Supporting Information for

Photoelectron Spectroscopy and Density Functional Theory Studies of $(FeS)_mH^-$ (m = 2 - 4) Cluster Anions: Effects of the Single Hydrogen

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The following results are supplied as additional detailed information for these studies: 1. The relative energy of $(FeS)_{2\text{-}4}H^-$ cluster anions with different spin multiplicities at BPW91/TZVP level in Figure S1 to S3, respectively; and 2. The first experimental and calculated VDEs (in eV) for $(FeS)_m^-$ (m = 2 - 8) cluster anions (taken from ref.[1]).

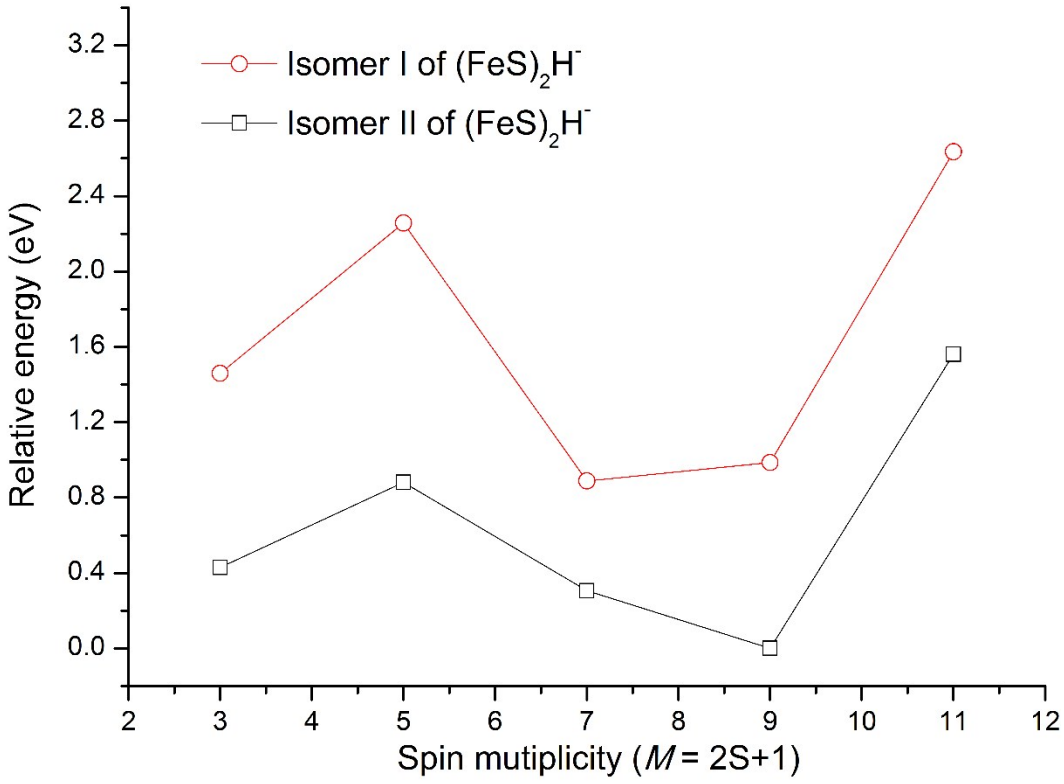

Figure S1. The relative energy of $(FeS)_2H^-$ clusters with different spin multiplicities at BPW91/TZVP level [Isomer I, SH-type] and [isomer II, FeH-type].

