Supplementary Information

Molecular mechanism of elemental sulfur dissolution in H₂S under stratal conditions

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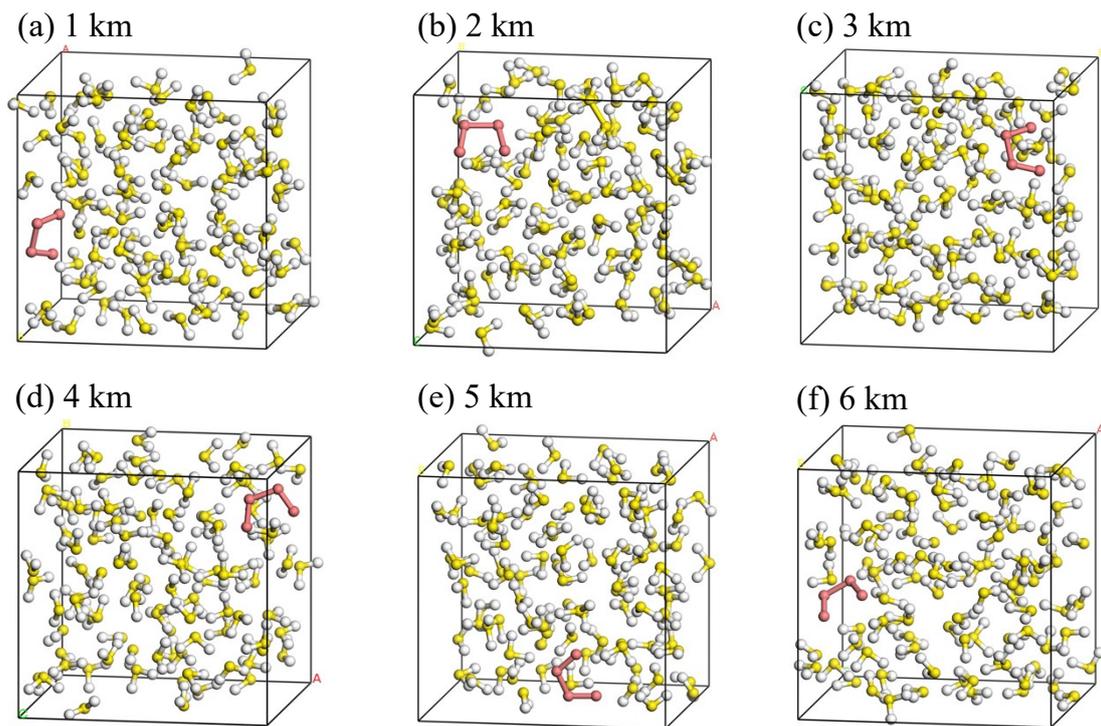
Fig. S1. Snapshots of the molecular configurations of S_4 in H_2S at a varying stratigraphic depth. (Red balls are for S atoms in S_4, others for atoms in H_2S).
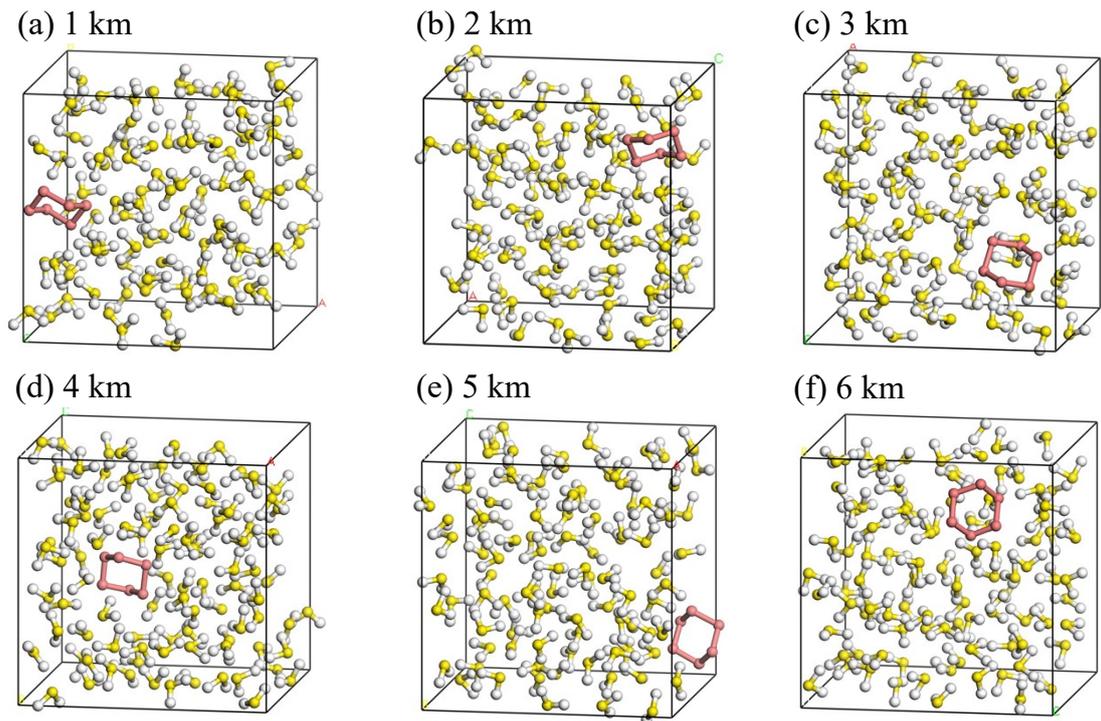
Fig. S2. Snapshots of the molecular configurations of S_6 in H_2S at a varying