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

Supporting Information

Stability of sulfur molecules and insights into sulfur allotropy

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S1. Atomic coordinates and total energies of all calculated ground-state structures of S_n molecules ($2 \leq n \leq 21$) in the XYZ format.

2
E_tot = -21671.58415 eV
S 0.0000000000 0.0000000000 0.9637190000
S 0.0000000000 0.0000000000 -0.9637190000

3
E_tot = -32507.32539 eV
S 1.6746230000 -0.3343910000 0.0000000000
S 0.0000000000 0.6687750000 -0.0000000000
S -1.6746230000 -0.3343840000 -0.0000000000

4
E_tot = -43343.45311 eV
S -1.6049580000 0.9354490000 0.0000240000
S -1.1128590000 -0.9354840000 -0.0000350000
S 1.1129120000 -0.9354620000 0.0000350000
S 1.6049040000 0.9354960000 -0.0000240000

5
E_tot = -54179.80544 eV
S -1.5206900000 -0.5565990000 -0.4631940000
S -1.1227180000 1.3769360000 0.1641920000
S -0.0058800000 -1.6217630000 0.5982530000
S 1.5165210000 -0.5677300000 -0.4626250000
S 1.1327670000 1.3691560000 0.1633740000

6
E_tot = -65016.34205 eV
S 1.8434330000 0.5277580000 -0.4522230000
S 1.3782040000 -1.3331270000 0.4522270000
S -0.4648300000 -1.8595930000 -0.4525100000
S -1.8435120000 -0.5275770000 0.4522140000
S -1.3783590000 1.3330030000 -0.4521840000
S 0.4650640000 1.8595360000 0.4524770000

7
E_tot = -75852.57994 eV
S -0.4543020000 -1.7822500000 0.7494920000
S -2.0213160000 -1.1352070000 -0.3628840000
S 2.3236290000 0.0005270000 0.2275120000
S 1.3151200000 -1.6890430000 -0.5002040000

S 1.3141290000 1.6896010000 -0.4999850000
S -0.4554530000 1.7823330000 0.7493640000
S -2.0218070000 1.1340390000 -0.3632960000

8
E_tot = -86689.01395 eV
S 0.9290290000 2.2445550000 0.4968070000
S 2.2445550000 -0.9290290000 0.4968070000
S -0.9290290000 -2.2445550000 0.4968070000
S -2.2445550000 0.9290290000 0.4968070000
S -0.9292710000 2.2445550000 -0.4968070000
S 2.2445550000 0.9292710000 -0.4968070000
S 0.9292710000 -2.2445550000 -0.4968070000
S -2.2445550000 -0.9292710000 -0.4968070000

9
E_tot = -97524.88454 eV
S -1.9252810000 -0.9613700000 1.0744450000
S -1.1177920000 1.4460550000 -1.2461830000
S -1.0501260000 -2.4302730000 -0.1513720000
S -2.7003360000 0.5738580000 -0.1913420000
S -0.0001070000 2.7422220000 -0.0001500000
S 1.9254920000 -0.9607570000 -1.0743820000
S 1.0505140000 -2.4301510000 0.1511630000
S 1.1173220000 1.4463940000 1.2461630000
S 2.7003140000 0.5740220000 0.1916580000

10
E_tot = -108361.02298 eV
S 2.8572120000 -0.0037340000 1.0471000000
S -2.8572120000 -0.0037340000 -1.0471000000
S 2.8572120000 0.0037340000 -1.0471000000
S -2.8572120000 0.0037340000 1.0471000000
S 1.2451710000 -1.2359690000 1.6877600000
S -1.2451710000 -1.2359690000 -1.6877600000
S 1.2451710000 1.2359690000 -1.6877600000
S -0.0000000000 0.0000000000 -2.8478380000
S 0.0000000000 -0.0000000000 2.8478380000
S -1.2451710000 1.2359690000 1.6877600000

11
E_tot = -119197.16088 eV
S -0.6802740000 2.7173010000 -0.8348620000
S 2.8296600000 -1.3288080000 -0.8111680000

S 2.5245240000 1.9507940000 0.2251390000
S 2.7592450000 -0.0661330000 0.8649150000
S 0.6820020000 2.7169760000 0.8348600000
S 0.8561710000 -1.7540510000 -1.4326540000
S -2.5232270000 1.9524450000 -0.2252100000
S -0.0010910000 -3.0428960000 -0.0001850000
S -2.7591860000 -0.0646420000 -0.8647050000
S -0.8572070000 -1.7539640000 1.4326140000
S -2.8306180000 -1.3270210000 0.8112560000

