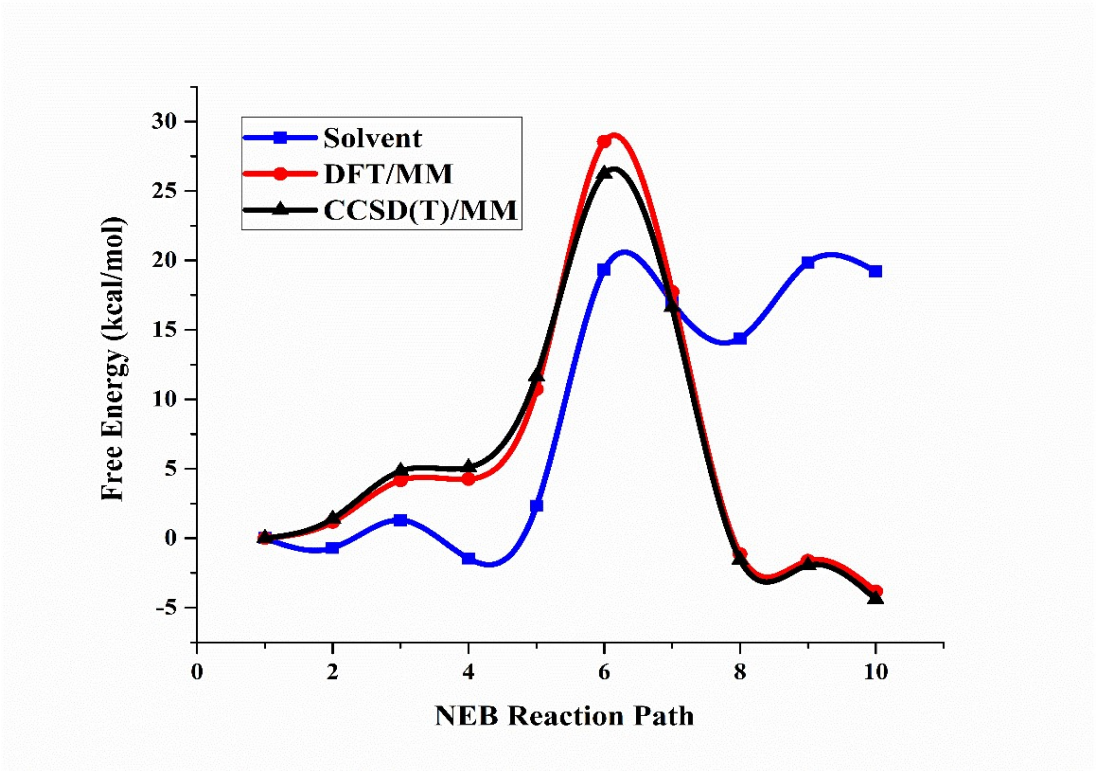

Fig. S12 The potentials of mean force calculated at DFT/MM and CCSD(T)/MM levels of theory and solvent energy contribution with the reactant complex as the energy reference point for the $SH^- + CH_3Cl$ reaction in water solution.