stratigraphic depth. (Red balls are for S atoms in S_6, others for atoms in H_2S).
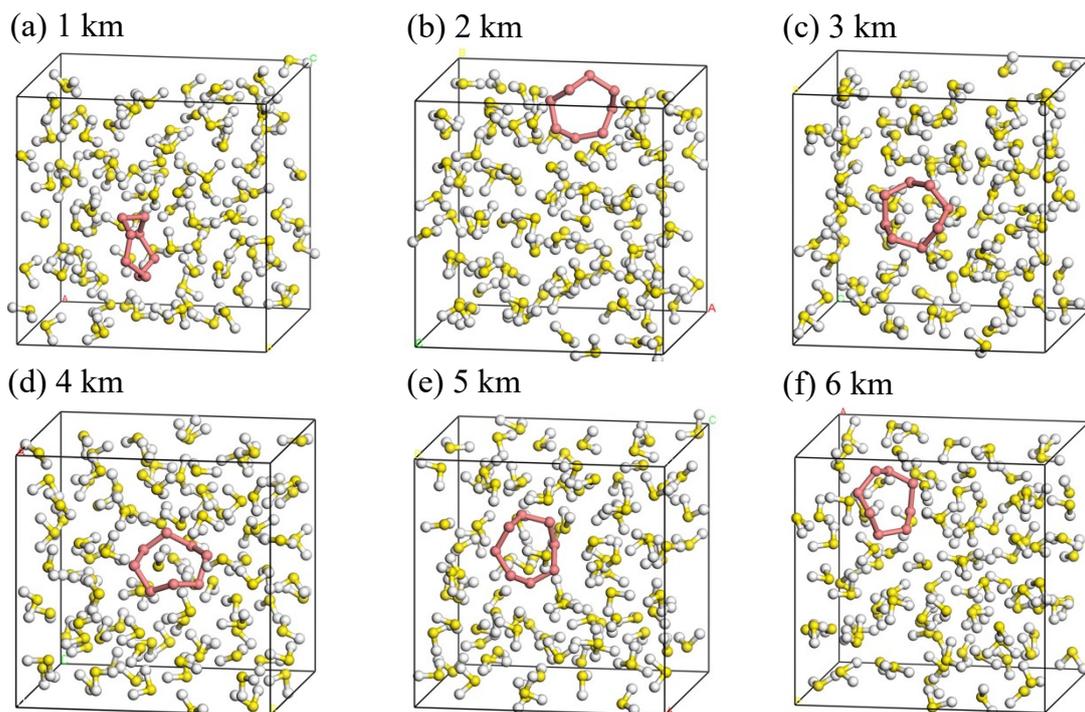
Fig. S3. Snapshots of the molecular configurations of S_8 in H_2S at a varying stratigraphic depth. (Red balls are for S atoms in S_8, others for atoms in H_2S).
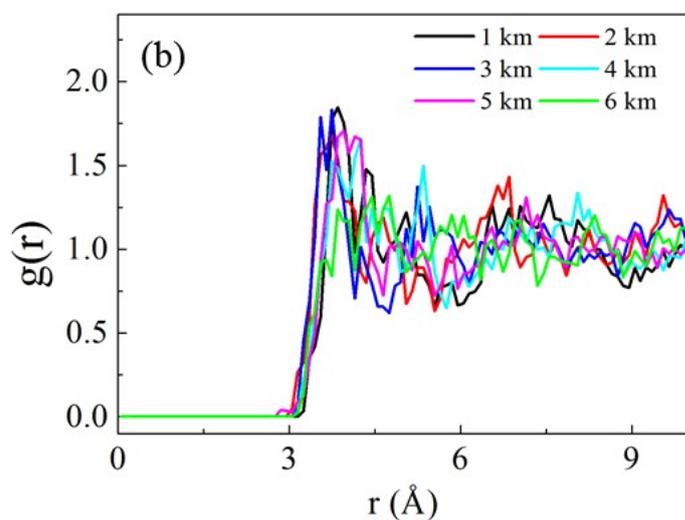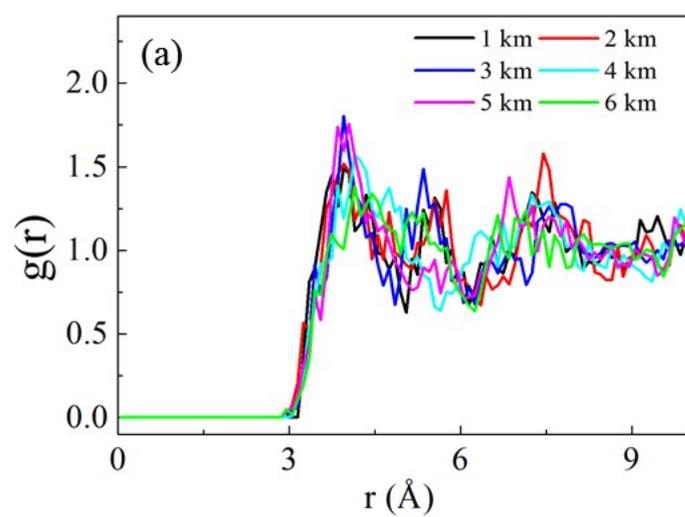
Fig. S4. RDFs of the terminal (a) and central (b) S atoms in S_4 with the S atom in H_2S at the stratigraphic depths of 1–6 km.

