Supporting Information:
Quantum Molecular Motion in the Mixed Ion-Radical Complex, \([\text{\(H_2O\)}(\text{\(H_2S\)})]^+\)

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Fig. S1. Comparison of harmonic spectra (left) and bond distributions (right) from the CCSD and MPW1K methods for the PTO isomer. Colors are consistent in the two plots.

Fig. S2. Potential energy scan along the proton-stretch normal mode of the PTO isomer, using CCSD and MPW1K. For the latter, two basis sets were considered, the results of which nearly overlap in the plot.

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Table S1. Additional density functional theory relative energies for the three stable isomers of (H₂O)(H₂S)⁺. Note that the HB relative energy is severely underestimated in each method, with both BLYP and B97M-V incorrectly predicting the sign of the energy of the HB isomer.