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

Supplementary Information for

Chemical Dynamics Study on the Gas-Phase Reaction of the D1-Silylidyne Radical (SiD; $X^2\Pi$) with Deuterium Sulfide (D_2S) and Hydrogen Sulfide (H_2S)

Shane J. Goettl,[a] Srinivas Doddipatla,[a] Zhenghai Yang,[a] Chao He,[a] Ralf I. Kaiser[a,*]

[a] *Department of Chemistry, University of Hawai'i at Manoa, Honolulu, Hawaii 96822, USA*

Corresponding Author: ralfk@hawaii.edu

Mateus Xavier Silva,[b] Breno R. L. Galvão[b,*]

[b] *Centro Federal de Educação Tecnológica de Minas Gerais, CEFET-MG, Av. Amazonas 5253, 30421-169 Belo Horizonte, Minas Gerais, Brazil*

Corresponding Author: brenogalvao@gmail.com

Tom J. Millar[c,*]

[c] *School of Maths and Physics, Queen's University Belfast, University Road, Belfast BT7 1NN, Northern Ireland*

Corresponding Author: Tom.Millar@qub.ac.uk

Supplementary Note 1. Pulse Sequence.

An optimized pulse sequence (Figure S1) was used to coordinate the data collection. A 17.0 ± 0.1 cm diameter, four-slot (0.76 ± 0.01 mm) chopper wheel rotating at 120 Hz provided with an infrared photodiode pulse initiated the trigger (T_0 = 0 μs) for the synchronization of the equipment. The photodiode sent a 480 Hz signal that was divided to 60 Hz and conveyed to three pulse/delay generators (PDG I-III; DG535, Stanford Research Systems). For the SiD/D_2S reaction, the PDG I outputs (+4 V, 50 Ω) AB ($A_I = T_0 + 1859$ μs, $B_I = A_I + 80$ μs) and CD ($C_I = A_I - 22$ μs, $D_I = C_I + 80$ μs) were sent through a pulse shaper and pulse amplifier (E-421, Physik Instrumente) and were received by the primary and secondary Proch-Trickl[1] pulsed valves, which each contain a piezoelectric disk translator (P-286.23, Physik Instrumente). This allows for a pulsed valve open time of 80 μs when operating at an amplitude of −400 V. The output from PDG I A (TTL, high impedance) was divided to 30 Hz and directed to PDG II and III, which were used for background subtraction. PDG II AB ($A_{II} = A_I + 16654$ μs, $B_{II} = A_{II} + 5$ μs) and CD ($C_{II} = A_{II} + 186$ μs, $D_{II} = C_{II} + 5$) triggered the flashlamps and Q-switch, respectively, of a neodymium-doped yttrium aluminum garnet (Nd:YAG) laser (Quanta-Ray Pro 270, Spectra-Physics) and PDG III AB ($A_{III} = A_I + 16666.66$ μs, $B_{III} = A_{III} + 5$ μs) triggered the MCS. For the SiD/H_2S reaction, the delay times were as follows: PDG I AB ($A_I = T_0 + 1868$ μs, $B_I = A_I + 80$ μs) and CD ($C_I = A_I - 22$ μs, $D_I = C_I + 80$ μs); PDG II AB ($A_{II} = A_I + 16643$ μs, $B_{II} = A_{II} + 5$ μs) and CD ($C_{II} = A_{II} + 186$ μs, $D_{II} = C_{II} + 5$); PDG III AB ($A_{III} = A_I + 16666.66$ μs, $B_{III} = A_{III} + 5$ μs).