Table S1. Structure and coordinates of S_2 reacting with a H_2S molecule optimized at the B3LYP/6-311++G(d,p) level. S and T denote the singlet and triplet states, respectively.

Name	Structure	Numbering	X	Y	Z
$IM1^T$		1	2.63349	-0.00026	0.000160
		2	1.70046	0.68505	-0.69003
		3	1.69900	-0.68717	0.68679
		4	-1.42371	-0.96330	-0.03062
		5	-1.42225	0.963670	0.03066
$TS1^S$		1	-1.79109	-0.28772	-0.05616
		2	-0.50825	-1.30131	-0.52196
		3	-1.76447	-0.83157	1.18843
		4	0.16856	0.87175	0.00733
		5	1.76457	-0.45072	0.00717
$TS1^T$		1	-2.22613	0.11759	-0.07727
		2	-0.42047	-0.89533	-0.04122
		3	-2.16991	0.30430	1.26075
		4	1.38627	0.93707	-0.00825
		5	1.00176	-1.01772	0.00930
$P1^S$		1	-1.71450	-0.38562	-0.08526
		2	1.88132	-0.58390	-1.24319
		3	-1.88145	-0.58386	1.24319
		4	-0.00006	0.84418	-0.00001
		5	1.71456	-0.38558	0.08526
$P1^T$		1	-2.04940	-0.28098	-0.07078
		2	0.50317	-1.53395	0.07574
		3	-2.29727	0.29644	1.12437
		4	0.58301	1.05538	-0.02077
		5	1.57852	-0.69706	0.01654