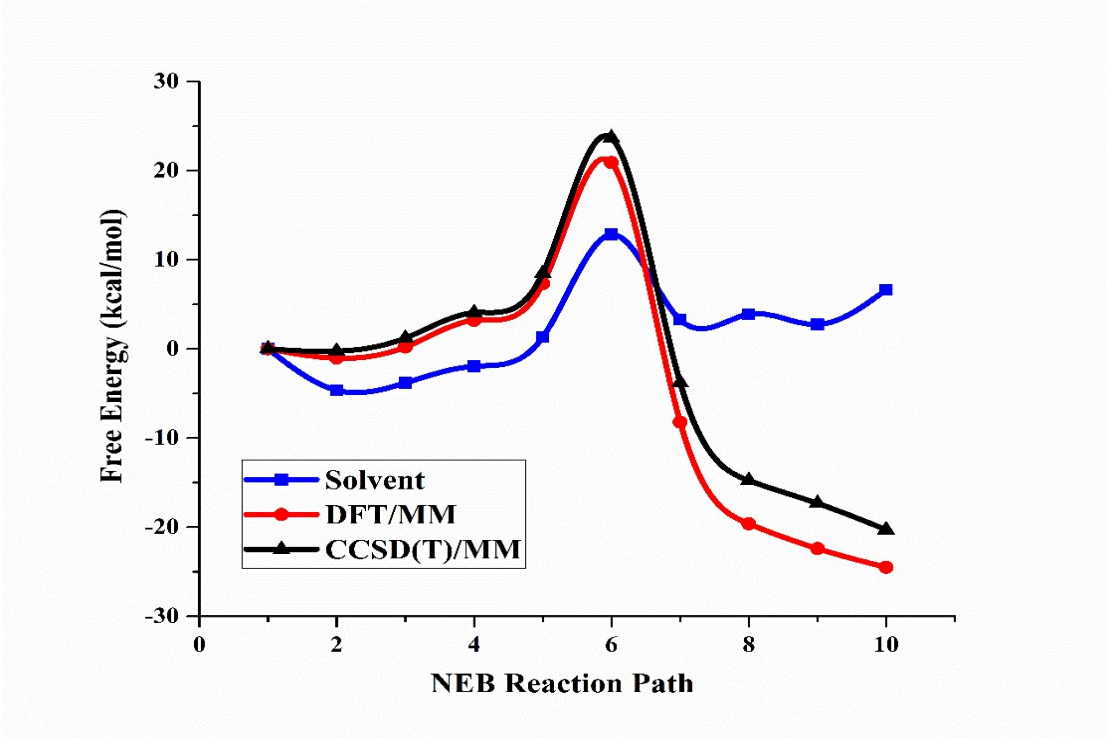

Fig. S13 The potentials of mean force calculated at DFT/MM and CCSD(T)/MM levels of theory and solvent energy contribution with the reactant state as the energy reference point for the $SH^- + CH_3Br$ reaction in water solution.

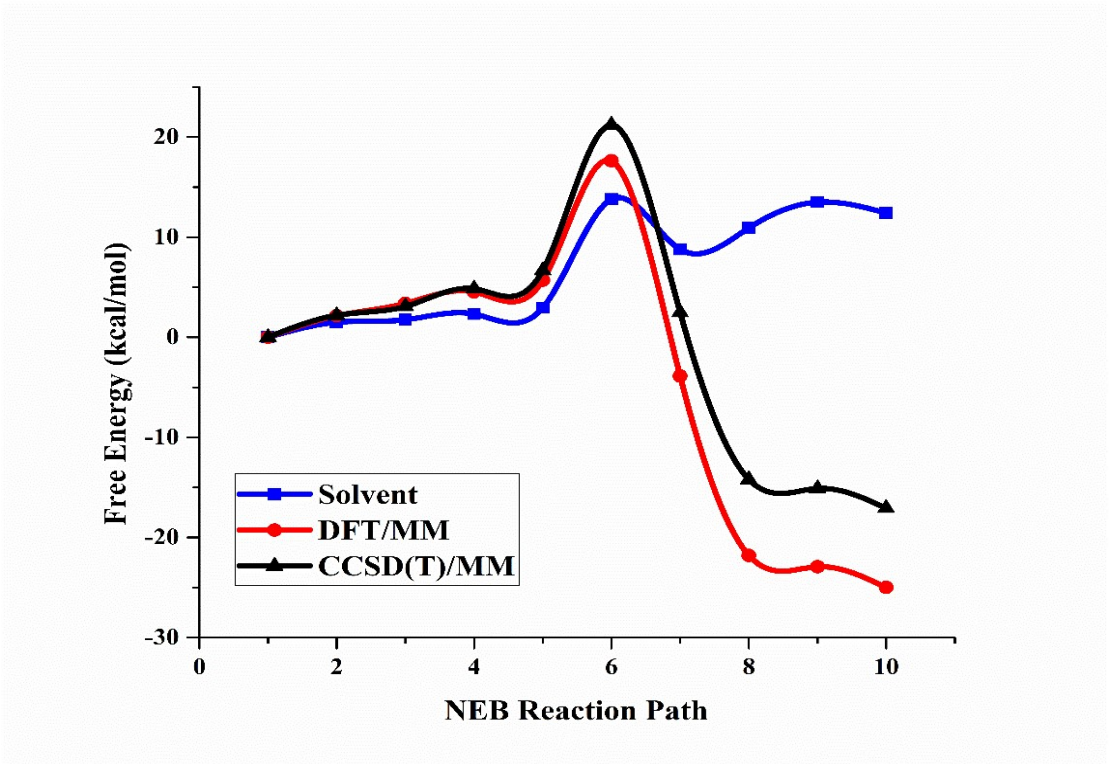

Fig. S14 The potentials of mean force calculated at DFT/MM and CCSD(T)/MM levels of theory and solvent energy contribution with the reactant complex as the energy reference point for the $SH^- + CH_3I$ reaction in water solution.