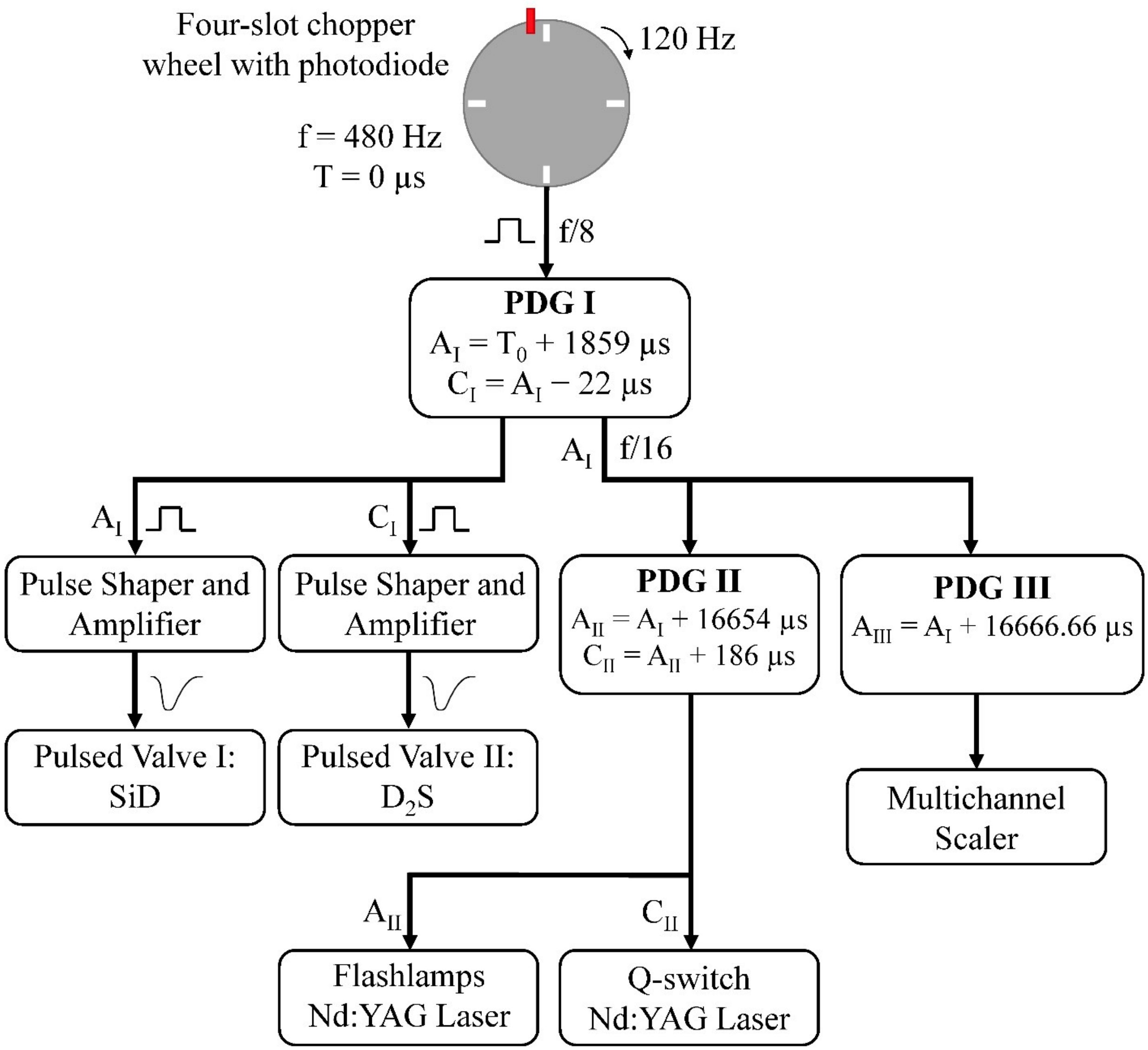


Figure S1. Pulse sequence for the crossed molecular beam reaction of the D1-silylidyne radical (SiD; $X^2\Pi$) with deuterium sulfide (D_2S) and hydrogen sulfide (H_2S).