Table S2. Structure and coordinates of S_2 reacting with a H_2S molecule optimized at the M06-2X/6-311++G(2d,2p) level. S and T denote the singlet and triplet states, respectively.
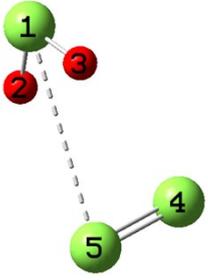
Name	Strcture	Numbering	X	Y	Z
IM1[T]		1	-2.55141	-0.00713	-0.00532
		2	-1.68304	0.16053	0.99609
		3	-1.57762	-0.01866	-0.91834
		4	1.37800	-0.95263	0.00607
		5	1.37720	0.95089	-0.00560
TS1[S]		1	-1.49858	-0.36654	-0.05525
		2	-0.37563	-1.18324	-0.50411
		3	-1.36683	-0.89834	1.17653
		4	0.11275	1.01026	0.01005
		5	1.49473	-0.51362	0.00317
TS1[T]		1	-1.83317	-0.12941	-0.07763
		2	-0.28441	-1.07909	-0.04008
		3	-1.86367	-0.05292	1.25894
		4	0.74350	1.05645	-0.00384
		5	1.22393	-0.85629	0.00529
P1[S]		1	1.65858	-0.38920	-0.08461
		2	-1.81868	-0.55399	-1.23429
		3	1.81909	-0.55460	1.23417
		4	-0.00001	0.84774	0.00004
		5	-1.65859	-0.38925	0.08458
P1[T]		1	-1.97279	-0.26730	-0.07389
		2	0.44019	-1.49825	0.03878
		3	-2.10923	0.13299	1.19593
		4	0.55571	1.04076	-0.01638
		5	1.52140	-0.68813	0.01310
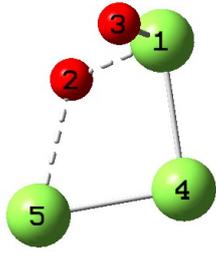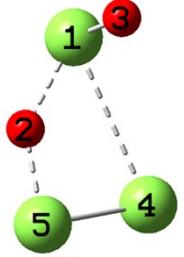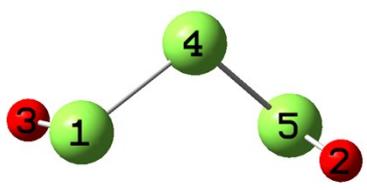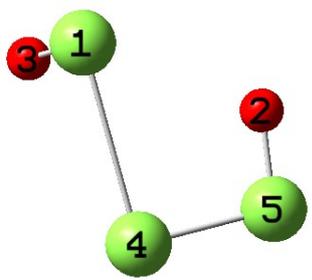
Table S3. Structure and coordinates of S_2 reacting with two H_2S molecule optimized at the B3LYP/6-311++G(d,p) level. S and T denote the singlet and triplet states, respectively.
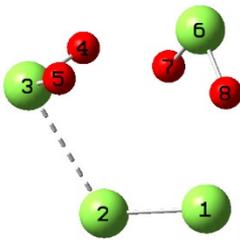
Name	Structure	Numbering	X	Y	Z
R2^S		1	1.17842	-1.58838	-0.52355
		2	1.43553	-0.09502	0.71433
		3	0.16025	2.18205	-0.21899
		4	-0.98284	1.44513	-0.29819
		5	0.48350	1.97156	-1.51210
		6	-2.51162	-0.59331	0.06336
		7	-2.29328	-0.54401	1.39306
		8	-1.40856	-1.35824	-0.14526
R2^T		1	-2.55254	-0.13787	0.08951
		2	-1.28131	1.30167	-0.10907
		3	2.50931	1.41441	-0.03734
		4	2.10860	0.12446	0.02702
		5	2.55833	1.53045	1.30490
		6	0.99005	-2.39469	0.05003
		7	0.97783	-2.61338	-1.28027
		8	-0.29284	-1.97787	0.05822
TS2^S		1	0.73177	1.64642	0.39903
		2	1.45854	0.01030	-0.55687
		3	0.29276	-1.84179	0.23859
		4	-1.05251	-1.01400	0.13066
		5	0.46366	-1.64314	1.56704
		6	-2.24731	0.26479	-0.09919
		7	-2.14210	0.21422	-1.44402
		8	-1.04108	1.16739	0.04124
TS2^T		1	-1.69294	-1.00626	0.02230
		2	-1.50355	0.97829	-0.03040
		3	1.34840	1.71989	-0.06677
		4	1.60320	-0.05719	0.02527
		5	1.28270	1.84823	1.27563
		6	1.57161	-1.60754	0.07028
		7	1.67228	-1.71941	-1.27076
		8	-0.13463	-1.42167	0.04315
P2^S		1	-0.67599	1.77644	-0.42358
		2	-1.13498	0.13032	0.80609
		3	-1.05973	-1.63506	-0.36077
		4	2.01443	-1.01408	-0.75646
		5	-2.30881	-1.59444	-0.87923
		6	2.72413	-0.18313	0.03455
		7	1.96361	-0.47001	1.11116
		8	0.67600	1.66139	-0.37607
P2^T		1	-1.14164	-1.71079	-0.01121
		2	-1.84532	0.18129	0.00582
		3	0.17885	2.25024	-0.08770
		4	1.92685	0.46695	0.10761
		5	-0.09755	2.43401	1.22145
		6	2.50884	-0.76570	0.08789
		7	2.74066	-0.70803	-1.23933
		8	0.21832	-1.47367	-0.00654
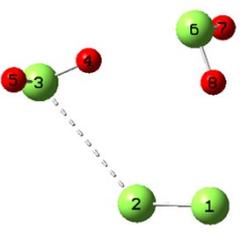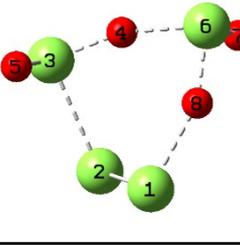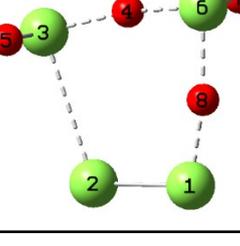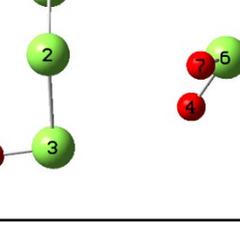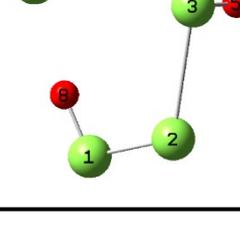
Table S4. Structure and coordinates of S_2 reacting with two H_2S molecule optimized at the M06-2X/6-311++G(2d,2p) level. S and T denote the singlet and triplet states, respectively.
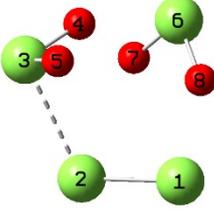
Name	Structure	Numbering	X	Y	Z
R2^S		1	0.98574	-1.62080	-0.52744
		2	1.23977	-0.21614	0.78416
		3	0.51623	1.98570	-0.24283
		4	-0.69568	1.46022	-0.51465
		5	1.02860	1.66558	-1.43609
		6	-2.53043	-0.26711	0.03589
		7	-2.20220	-0.10821	1.32237
		8	-1.51168	-1.12403	-0.16795
R2^T		1	-2.62994	0.30878	0.20352
		2	-0.96199	1.08995	-0.28471
		3	2.69010	1.18180	0.03612
		4	2.17481	-0.05504	0.04602
		5	2.29306	1.41460	1.28993
		6	0.64214	-2.41448	-0.00764
		7	0.07457	-2.09965	-1.17584
		8	-0.38729	-1.91668	0.68328
TS2^S		1	0.66175	-1.62259	-0.41357
		2	1.37227	-0.04220	0.62584
		3	0.45237	1.70607	-0.28443
		4	-0.92733	1.07716	-0.19555
		5	0.66305	1.36592	-1.56653
		6	-2.26776	-0.12568	0.09752
		7	-2.09687	-0.05098	1.42259
		8	-1.13697	-1.04172	-0.06617
TS2^T		1	-1.57280	-1.12753	0.02353
		2	-1.52224	0.83766	-0.03294
		3	1.12034	1.80401	-0.06288
		4	1.56227	0.07539	0.01398
		5	1.00654	1.87335	1.26836
		6	1.70329	-1.45200	0.06825
		7	1.77331	-1.54600	-1.26384
		8	0.00065	-1.39683	0.04611
P2^S		1	0.75317	-1.70154	-0.42492
		2	1.13848	-0.08151	0.80204
		3	0.91290	1.62019	-0.36431
		4	-1.93418	0.74559	-0.85902
		5	2.13918	1.63592	-0.90123
		6	-2.66589	0.09138	0.05060
		7	-1.83914	0.44506	1.04196
		8	-0.58433	-1.68290	-0.29639
P2^T		1	-0.84959	-1.63891	-0.06932
		2	-2.08420	-0.09537	0.08419
		3	-0.25983	1.97142	-0.12953
		4	2.11355	0.72573	0.25799
		5	-0.65809	2.31130	1.10204
		6	2.89358	-0.35576	0.11170
		7	3.01319	-0.15921	-1.20431
		8	0.33207	-0.97980	-0.10841
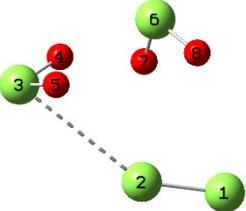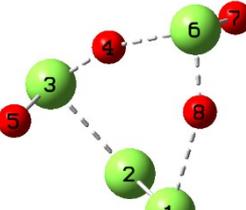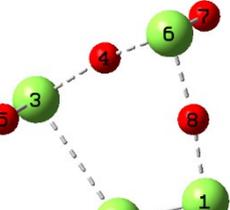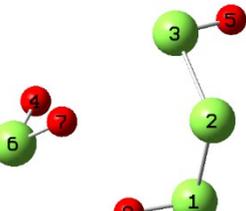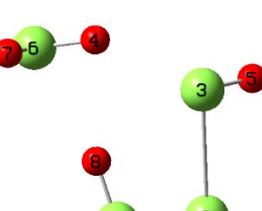
Table S5. Thermodynamic parameters of S_2 reacting with H_2S calculated with B3LYP/6-311++G(d,p). (Values in the parentheses are in triplet state.)

