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

Supporting Information

for

New accurate diabatic potential energy surfaces for the lowest two ^{1}A" states of H_2S and photodissociation dynamics in its first absorption band

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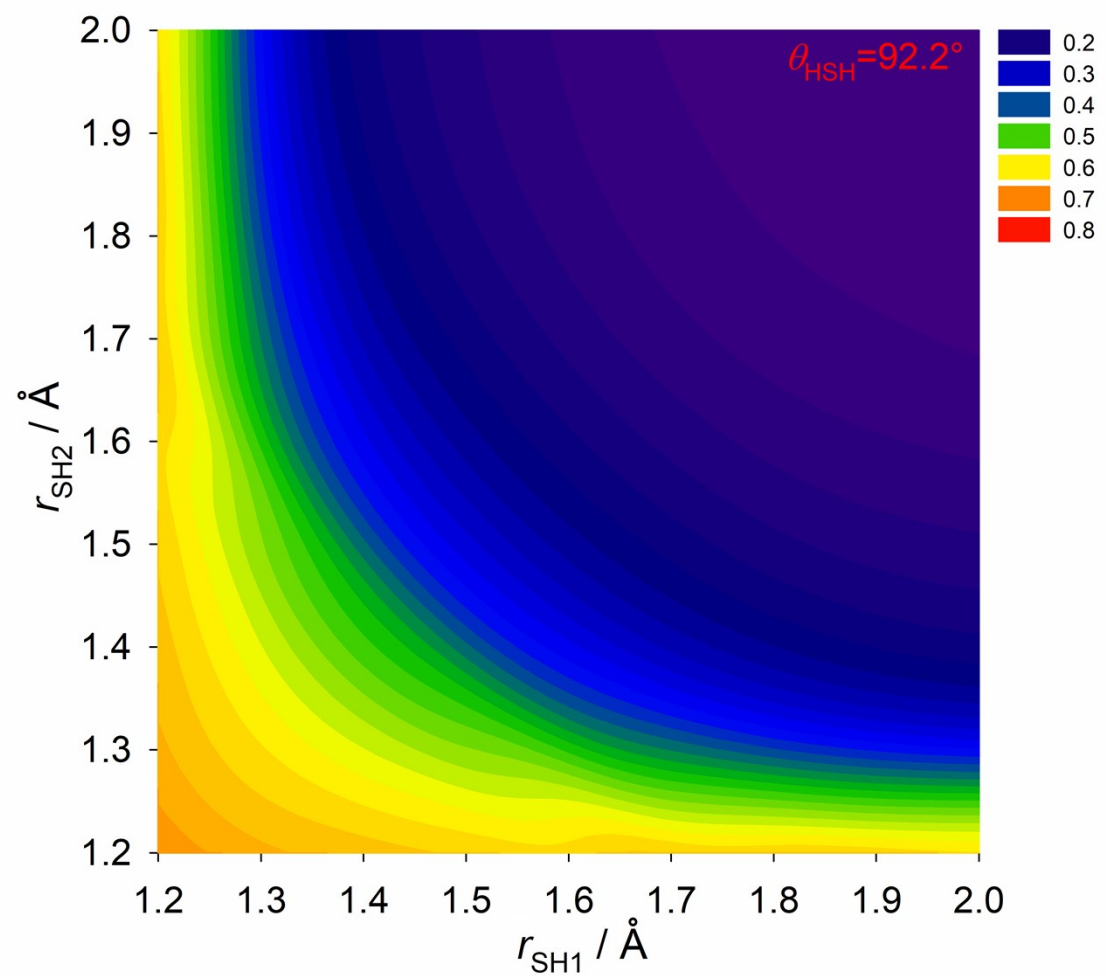

Fig. S1 Diabatic transition dipole surface (μd B) for the $1^1B_1 \leftarrow \tilde{X}^1A_1$ transition as a function of two bond S-H lengths with the inter-bond angle θ_{HSH} fixed at 92.2°. The contour interval is 0.1 a.u.