12
E_tot = -130033.50977 eV
S -2.0489450000 1.4862220000 -1.1489010000
S 2.3120550000 1.0309620000 -1.1487010000
S -0.2630080000 -2.5188960000 -1.1475790000
S -2.3120550000 -1.0309620000 1.1487010000
S 2.0489450000 -1.4862220000 1.1489010000
S 0.2630080000 2.5188960000 1.1475790000
S -1.3968490000 3.1328630000 -0.0016760000
S -3.4112110000 0.3564970000 0.0004590000
S 3.4112110000 -0.3564970000 -0.0004590000
S 2.0145750000 2.7764120000 -0.0002710000
S -2.0145750000 -2.7764120000 0.0002710000
S 1.3968490000 -3.1328630000 0.0016760000

13
E_tot = -140869.42193 eV
S 2.1389460000 2.9478860000 -0.0950660000
S 0.3740380000 2.5277830000 -1.1704970000
S -1.2489240000 3.3516220000 -0.0867760000
S -2.1475870000 1.9346470000 1.1498980000
S 3.8357840000 0.0007920000 -0.0006350000
S 2.6006380000 1.2909020000 1.1217840000
S -3.6381630000 -1.0181340000 0.1372650000
S -2.1464090000 -1.9362060000 -1.1496540000
S -3.6381200000 1.0165550000 -0.1387170000
S -1.2472340000 -3.3518730000 0.0883480000
S 0.3756400000 -2.5268390000 1.1710880000
S 2.6010190000 -1.2902190000 -1.1223680000
S 2.1403730000 -2.9469170000 0.0953300000

14
E_tot = -151705.69286 eV
S -1.6777500000 2.3342020000 -1.1158580000

S -0.8262690000 3.3890470000 0.5036780000
S -3.5989740000 1.7254730000 -0.4972200000
S -1.6791090000 -2.3336510000 -1.1160410000
S -3.4448260000 0.0006600000 0.7052630000
S -3.6000220000 -1.7238250000 -0.4973040000
S 2.8553640000 1.7322110000 -1.0818680000
S 2.4429400000 2.6070200000 0.7959950000
S 0.5181120000 2.0591350000 1.4492970000
S 4.0257950000 -0.0009250000 -0.8136180000
S 0.5167430000 -2.0592110000 1.4492270000
S -0.8281130000 -3.3886640000 0.5034960000
S 2.4413640000 -2.6079480000 0.7965120000
S 2.8547450000 -1.7335240000 -1.0815590000

15
E_tot = -162541.79870 eV
S -3.2691130000 -1.3262090000 -0.9151980000
S -4.0203180000 0.6346250000 -1.0512380000
S -2.4502580000 2.0063950000 -1.3935590000
S -0.3646260000 2.2881130000 1.3703150000
S -2.0766190000 3.0530620000 0.4070630000
S 1.2751500000 3.4339660000 0.6935900000
S 2.2332860000 2.3801380000 -0.8669900000
S -1.0584060000 -1.3860650000 1.6343370000
S -3.0521650000 -1.8343620000 1.1276630000
S 0.1221670000 -3.1118620000 1.4088550000
S 0.4333050000 -3.4909190000 -0.6518750000
S 3.4125210000 -1.8138490000 -0.8782420000
S 1.4058790000 -1.8469800000 -1.5307890000
S 3.4559250000 -0.4364620000 0.7218550000
S 3.9532740000 1.4504090000 -0.0757870000

16
E_tot = -173377.89488 eV
S 3.4374160000 0.4398790000 1.1159180000
S 3.8234910000 2.1888120000 0.0003270000
S 4.2517040000 -1.1556610000 0.0007580000
S 2.7418860000 -2.1192440000 -1.1148210000
S -1.1555810000 -4.2507320000 -0.0006770000
S 0.4394770000 -3.4363990000 1.1151850000
S 2.1889780000 -3.8229330000 0.0005690000
S -0.4399190000 3.4365370000 1.1152100000
S -2.7414030000 2.1190900000 -1.1155880000
S -3.4377140000 -0.4398450000 1.1151330000

S -2.1194680000 -2.7408070000 -1.1157600000
S -3.8235200000 -2.1888870000 -0.0004280000
S 1.1556400000 4.2507700000 -0.0000820000
S -2.1889210000 3.8229280000 -0.0001870000
S -4.2515980000 1.1556080000 -0.0004190000
S 2.1195340000 2.7408850000 -1.1151410000