	R1	IM1	TS1	P1	R2	TS2	P2
S (cal/mol·K)	101.5930	-	70.4070	70.9130	95.2130	83.2820	94.3320
	(103.7690)	(86.2430)	(78.1540)	(80.3930)	(108.0650)	(89.0300)	(97.79600)
U (Hartree)	-1195.7810	-	-1195.7592	-1195.8334	-1595.1996	-1595.1940	-1595.2428
	(-1195.8171)	(-1195.8170)	(-1195.7725)	(-1195.7751)	(-1595.2248)	(-1595.1830)	(-1595.1876)
H (Hartree)	-1195.7791	-	-1195.7582	-1195.8324	-1595.1999	-1595.1931	-1595.2419
	(-1195.8152)	(-1195.8161)	(-1195.7715)	(-1195.7742)	(-1595.2239)	(-1595.1821)	(-1595.1867)
G (Hartree)	-1195.8273	-	-1195.7917	-1195.8661	-1595.2439	-1595.2326	-1595.2867
	(-1195.8645)	(-1195.8571)	(-1195.8087)	(-1195.8124)	(-1595.2752)	(-1595.2244)	(-1595.2332)

Table S6. Thermodynamic parameters of S_2 reacting with H_2S calculated with CCSD(T)/aug-cc-pVQZ on the B3LYP/6-311++G(d,p) optimized structures. (Values in the parentheses are in triplet state.)

	R1	IM1	TS1	P1	R2	TS2	P2
S (cal/mol·K)	101.5930	-	70.4070	70.9130	95.213	83.2820	94.3320
	(103.7690)	(86.2430)	(78.1540)	(80.3930)	(108.0650)	(89.0300)	(97.7960)
U (Hartree)	-1194.4023	-	-1194.3560	-1194.4550	-1593.3470	-1593.3408	-1593.3975
	(-1194.4293)	(-1194.4289)	(-1194.3754)	(-1194.3814)	(-1593.3696)	(-1593.3124)	(-1593.3241)
H (Hartree)	-1194.4004	-	-1194.3550	-1194.4540	-1593.3461	-1593.3398	-1593.3966
	(-1194.4274)	(-1194.4280)	(-1194.3744)	(-1194.3804)	(-1593.3687)	(-1593.3115)	(-1593.3232)
G (Hartree)	-1194.4486	-	-1194.3885	-1194.4877	-1593.3913	-1593.3794	-1593.4414
	(-1194.4767)	(-1194.4689)	(-1194.4116)	(-1194.4186)	(-1593.4200)	(-1593.3538)	(-1593.3696)

Table S7. Thermodynamic parameters of S_2 reacting with H_2S calculated with CCSD(T)/aug-cc-pVTZ on the B3LYP/6-311++G(d,p) optimized structures. (Values in the parentheses are in triplet state.)