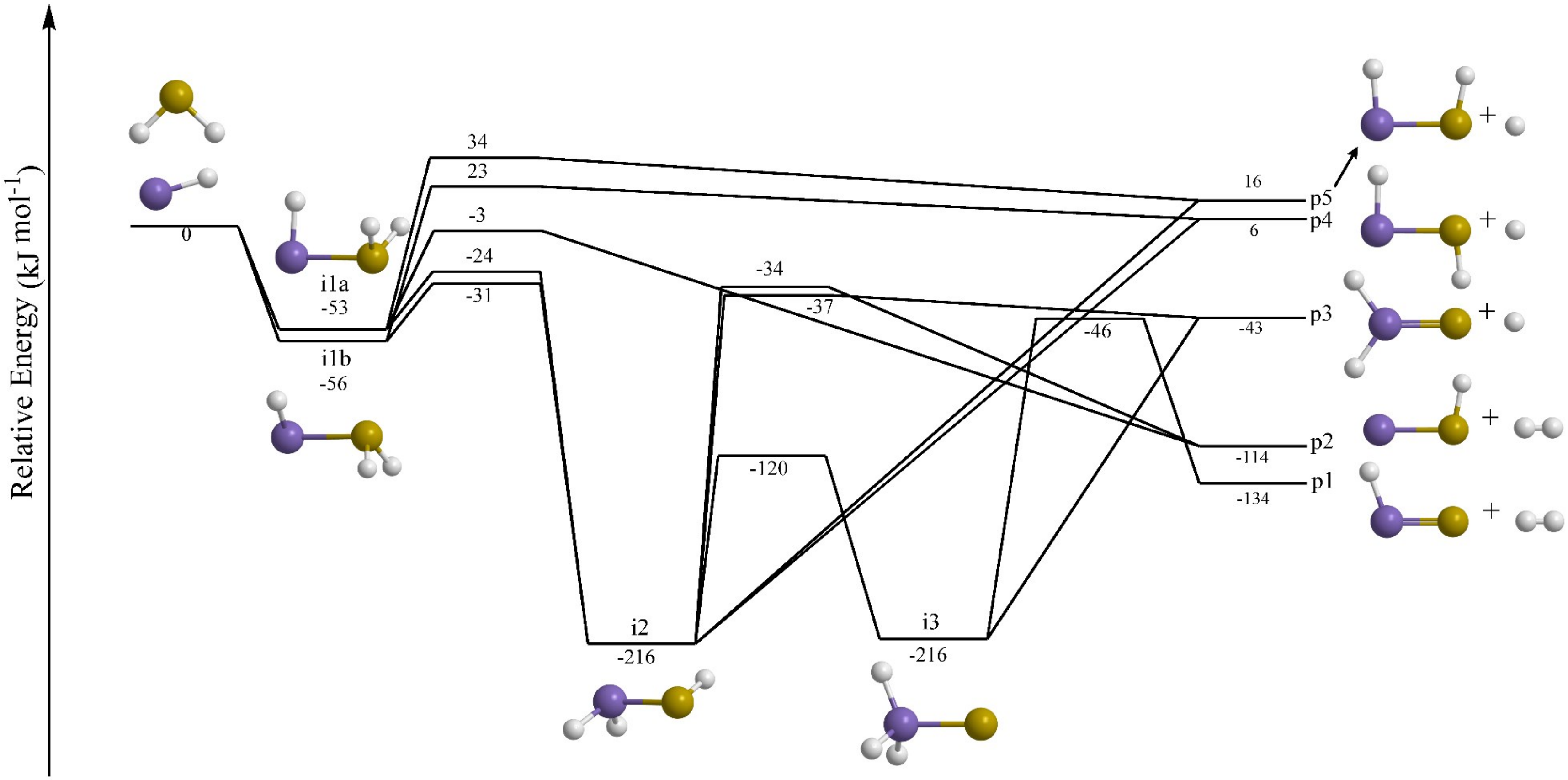


Figure S2. Schematic representation of the potential energy surface at the CCSD(T)-F12/aug-cc-pV(T+d)Z//CCSD(T)/aug-cc-pV(T+d)Z+ZPE(CCSD(T)/aug-cc-pV(T+d)Z) level for the non-deuterated (H_2S+SiH) case including transition states not accessible in our experiments.

