Supporting Information

for

Cooperative nature of sulfur centered hydrogen bond: Investigation of $(H_2S)_n$ (n = 2-4) clusters using an affordable yet accurate level of theory

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Table S1: Optimized geometries in Cartesian coordinates and normal mode frequencies of H_2S-dimer calculated at MP2/aug-cc-pV(X+d)Z (X = D, T, Q) level of theories

Lavel of theory	Cartesian Coordinate ($\AA$)	Frequencies (cm^{-1})
MP2/ aug-cc-pV(D+d)Z	H -2.31234000 1.23790500 0.00134500 H -0.74642500 0.08160500 0.00015900 H 2.10622400 -0.81389000 -0.97557700 H 2.10490500 -0.82322400 0.96784200 S 2.01220400 0.10729400 0.00051500 S -2.08422700 -0.08744400 -0.00012600	43.3 71.1 93.8 95.8 177.5 313.6 1201.7 1208.7 2729.7 2760.9 2779.2 2784.7
MP2/ aug-cc-pV(T+d)Z	H 2.30259000 1.22666800 0.00157100 H 0.74401700 0.09282600 0.00043500 H -2.05402700 -0.82292000 0.95673500 H -2.05504400 -0.81078600 -0.96699800 S -2.00316300 0.10589300 0.00066100 S 2.06956700 -0.08625400 -0.00014500	36.8 65.0 76.9 82.0 163.3 290.2 1215.4 1221.8 2734.0 2773.7 2787.4 2792.6
MP2/ aug-cc-pV(Q+d)Z	H 2.31879500 1.22333700 0.00149800 H 0.74874800 0.10435900 0.00062900 H -2.05656100 -0.82210300 0.95715400 H -2.05730400 -0.81040200 -0.96706700 S -2.00684900 0.10578900 0.00063100 S 2.07224400 -0.08673900 -0.00014400	35.4 62.3 70.8 79.4 158.7 280.7 1214.1 1219.9 2735.2 2775.7 2789.7 2794.8

Table S2: Optimized geometries in Cartesian coordinates and normal mode frequencies of H_2S-dimer calculated at MP2-CP/aug-cc-pV(X+d)Z (X = D, T, Q) level of theories

Lavel of theory	Cartesian Coordinate ($\AA$)	Frequencies (cm^{-1})
MP2-CP/ aug-cc-pV(D+d)Z	H 2.41002300 1.23144700 -0.00058700 H 0.81920700 0.11040600 0.00011800 S 2.15210400 -0.08842800 0.00005400 H -2.16816500 -0.81769900 0.97315700 H -2.16702400 -0.82149000 -0.97007600 S -2.08298200 0.10701200 -0.00021700	36.4 55.4 64.0 70.7 146.2 255.3 1201.0 1205.7 2739.6 2762.2 2780.4 2786.0
MP2-CP/ aug-cc-pV(T+d)Z	H 2.35274200 1.22231700 0.00151700 H 0.77842600 0.11099600 0.00057800 S 2.10069500 -0.08709100 -0.00014400 H -2.08846200 -0.82273700 0.95675200 H -2.08918500 -0.81082400 -0.96685200 S -2.03529000 0.10585700 0.00064400	33.8 58.3 66.5 74.6 150.9 268.0 1215.3 1220.5 2740.7 2774.1 2787.9 2793.0
MP2-CP/ aug-cc-pV(Q+d)Z	H 2.33391100 1.22320600 -0.00062000 H 0.76614800 0.10110200 0.00007800 S 2.08974200 -0.08730600 0.00005700 H -2.10325900 -0.81132600 0.96389700 H -2.10221100 -0.81552100 -0.96045400 S -2.02065400 0.10621500 -0.00023900	37.5 59.6 65.8 75.7 152.7 271.5 1214.0 1219.6 2739.1 2776.1 2789.9 2795.1

Table S3: Optimized geometries in Cartesian coordinates and normal mode frequencies of all species calculated at MP2-CP/aug-cc-pV(Q+d)Z level of theory