	R1	IM1	TS1	P1	R2	TS2	P2
S (cal/mol·K)	101.5930	-	70.4070	70.9130	95.2130	83.2820	94.3320
	(103.7690)	(86.2430)	(78.1540)	(80.3930)	(108.0650)	(89.0300)	(97.7960)
U (Hartree)	-1194.3543	-	-1194.3072	-1194.4054	-1593.2827	-1593.2755	-1593.3318
	(-1194.3819)	(-1194.3816)	(-1194.3288)	(-1194.3344)	(-1593.3062)	(-1593.3124)	(-1593.2612)
H (Hartree)	-1194.3524	-	-1194.3063	-1194.4044	-1593.2817	-1593.3398	-1593.3308
	(-1194.3800)	(-1194.3907)	(-1194.3278)	(-1194.3335)	(-1593.3053)	(-1593.3115)	(-1593.2602)
G (Hartree)	-1194.4006	-	-1194.3397	-1194.4381	-1593.3270	-1593.3794	-1593.3757
	(-1194.4293)	(-1194.4216)	(-1194.3650)	(-1194.3717)	(-1593.3566)	(-1593.3538)	(-1593.3067)

Table S8. Thermodynamic parameters of S_2 reacting with H_2S calculated with M06-2X/6-311++G(2d,2p). (Values in the parentheses are in triplet state.)

	R1	IM1	TS1	P1	R2	TS2	P2
S (cal/mol·K)	101.3930	-	69.9230	72.5170	93.8460	82.8970	91.5780
	(103.5790)	(84.6600)	(74.8770)	(79.0650)	(94.2280)	(90.3860)	(99.0180)
U (Hartree)	-1195.6768	-	-1195.6658	-1195.7395	-1595.0502	1595.0511	-1595.1045
	(-1195.7108)	(-1195.7102)	(-1195.6630)	(-1195.6671)	(-1595.0760)	(-1595.0266)	(-1595.0334)
H (Hartree)	-1195.6749	-	-1195.6648	-1195.7385	-1595.0493	-1595.0501	-1595.1036
	(-1195.7089)	(-1195.7092)	(-1195.6621)	(-1195.6661)	(-1595.0751)	(-1595.0257)	(-1595.0325)
G (Hartree)	-1195.7231	-	-1195.6981	-1195.7730	-1595.0936	-1595.0895	-1595.1471
	(-1195.7581)	(-1195.7494)	(-1195.6977)	(-1195.7037)	(-1595.1199)	(-1595.0686)	(-1595.0795)

Table S9. Thermodynamic parameters of S_2 reacting with H_2S calculated with CCSD(T)/aug-cc-pVQZ on the M06-2X/6-311++G(2d,2p) optimized structures. (Values in the parentheses are in triplet state.)

	R1	IM1	TS1	P1	R2	TS2	P2
S (cal/mol·K)	101.3930	-	69.9230	72.5170	93.8460	82.8970	91.5780
	(103.5790)	(84.6600)	(74.8770)	(79.0650)	(94.2280)	(90.3860)	(99.0180)
U (Hartree)	-1194.4044	-	-1194.3896	-1194.4567	-1593.3463	-1593.3445	-1593.3986
	(-1194.4319)	(-1194.4353)	(-1194.3778)	(-1194.3823)	(-1593.3712)	(-1593.3148)	(-1593.3249)
H (Hartree)	-1194.4010	-	-1194.3844	-1194.4558	-1593.3453	-1593.3435	-1593.3976
	(-1194.4285)	(-1194.4279)	(-1194.3768)	(-1194.3813)	(-1593.3702)	(-1593.3138)	(-1593.3240)
G (Hartree)	-1194.4482	-	-1194.4177	-1194.4902	-1593.3896	-1593.3829	-1593.4411
	(-1194.4767)	(-1194.4681)	(-1194.4124)	(-1194.4189)	(-1593.4150)	(-1593.3568)	(-1593.3710)

Table S10. Thermodynamic parameters of S_2 reacting with H_2S calculated with CCSD(T)/aug-cc-pVTZ on the M06-2X/6-311++G(2d,2p) optimized structures. (Values in the parentheses are in triplet state.)

	R1	IM1	TS1	P1	R2	TS2	P2
S (cal/mol·K)	101.3930	-	69.9230	72.5170	93.8460	82.8970	91.5780
	(103.5790)	(84.6600)	(74.8770)	(79.0650)	(94.2280)	(90.3860)	(99.0180)
U (Hartree)	-1194.3535	-	-1194.3349	-1194.4063	-1593.2819	-1593.2780	-1593.3320
	(-1194.3815)	(-1194.3811)	(-1194.3301)	(-1194.3347)	(-1593.3072)	(-1593.2508)	(-1593.2611)
H (Hartree)	-1194.3516	-	-1194.3339	-1194.4053	-1593.2799	-1593.2770	-1593.3311
	(-1194.3796)	(-1194.3802)	(-1194.3292)	(-1194.3338)	(-1593.3063)	(-1593.2499)	(-1593.2602)
G (Hartree)	-1194.3998	-	-1194.3671	-1194.4398	-1593.3242	-1593.3164	-1593.3746
	(-1194.4289)	(-1194.4204)	(-1194.3647)	(-1194.3713)	(-1593.3510)	(-1593.2928)	(-1593.3072)

Table S11. Thermodynamic parameters of S_2 reacting with H_2S calculated with CCSD(T)/CBS on the M06-2X/6-311++G(2d,2p) optimized structures. (Values in the parentheses are in triplet state.)