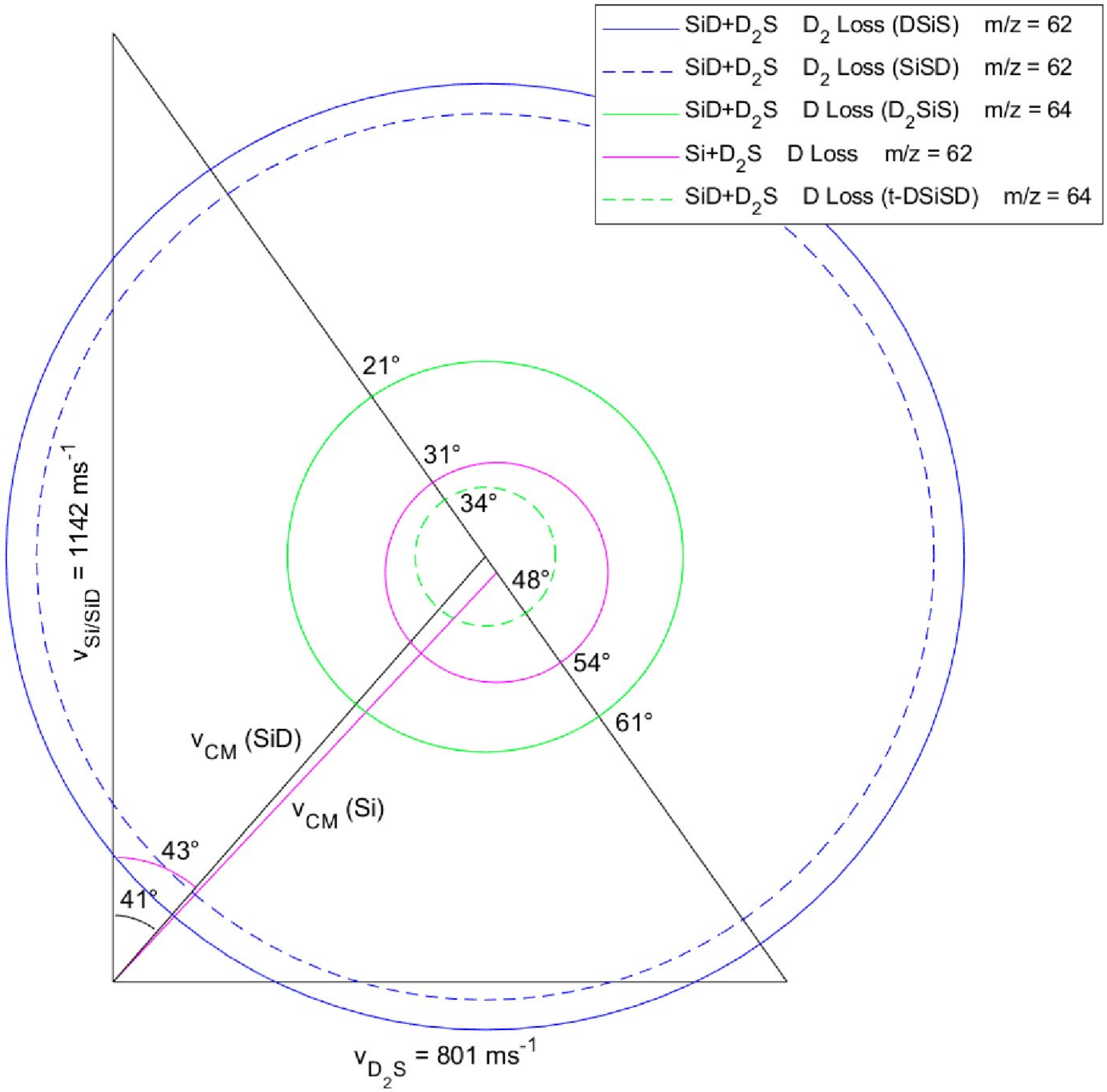


Figure S3. Newton circle diagram for the reaction of ground state atomic silicon (Si(^{3}P)) with deuterium sulfide (D_2S) and of the D1-silylidyne radical (SiD; $X^2\Pi$) with deuterium sulfide (D_2S). The diagram incorporates all reaction pathways below the reaction collision energy of 15.9 kJ mol^{-1}. Each Newton circle has a radius equal to the maximum CM recoil velocity of its corresponding heavy product, and a maximum laboratory angular scattering range for observation of products by the detector.