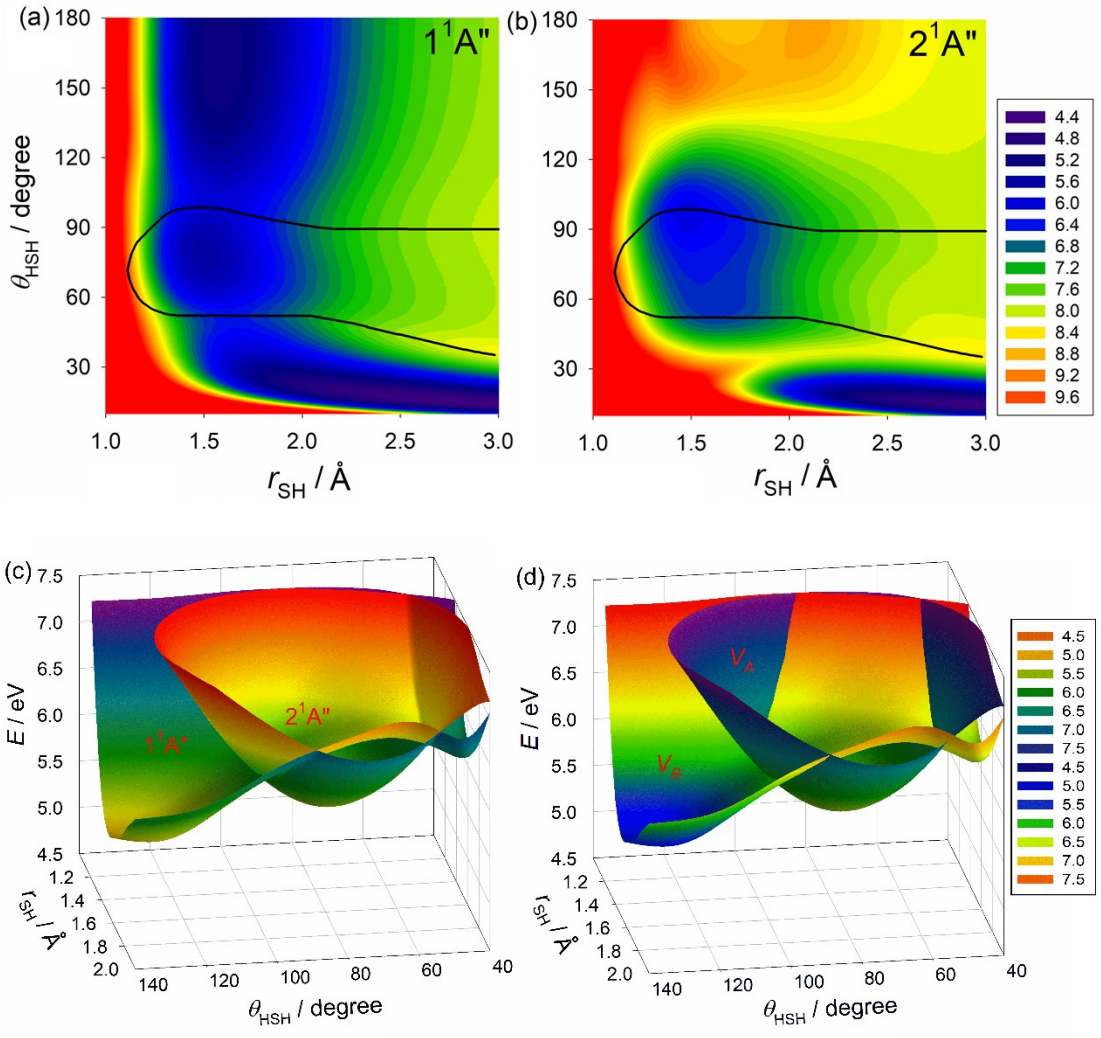

Fig. S2 Contour plots of adiabatic PESs for the singlet (a)1 ^1A" and (b) 2^1A" states, 3D plots for the adiabatic PESs (c) and diagonal diabatic PESs(d) as a function of equivalent S-H bond lengths and inter-bond angle. The CI seam between the two PESs is shown by a solid black line.