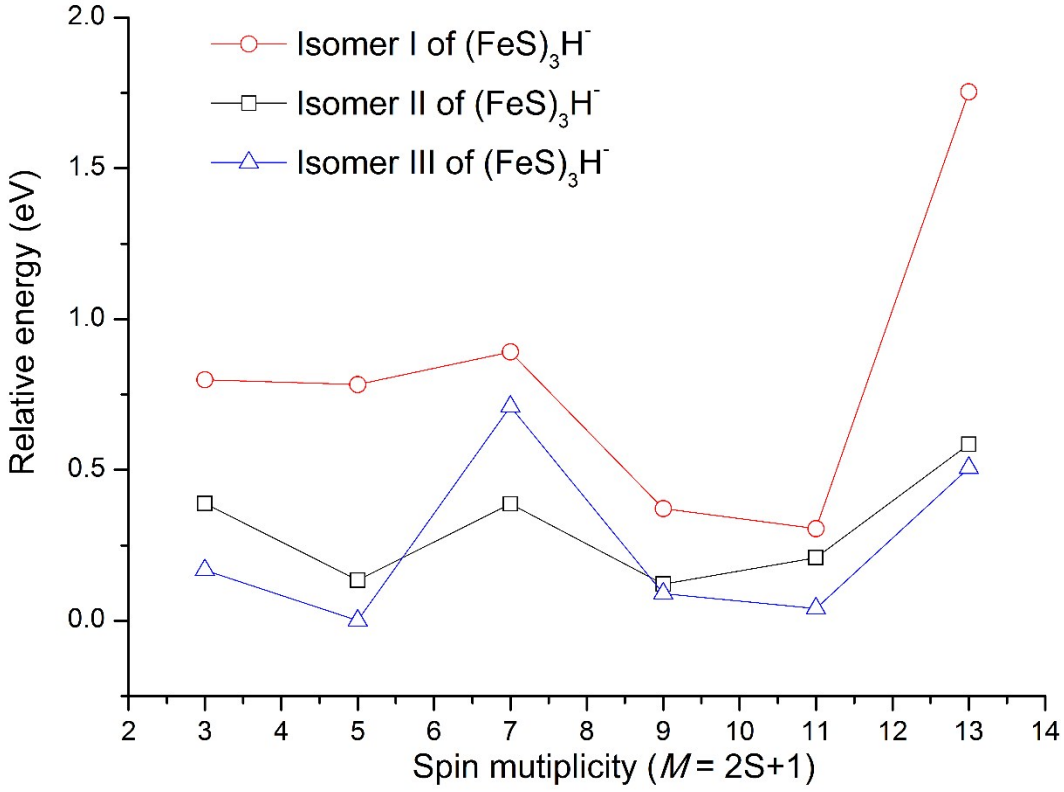

Figure S2. The relative energy of $(FeS)_3H^-$ clusters with different spin multiplicities at BPW91/TZVP level [isomer III, Fe_3H-type].

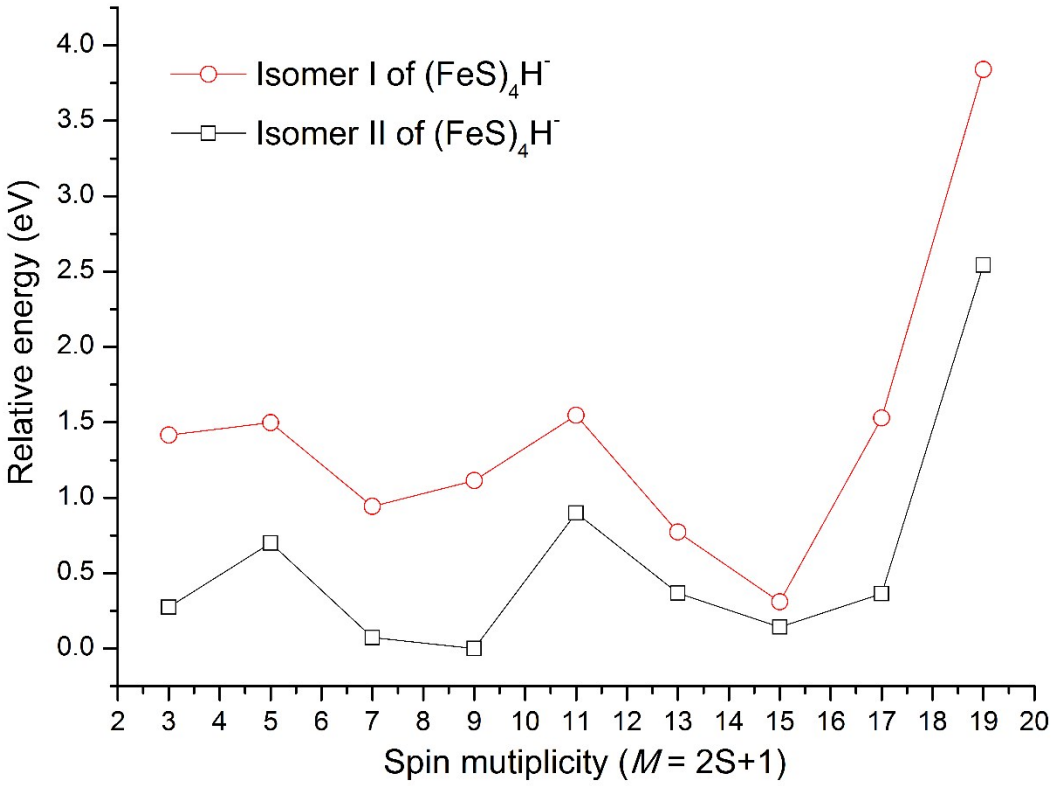

Figure S3. The relative energy of $(FeS)_4H^-$ clusters with different spin multiplicities at BPW91/TZVP level.

Table S1. The first calculated VDEs (in eV) for $(FeS)_m^-$ (m = 2 - 8) at the BPW91/TZVP level, as well as the experimental results for comparison. Different spin multiplicities of each cluster are displayed in order of their relative energy low to high from top to bottom. All calculated and experimental data are taken from ref. [1].

Cluster	Spin multiplicity	VDE (eV)	
		Calculated	Experimental
$(FeS)_2^-$	8	2.04	2.34
	2	1.88	
$(FeS)_3^-$	10	3.24	3.57
	12	2.98	
$(FeS)_4^-$	16	2.87	2.71
	8	2.20	
	14	2.76	
	10	1.83	
	2	2.29	
$(FeS)_5^-$	12	3.08	3.54
	18	3.13	
	10	3.06	
	20	3.26	

	16	3.02	
	4	3.04	
	8	2.56	
	6	2.86	
$(FeS)_6^-$	20	3.06	3.71
	22	3.08	
	16	4.33	
	2	4.47	
	8	6.03	
	6	3.45	
	24	3.27	
	18	2.85	
$(FeS)_7^-$	10	3.50	3.83
	8	3.59	
	6	3.63	
	14	3.84	
	2	3.73	
	16	3.47	
$(FeS)_8^-$	8	4.10	3.85
	4	3.68	
	10	4.64	

Reference

1. Yin, S.; Bernstein, E. R., Photoelectron Spectroscopy and Density Functional Theory Studies of Iron Sulfur $(FeS)_m^-$ (m = 2–8) Cluster Anions: Coexisting Multiple Spin States. *J. Phys. Chem. A* **2017,** *121*, 7362-7373.