17
E_tot = -184214.09871 eV
S 0.3835170000 -3.1017390000 0.8744850000
S 1.3560620000 1.0279640000 1.6970250000
S 0.4496110000 2.8700930000 1.2227470000
S -4.8505420000 -0.0003150000 0.0003120000
S -3.6362440000 -1.6439180000 -0.5220160000
S -2.9771520000 -2.5786560000 1.2541600000
S -2.9775580000 2.5781550000 -1.2539150000
S -3.6364020000 1.6435590000 0.5223660000
S -1.0638180000 -1.7829040000 1.6574450000
S 3.4212650000 1.2680150000 2.0207650000
S 4.4930470000 1.0369870000 0.2194720000
S -1.0640280000 1.7828050000 -1.6572880000
S 0.3830150000 3.1023620000 -0.8751220000
S 4.4924700000 -1.0379170000 -0.2187320000
S 3.4214740000 -1.2681050000 -2.0206150000
S 0.4490770000 -2.8690640000 -1.2233480000
S 1.3562060000 -1.0273230000 -1.6977430000

18
E_tot = -195050.32884 eV
S -3.4421840000 0.0505240000 -1.6809010000
S -3.0072380000 -2.8833830000 0.0356950000
S -4.0053630000 -1.9824720000 -1.5906260000
S 3.4420650000 -0.0507580000 -1.6809560000
S -1.0945810000 -3.4840310000 -0.6258600000
S 2.7229740000 -2.7438390000 1.7097690000
S 4.8027640000 -1.2028150000 -0.5545150000
S 4.1785680000 -1.2387190000 1.4617550000
S 0.8444470000 -1.7859800000 1.6246140000
S 0.1753480000 -1.8196550000 -0.3794940000
S 4.0057140000 1.9821310000 -1.5903720000
S 3.0074190000 2.8831290000 0.0357460000
S 1.0949720000 3.4841360000 -0.6262090000
S -0.8445420000 1.7867820000 1.6243700000
S -0.1753740000 1.8201410000 -0.3797580000

S -2.7232870000 2.7441580000 1.7092040000
S -4.1785300000 1.2385480000 1.4618110000
S -4.8031730000 1.2021060000 -0.5542730000

19
E_tot = -205886.44649 eV
S -4.7156160000 0.0166930000 1.2439230000
S -3.6395730000 2.6562520000 -0.6943700000
S -5.1717960000 1.9647050000 0.5818940000
S -2.1197390000 3.5121150000 0.4950100000
S 2.1195990000 3.5120100000 -0.4950710000
S 0.6543310000 2.0305190000 -0.8286520000
S -0.6544270000 2.0307070000 0.8288630000
S -5.4310240000 -1.3580600000 -0.1916170000
S -3.8373240000 -1.7521290000 -1.5174150000
S -2.7876470000 -3.4386280000 -0.8161790000
S 4.7157660000 0.0164950000 -1.2438470000
S 2.7879520000 -3.4384860000 0.8161090000
S 3.6396250000 2.6563030000 0.6942330000
S 5.1717090000 1.9647560000 -0.5821170000
S 5.4312050000 -1.3577840000 0.1918790000
S 3.8370330000 -1.7521710000 1.5175070000
S 1.5426760000 -2.8221580000 -0.7772630000
S 0.0000740000 -1.6187870000 0.0000230000
S -1.5428240000 -2.8223530000 0.7770920000

20
E_tot = -216722.46678 eV
S 2.8566850000 3.8417290000 0.4539030000
S 0.0000350000 1.9849410000 0.0000890000
S 1.4392020000 3.1832290000 -0.9618200000
S 3.9604100000 2.1626410000 1.1074160000
S 5.1534010000 1.5312440000 -0.5092560000
S 4.0883930000 -0.0601220000 -1.4143590000
S -2.8565490000 3.8418960000 -0.4540030000
S -1.4391030000 3.1834900000 0.9617650000
S -3.9603750000 2.1627410000 -1.1074460000
S -5.1532450000 1.5313330000 0.5092880000
S -4.0883050000 -0.0600470000 1.4144100000
S -2.5989460000 -3.7419390000 -0.7824360000
S -4.2625240000 -2.4639500000 -1.0985740000
S -0.0001080000 -1.5811920000 -0.0000730000
S 0.8577390000 -2.8039440000 1.4907340000
S 4.9954200000 -1.8510460000 -0.7780450000