	R1	IM1	TS1	P1	R2	TS2	P2
S (cal/mol·K)	101.3930	-	69.9230	72.5170	93.8460	82.8970	91.5780
	(103.5790)	(84.6600)	(74.8770)	(79.0650)	(94.2280)	(90.3860)	(99.0180)
U (Hartree)	-1194.4163	-	-1194.4003	-1194.4716	-1593.3653	-1593.3639	-1593.4180
	(-1194.4436)	(-1194.4429)	(-1194.3919)	(-1194.3964)	(-1593.3898)	(-1593.3335)	(-1593.3435)
H (Hartree)	-1194.4144	-	-1194.3994	-1194.4707	-1593.3644	-1593.3630	-1593.4170
	(-1194.4417)	(-1194.4420)	(-1194.3909)	(-1194.3953)	(-1593.3889)	(-1593.3326)	(-1593.3426)
G (Hartree)	-1194.4625	-	-1194.4326	-1194.5051	-1593.4087	-1593.4024	-1593.4605
	(-1194.4909)	(-1194.4822)	(-1194.4265)	(-1194.4329)	(-1593.4337)	(-1593.3755)	(-1593.3896)

Table S12. Structure and coordinates of S_4 reacting with H_2S molecule optimized at the M06-2X/6-311++G(2d,2p) level.

Name	Structure	Numbering	X	Y	Z
IM3		1	-0.55245	1.18173	-0.86047
		2	-1.17393	-0.78005	-0.89159
		3	-0.15245	1.64795	0.95142
		4	-1.12612	-1.43978	0.91077
		5	2.69434	-0.44424	-0.11662
		6	1.78803	-1.04269	0.66330
		7	3.18163	-1.60704	-0.55948
TS3		1	-0.25313	1.64354	-0.27385
		2	-1.72853	0.10700	-0.52094
		3	1.14581	0.91514	0.82172
		4	-1.19724	-1.44731	0.61776
		5	1.90725	-1.09016	-0.53286
		6	0.55894	-1.52439	-0.12951
		7	1.45440	-0.52706	-1.65974
P3		1	-0.00217	1.24909	0.32682
		2	-1.33322	0.29956	-0.94217
		3	1.30467	-0.23327	0.94799
		4	-2.68454	-0.67986	0.28053
		5	2.62126	-0.54788	-0.61925
		6	-1.99010	-1.81961	0.40020
		7	3.49394	0.41737	-0.30283

Table S13. Structure and coordinates of S_6 reacting with H_2S molecule optimized at the M06-2X/6-311++G(2d,2p) level.

Name	Structure	Numbering	X	Y	Z
IM4		1	0.03036	-1.18139	1.18860
		2	1.95993	-0.52873	0.98906
		3	1.68201	1.51612	0.54365
		4	0.01537	1.45513	-0.75068
		5	0.42550	-0.17510	-1.91264
		6	-0.43194	-1.75383	-0.78750
		7	-3.23182	0.67239	0.69978
		8	-4.47708	0.20703	0.55834
		9	-2.71339	-0.28046	-0.08252
TS4		1	-0.29811	1.30973	-0.91613
		2	-2.14459	0.80338	-0.65008
		3	-2.05838	-1.13124	0.20524
		4	-0.19880	-1.19143	1.19236
		5	1.23706	-1.88778	-0.11850
		6	2.23062	-0.35783	-0.99569
		7	1.01270	2.17783	1.20133
		8	1.66651	3.20132	0.63440
		9	1.84546	1.23617	0.66926
P4		1	-2.06350	0.27920	-0.78533
		2	-1.62200	-1.54018	0.10648
		3	0.31187	-2.03401	-0.41586
		4	1.54468	-1.02367	0.92271
		5	2.53857	0.36833	-0.23576
		6	1.29769	2.01135	-0.44603
		7	-1.90958	1.67755	0.73710
		8	-3.17703	1.56957	1.15849
		9	1.61346	2.61304	0.70873
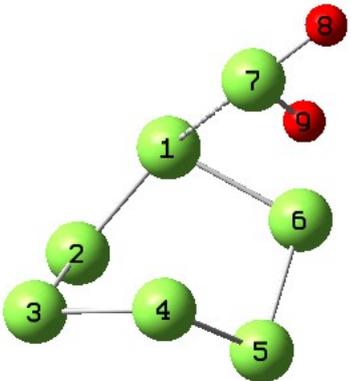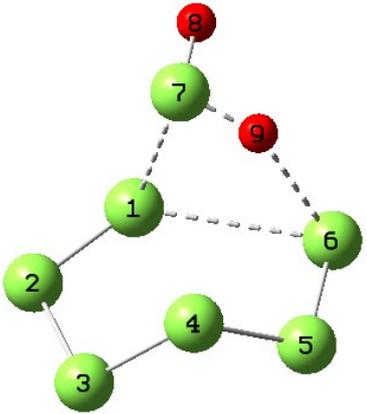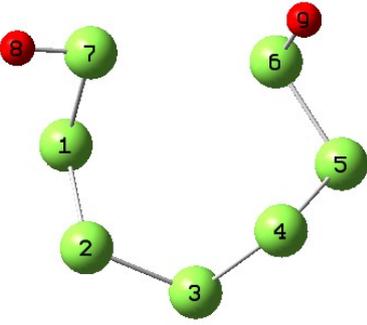
Table S14. Structure and coordinates of S_8 reacting with H_2S molecule optimized at the M06-2X/6-311++G(2d,2p) level.