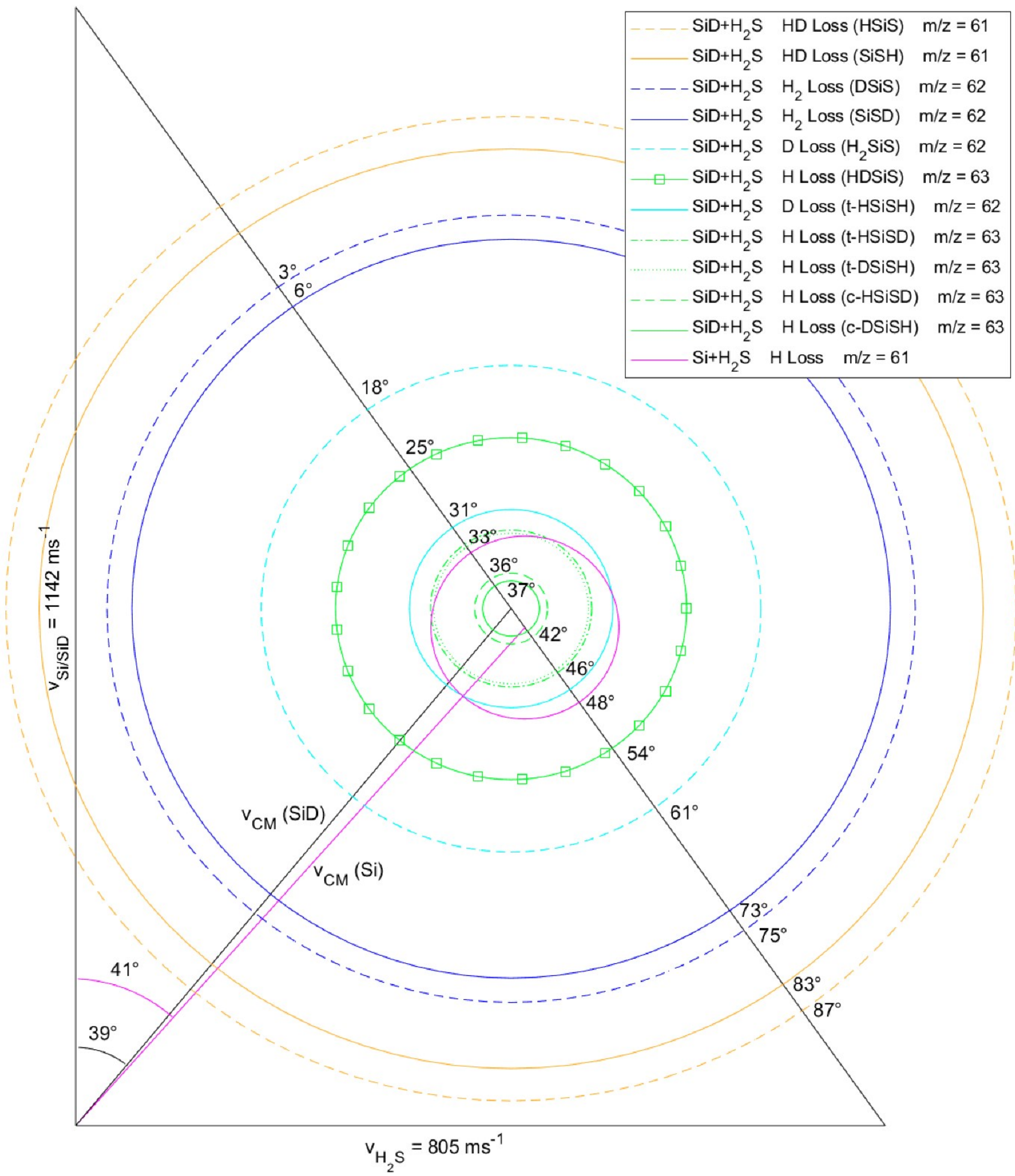


Figure S4. Newton circle diagram for the reaction of ground state atomic silicon (Si(^{3}P)) with hydrogen sulfide (H_2S) and of D1-silylidyne radical (SiD; $X^2\Pi$) with hydrogen sulfide (H_2S). The diagram incorporates all reaction pathways below the reaction collision energy of 15.6 kJ mol^{-1}. Each Newton circle has a radius equal to the maximum CM recoil velocity of its corresponding heavy product, and a maximum laboratory angular scattering range for observation of products by the detector.