S 2.5987750000 -3.7418590000 0.7825210000
S 4.2624850000 -2.4640620000 1.0986330000
S -4.9954690000 -1.8509190000 0.7780540000
S -0.8579210000 -2.8041640000 -1.4908010000

21
E_tot = -227558.63640 eV
S 1.5768550000 1.4828340000 -0.6845360000
S 4.7270090000 2.4464640000 0.2422710000
S -2.3915250000 3.3589640000 -0.8704320000
S -5.5102370000 0.4379910000 0.6904860000
S -3.7049260000 1.2410670000 1.4237350000
S -0.5582320000 4.1589610000 -0.2010940000
S 0.5655520000 2.6546530000 0.7516270000
S -3.6721870000 3.2641040000 0.8083800000
S 1.4317320000 -2.2741940000 1.8075270000
S 2.0046250000 -3.3690760000 0.0931450000
S 5.6410160000 -0.8376620000 0.7513280000
S 6.1696100000 0.9822460000 -0.1962690000
S 3.2833630000 2.5581170000 -1.3007380000
S 3.0652330000 -2.0839420000 -1.1969620000
S 5.1209930000 -2.2218380000 -0.7469810000
S -2.8982870000 -2.5698330000 -1.6159710000
S -0.2581070000 -1.1292910000 1.2839800000
S -2.3455150000 -3.5961740000 0.1298240000
S -2.0037770000 -2.2300220000 1.7054640000
S -5.2644550000 -0.1002710000 -1.3415380000
S -4.9787430000 -2.1730990000 -1.5332450000

S2. Frequencies of S_n molecules ($2 \leq n \leq 21$)

S_2:
682.9

S_3:
258.4 561.9 638.8

S_4:
85.8 204.4 304.3
318.8 622.1 648.6

S_5:
93.1 217.3 273.2
285.1 303.5 305.5
397.3 473.0 479.7

S_6:
157.8 158.4 195.4
195.6 252.6 305.3
308.7 404.5 404.95
428.7 429.0 450.95

S_7:
57.2 124.2 147.8
163.8 188.6 226.8
257.8 281.6 314.5
331.3 345.0 420.9
454.2 491.5 501.2

S_8:
71.2 71.97 140.9
141.0 185.8 185.8
207.8 235.1 241.0
241.0 342.5 376.6
376.6 431.2 432.7
437.9 447.9

S_9:
48.7 64.5 79.9
91.1 138.8 149.7
168.4 206.6 208.8
240.2 244.1 293.0
348.6 352.5 386.1
395.7 422.6 426.2
428.6 447.7 453.1

S_{10}:
32.5 32.6 68.9
68.9 143.5 143.5

167.0	175.4	175.4
189.6	199.9	200.0
207.9	207.9	333.1
368.4	368.6	412.8
413.0	434.9	435.0
435.1	435.3	444.2

S_{11}:

29.8	38.3	52.3
56.5	89.9	102.2
125.9	155.9	161.8
164.0	193.5	204.8
211.1	234.8	253.5
275.1	334.6	346.7
385.9	386.4	419.4
429.4	429.9	434.2
445.0	445.7	453.8

S_{12}:

40.3	40.5	41.8
42.0	66.0	75.0
100.4	140.2	152.3
152.4	173.7	174.0
232.9	232.9	244.7
244.8	264.9	281.9
338.3	360.8	360.9
400.4	400.6	426.7
428.2	429.3	434.3
434.3	441.4	441.5

S_{13}:

12.6	29.5	36.7
39.3	57.4	67.5
82.9	98.1	120.4
127.9	152.7	160.7
174.7	178.9	219.7
221.9	228.7	236.9
257.4	267.8	336.6
345.6	373.1	376.2
405.7	411.0	429.8
433.1	437.5	440.5
448.7	451.5	476.4

S_{14}:

23.8	29.7	30.5
36.7	57.6	60.6
61.8	68.6	108.8

114.6	152.5	155.8
160.5	178.9	185.5
206.4	222.5	232.2
235.8	244.5	251.6
265.2	338.9	355.9
357.4	391.1	391.2
418.8	421.4	429.4
431.6	436.6	436.8
438.1	446.6	451.4

S_{15}:

15.9	24.6	27.3
40.0	49.6	50.5
55.7	58.2	73.5
95.0	108.3	146.3
156.5	158.4	171.9
179.7	197.9	217.5
227.4	228.9	244.2
250.3	258.9	278.9
341.1	348.3	369.0
370.6	401.1	402.6
418.7	426.6	427.0
431.0	436.2	439.5
443.0	446.6	450.8

S_{16}:

15.4	16.0	29.4
29.5	50.4	50.4
53.2	53.2	58.5
73.8	83.7	125.1
125.1	157.1	165.0
165.0	184.3	184.4
199.0	199.1	235.9
235.9	237.8	237.8
253.8	257.1	338.1
351.9	351.9	381.0
381.1	409.5	409.6
426.4	429.6	434.7
438.7	438.7	439.5
439.5	443.9	444.0

S_{17}:

19.1	20.3	32.4
32.4	40.2	41.8
46.7	48.9	60.9

63.1	72.5	99.1
106.9	126.2	129.8
155.4	163.6	178.7
194.4	207.9	216.7
222.5	239.0	248.7
254.0	259.2	267.8
274.6	342.1	344.8
362.4	366.5	392.0
394.7	417.9	419.1
422.7	425.5	429.0
433.4	434.5	435.0
441.6	449.8	450.3

S_{18}:

19.0	26.7	31.0
32.6	33.6	39.4
44.8	56.0	58.1
61.2	64.7	82.9
93.1	107.7	123.5
147.3	154.8	161.3
178.1	192.8	196.5
217.5	222.9	231.5
241.8	246.4	252.8
263.1	267.9	273.1
339.6	348.9	351.2
373.8	374.3	398.9
401.3	420.1	422.1
429.4	429.5	433.2
435.0	437.7	438.2
439.6	443.2	443.3

S_{19}:

16.8	19.0	24.3
28.6	32.0	35.8
36.1	41.9	47.7
53.0	58.4	64.2
81.3	83.1	97.6
112.6	144.2	146.7
161.6	164.8	186.6
192.3	209.0	218.6
238.4	239.4	248.8
250.2	262.9	266.3
273.9	284.5	341.7
342.2	358.1	361.3
385.1	385.2	408.8
409.7	423.2	426.0

427.9	428.3	431.7
432.0	433.9	438.5
438.7	443.7	444.3

S_{20}:

11.2	14.6	18.3
23.3	24.3	27.2
30.1	42.2	43.8
46.3	50.2	64.8
73.2	79.2	87.4
93.2	107.2	125.0
139.4	161.8	169.4
178.3	178.7	201.1
210.1	223.7	236.7
238.5	239.9	252.6
253.3	263.4	266.0
284.3	339.4	348.37
350.3	370.5	374.4
396.1	399.6	418.9
419.4	421.8	424.6
427.1	432.3	432.6
433.9	434.2	437.8

S_{21}:

12.9	14.0	20.6
25.1	27.5	28.6
32.1	35.4	41.4
45.8	53.3	54.4
59.6	68.6	78.6
91.2	104.4	121.1
136.3	145.3	157.9
168.6	169.7	182.9
194.9	204.5	209.6
222.4	231.3	234.7
240.4	246.1	261.0
262.6	265.9	271.7
339.6	340.8	355.4
356.3	378.0	380.8
402.2	403.6	420.6
421.3	426.0	427.8
431.5	432.6	434.2
435.2	435.8	440.7
443.6	444.4	449.2

Table S1. Fragmentation energies and fission products of S_n molecules with $n = 2 – 21$.

Molecule	Fission products	Fragmentation energy, eV
S_2	$S_1 + S_1$	4.07
S_3	$S_1 + S_2$	1.98
S_4	$S_2 + S_2$	0.28
S_5	$S_2 + S_3$	0.90
S_6	$S_2 + S_4$	1.30
S_7	$S_2 + S_5$	1.19
S_8	$S_2 + S_6$	1.09
S_9	$S_2 + S_7$	0.72
S_{10}	$S_2 + S_8$	0.42
S_{11}	$S_2 + S_9$	0.69
S_{12}	$S_6 + S_6$	0.83
S_{13}	$S_6 + S_7$	0.50
S_{14}	$S_6 + S_8$	0.34
S_{15}	$S_7 + S_8$	0.20
S_{16}	$S_8 + S_8$	-0.13
S_{17}	$S_8 + S_9$	0.20
S_{18}	$S_8 + S_{10}$	0.29
S_{19}	$S_8 + S_{11}$	0.27
S_{20}	$S_8 + S_{12}$	-0.06
S_{21}	$S_8 + S_{13}$	0.20