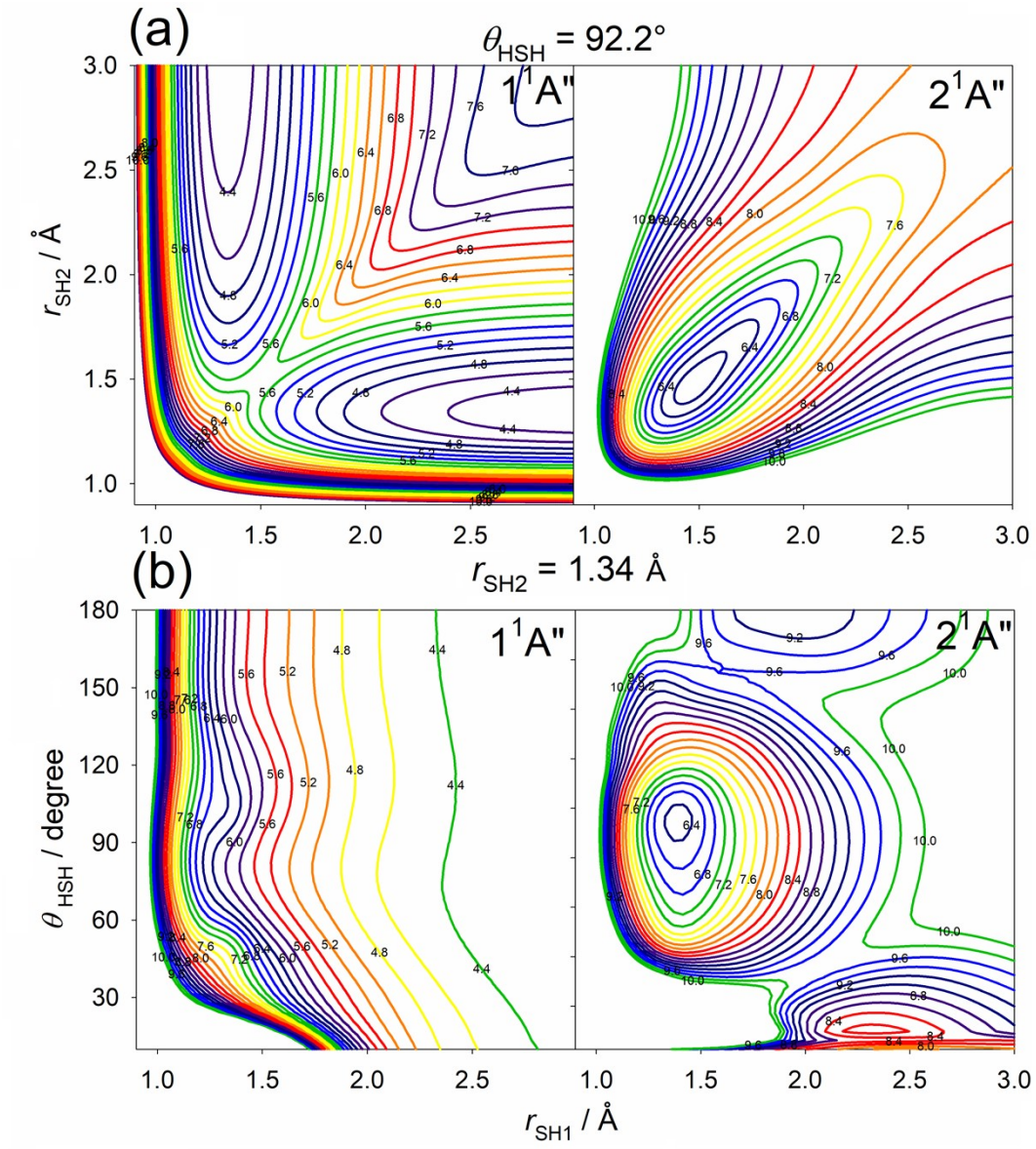

Fig. S3 Adiabatic PESs for the 1^1A" and the 2^1A" PESs: (a) as a function of r_{SH1} and r_{SH2}, with bond angle fixed at θ_{HSH}=92.2°. (b) PESs as a function of r_{SH1} and θ_{HSH}, with the other SH bond fixed at 1.34 Å. The contour intervals are 0.2 eV for all panels.

