

Description of Additional Supplementary Information

1. Supplementary Data File 1

This file contains the coordinates of B3LYP/aug-cc-pVTZ optimized geometries for the neutral molecules of H_2S_2 through H_2S_8 and S_8 .

2. Supplementary Data File 2

This file contains the error analysis of adiabatic ionization energies (IEs) of unique H_2S_x ($x=2-8$) isomers.