Name	Structure	Numbering	X	Y	Z
IM5		1	2.51784	0.29337	-1.13277
		2	1.86305	1.91464	-0.03814
		3	-0.21978	1.88995	-0.24848
		4	-1.03960	1.28822	1.51111
		5	-2.23946	-1.62600	-0.06782
		6	-0.38672	-1.82164	-0.55251
		7	0.78169	-1.31456	1.11619
		8	2.63079	-1.32427	0.18985
		9	-3.46244	0.61355	-0.79532
		10	-2.67305	1.12508	0.25135
		11	-4.45268	0.26295	0.03505
TS5		1	2.51784	0.29337	-1.13277
		2	1.86305	1.91464	-0.03814
		3	-0.21978	1.88995	-0.24848
		4	-1.03960	1.28822	1.51111
		5	-2.23946	-1.62600	-0.06782
		6	-0.38672	-1.82164	-0.55251
		7	0.78169	-1.31456	1.11619
		8	2.63079	-1.32427	0.18985
		9	-3.46244	0.61355	-0.79532
		10	-2.67305	1.12508	0.25135
		11	-4.45268	0.26295	0.03505
P5		1	0.86260	-1.28955	-1.43266
		2	2.60694	-0.50672	-0.63105
		3	2.13265	1.45265	-0.14659
		4	1.68809	1.51601	1.86819
		5	-2.13237	1.45281	0.14696
		6	-2.60704	-0.50664	0.63066
		7	-0.86297	-1.28984	1.43249
		8	-0.00016	-2.50616	-0.00020
		9	-1.68775	1.51694	-1.86781
		10	0.37115	1.28421	1.75058
		11	-0.37102	1.28393	-1.75035

Table S15. Thermodynamic parameters of S_4 reacting with H_2S calculated with M06-2X/6-311++G(2d,2p).

	R3	IM3	TS3	P3
S (cal/mol·K)	123.0590	91.5900	86.7710	89.3200
U (Hartree)	-1992.0745	-1992.0777	-1992.0564	-1992.1237
H (Hartree)	-1992.0726	-1992.0767	-1992.0554	-1992.1228
G (Hartree)	-1992.1311	-1992.1202	-1992.0967	-1992.1652

Table S16. Thermodynamic parameters of S_4 reacting with H_2S calculated with CCSD(T)/aug-cc-pVTZ on the M06-2X/6-311++G(2d,2p) optimized structures.

	R3	IM3	TS3	P3
S (cal/mol·K)	123.0590	91.5900	86.7710	89.3200
U (Hartree)	-1989.8668	-1989.8696	-1989.8696	-1989.8552
H (Hartree)	-1989.8649	-1989.8686	-1989.8686	-1989.8976
G (Hartree)	-1989.9234	-1989.9121	-1989.8822	-1989.9400

Table S17. Thermodynamic parameters of S_6 reacting with H_2S calculated with M06-2X/6-311++G(2d,2p).

	R4	IM4	TS4	P4
S (cal/mol·K)	133.6690	106.9400	105.6170	104.4290
U (Hartree)	-2788.5058	-2788.4865	-2788.4193	-2788.5076
H (Hartree)	-2788.5039	-2788.4856	-2788.4184	-2788.5066
G (Hartree)	-2788.5674	-2788.5364	-2788.4686	-2788.5563

Table S18. Thermodynamic parameters of S_6 reacting with H_2S calculated with CCSD(T)/aug-cc-pVTZ on the M06-2X/6-311++G(2d,2p) optimized structures.

	R4	IM4	TS4	P4
S (cal/mol·K)	133.6690	106.9400	105.6170	104.4290
U (Hartree)	-2785.3933	-2785.3756	-2785.3196	-2785.3914
H (Hartree)	-2785.3914	-2785.3747	-2785.3186	-2785.3905
G (Hartree)	-2785.4549	-2785.4255	-2785.3688	-2785.4401

Table S19. Thermodynamic parameters of S_8 reacting with H_2S calculated with M06-2X/6-311++G(2d,2p).

	R5	IM5	TS5	P5
S (cal/mol·K)	-148.9340	121.4350	119.0410	115.8910
U (Hartree)	-3584.9002	-3584.8869	-3584.8036	-3584.8987
H (Hartree)	-3584.8983	-3584.8859	-3584.8026	-3584.8977
G (Hartree)	-3584.9691	-3584.9436	-3584.8694	-3584.9516

Table S20. Thermodynamic parameters of S_8 reacting with H_2S calculated with CCSD(T)/aug-cc-pVTZ on the M06-2X/6-311++G(2d,2p) optimized structures.

	R4	IM4	TS4	P4
S (cal/mol·K)	148.9340	121.4350	119.0410	115.8910
U (Hartree)	-3580.8960	-3580.8836	-3580.8064	-3580.8954
H (Hartree)	-3580.8942	-3580.8827	-3580.8036	-3580.8925
G (Hartree)	-3580.9649	-3580.9404	-3579.0646	-3580.9474