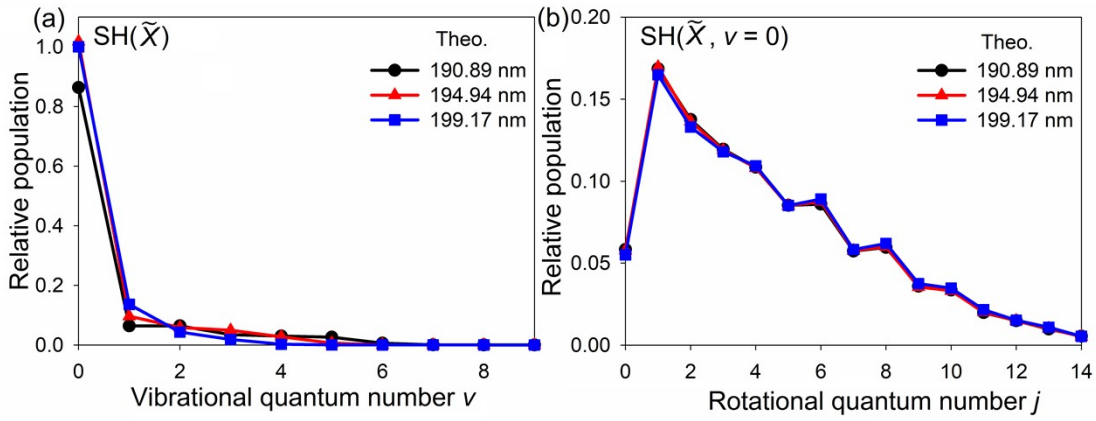

Fig. S4 (a) Theoretical SH($\tilde{X}$) vibrational distributions at three peak energies of the absorption spectrum. (b) Theoretical SH($\tilde{X}, v = 0$) rotational distributions at three peak energies of the absorption spectrum.

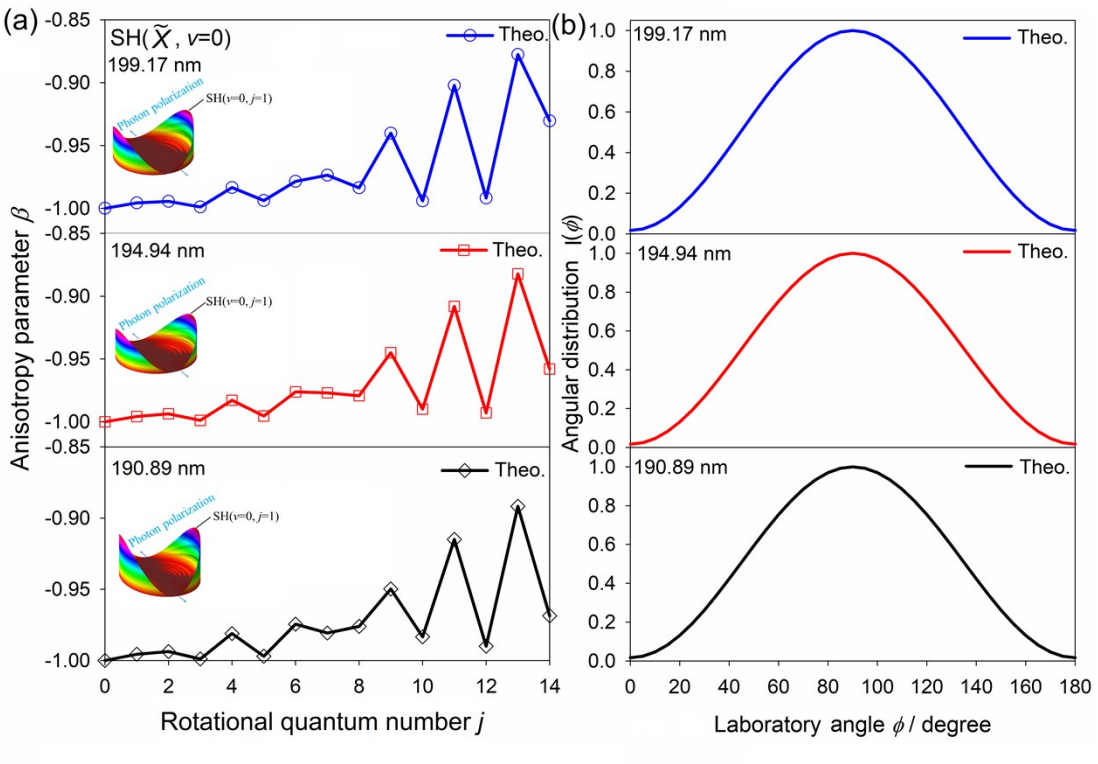

Fig. S5 (a) Calculated rotational state resolved anisotropy parameters β for SH($\tilde{X}$, $v = 0$) products at three peak energies of the absorption spectrum, and (b) angular distributions of recoiling H atom as a function of laboratory angle at three peak energies of the absorption spectrum. The inset shows calculated DCSs for SH($\tilde{X}$) fragments at corresponding energy.