Complex	Cartesian Coordinate ($\AA$)	Frequencies (cm^{-1})
monomer	S 0.00000000 0.00000000 0.10265900 H 0.00000000 0.96086000 -0.82127000 H 0.00000000 -0.96086000 -0.82127000	1216.3 2779.5 2798.6
dimer	H 2.33391100 1.22320600 -0.00062000 H 0.76614800 0.10110200 0.00007800 S 2.08974200 -0.08730600 0.00005700 H -2.10325900 -0.81132600 0.96389700 H -2.10221100 -0.81552100 -0.96045400 S -2.02065400 0.10621500 -0.00023900	37.5 59.6 65.8 75.7 152.7 271.5 1214.0 1219.6 2739.1 2776.1 2789.9 2795.1
anti-trimer	H 1.08832700 1.21411700 -0.03997500 H 0.38203600 2.57187900 -1.21831900 S 0.32242000 2.30492800 0.08696400 H 1.99942400 -1.53314900 1.24166700 H 0.51344100 -1.56567300 0.00935400 S 1.84292000 -1.43536200 -0.07916300 H -2.44529500 -0.89936000 1.21934300 H -1.60247500 0.33650300 -0.00099800 S -2.16130500 -0.87733600 -0.08349200	66.8 67.3 75.6 80.2 85.2 89.1 157.4 160.5 175.8 241.3 249.2 386.8 1216.5 1218.3 1218.8 2712.1 2722.9 2723.9 2785.2 2785.5 2785.7
syn-trimer	H -1.53270300 0.58515800 -0.02354300 H -2.48320100 -0.52009400 1.24152100 S -2.27543100 -0.52760400 -0.07579400 H 0.78892700 2.40447400 1.24218300 H 1.26958700 1.03284900 -0.02770900 S 0.68092000 2.23444200 -0.07613900 H 1.69802900 -1.88507000 1.24107100 H 0.25933300 -1.62524900 -0.01922200 S 1.59451200 -1.70634200 -0.07646100	65.8 66.0 79.7 79.8 81.9 97.6 165.4 166.1 182.6 239.7 240.3 383.9 1218.3 1219.1 1219.1 2711.2 2722.5 2722.8 2785.3 2785.4 2785.8
S_4-tetramer	H 1.96304000 -0.49701600 -0.28194800 H 3.35166400 0.80564100 0.04640900 S 2.45549700 0.57679900 -0.91458700 H 0.49683300 1.96343000 0.28103500 H -0.80629000 3.35197200 -0.04606100 S -0.57674400 2.45543800 0.91442600 H -1.96394100 0.49705800 -0.28100700 H -3.35220300 -0.80642500 0.04589900 S -2.45545000 -0.57677000 -0.91435800 H -0.49717200 -1.96332600 0.28196200 H 0.80557900 -3.35190400 -0.04622400 S 0.57685300 -2.45543200 0.91451600	6.9 8.7 73.5 79.4 79.4 79.8 101.5 106.3 106.3 112.6 135.3 151.7 151.7 164.9 291.3 332.9 333.0 397.7 1213.3 1216.9 1216.9 1220.3 2691.1 2703.2 2703.2 2710.0 2783.8 2784.0 2784.0 2784.3
C_i-tetramer	H -1.71865100 1.35495400 0.00533800 H -2.98201700 0.57479100 1.24330900 S -2.80132000 0.57001500 -0.07805500 H -1.34732200 -1.68602900 -0.04208300 H -0.69411100 -3.08345900 -1.20683100 S -0.56828000 -2.76914900 0.08307800 H 1.71871300 -1.35490000 -0.00402200 H 2.98590100 -0.57539100 -1.23849900 S 2.80110000 -0.56989100 0.08229400 H 1.34730400 1.68606900 0.04052000 H 0.69476700 3.08681300 1.20166400 S 0.56821300 2.76884700 -0.08727900	4.8 19.7 71.7 78.1 78.9 79.7 91.9 95.5 100.0 100.9 176.1 177.5 184.6 194.8 222.6 310.5 319.1 408.3 1214.6 1217.6 1218.8 1222.5 2692.8 2703.8 2706.4 2710.9 2784.8 2784.8 2785.4 2785.5