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$_3$F 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 $\text{PH}_2^− + \text{CH}_3\text{Cl}$ 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 $\text{PH}_2^-$ + $\text{CH}_3\text{Br}$ 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$_3$F 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 $\text{PH}_2^- + \text{CH}_3\text{Cl}$ 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 \( \text{PH}_2^- + \text{CH}_3\text{Br} \) reaction in water solution.
Fig. S7  Structural evolution along the NEB reaction path for the $\text{SH}^- + \text{CH}_3\text{F}$ 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 $\text{SH}^- + \text{CH}_3\text{Cl}$ 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 \( \text{SH}^- + \text{CH}_3\text{Br} \) 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 $\text{SH}^- + \text{CH}_3\text{I}$ 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 $\text{SH}^- + \text{CH}_3\text{F}$ 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 $\text{SH}^- + \text{CH}_3\text{Cl}$ 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 $\text{SH}^- + \text{CH}_3\text{Br}$ 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 $\text{SH}^- + \text{CH}_3\text{I}$ reaction in water solution.