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Electronic Supplementary Information

Quantum dynamics analysis of transition-state spectrum for the SH + H_2S → H_2S + SH reaction.

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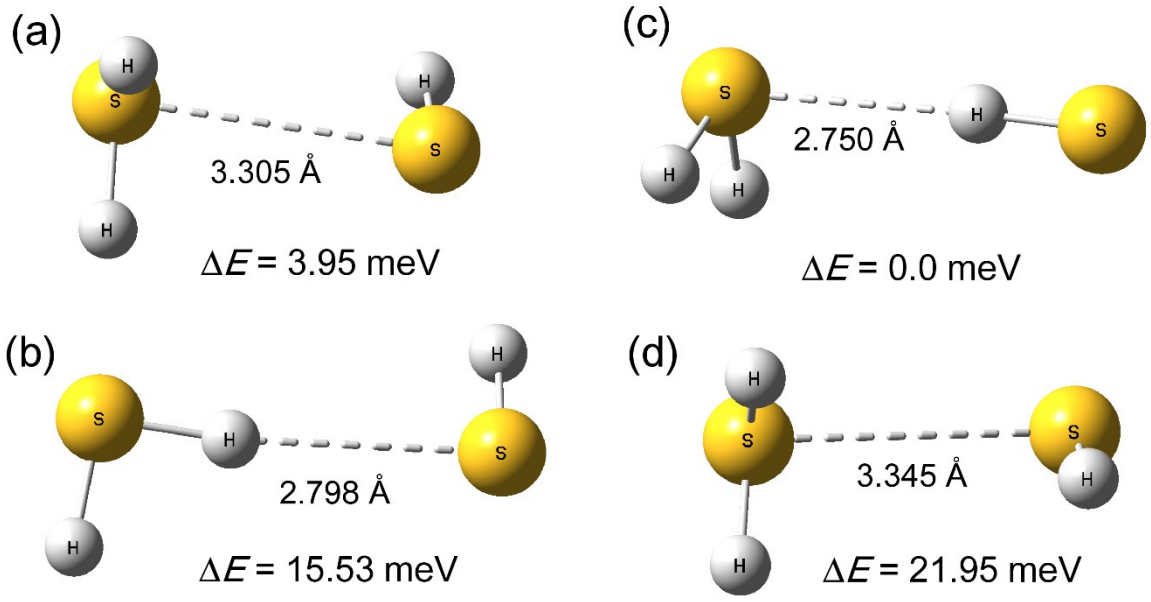

Fig. S1
Molecular structures of the SH···H_2S complex optimized at the MP2/aug-cc-pVDZ level of theory. Relative energies are also shown.

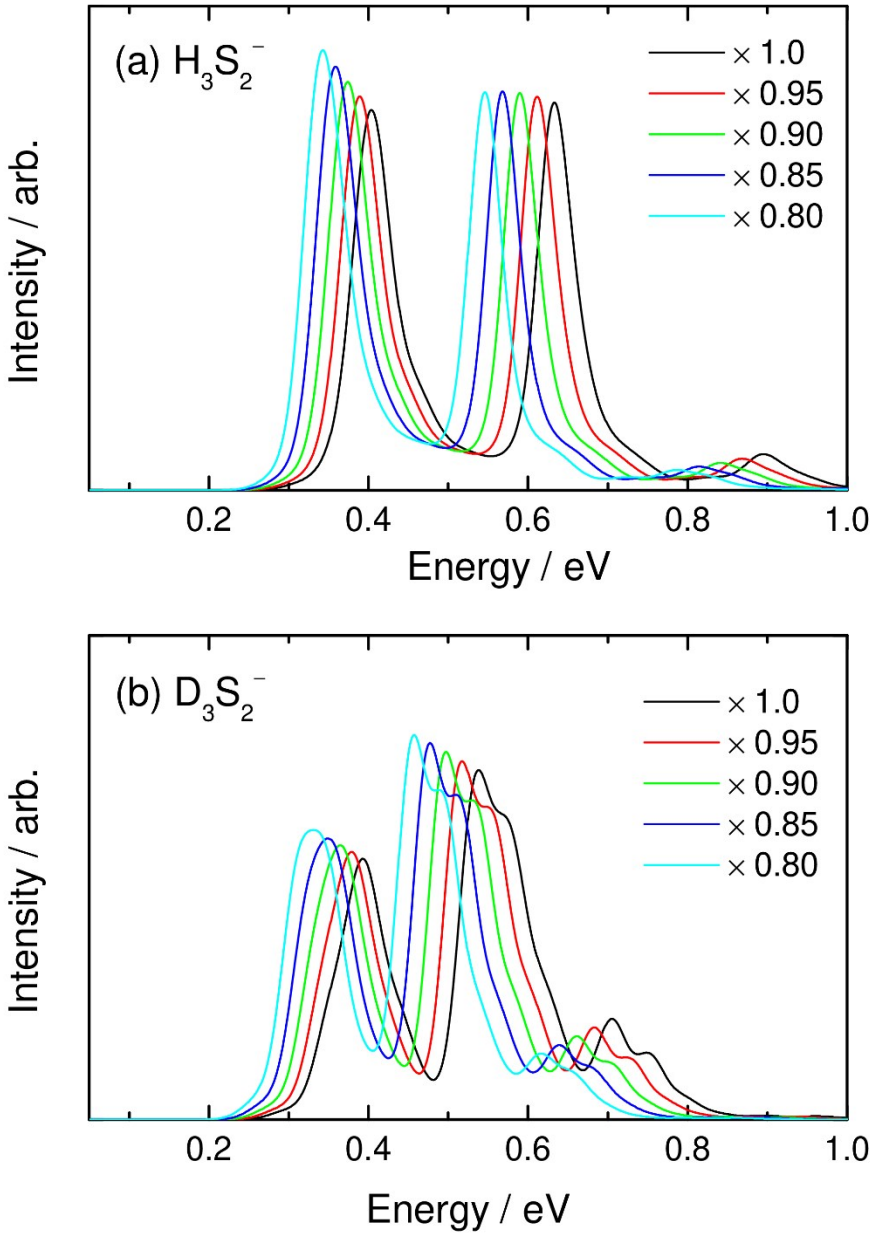

Fig. S2

Effect of a scale factor (0.80–1.0) on the calculated photodetachment spectra of the (a) $H_3S_2^-$ and (b) $D_3S_2^-$ anions. The neural MP2 potential energy surface is used for scaling. Energy is measured from the asymptotic SH + H_2S potential energy minimum.