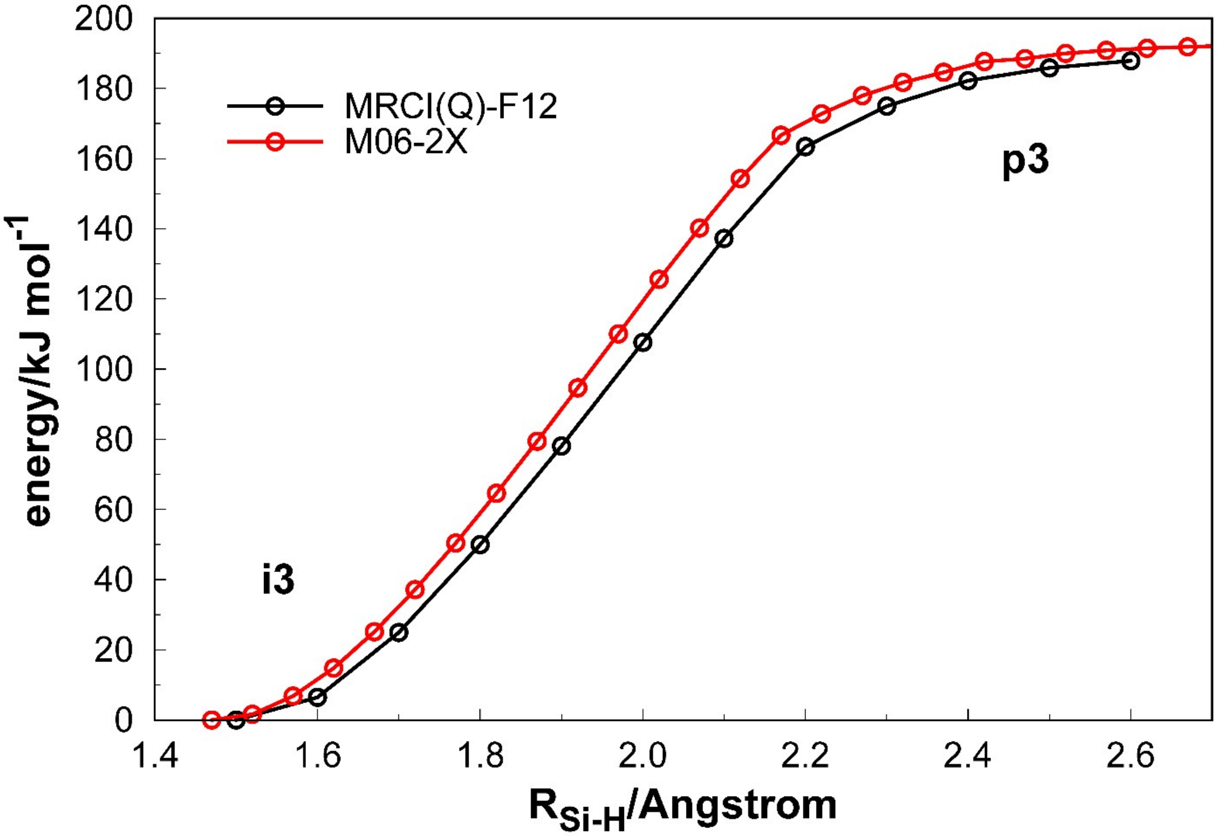
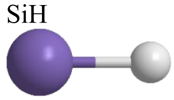
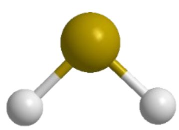
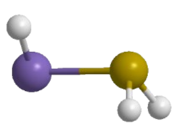
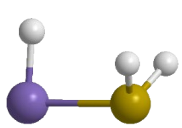
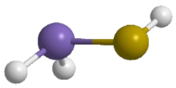
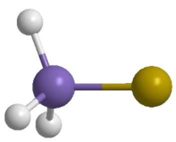
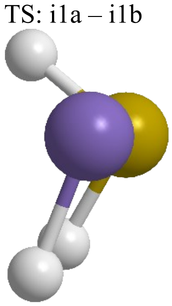
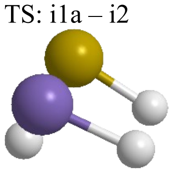
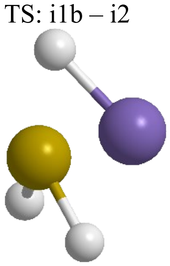


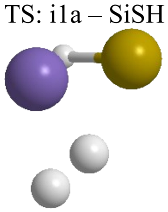
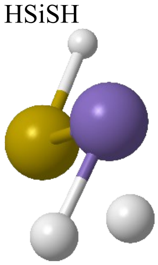
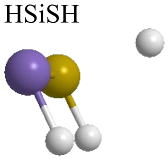
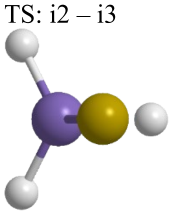
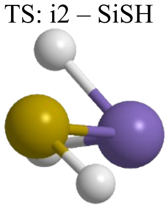
Figure S5. Optimized potential energy profile as a function of the Si-H bond for a hydrogen loss from **i3** to **p3**. To confirm the barrierless nature of this path obtained by the exploratory M06-2X/cc-pV(T+d)Z calculations (red line), a full valence CASSCF/cc-pV(T+d)Z optimization followed by single point energy refinement at the MRCI(Q)-F12 level[2] (black line) were performed. The energies are relative to the **i3** optimized structure for each method.

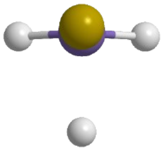
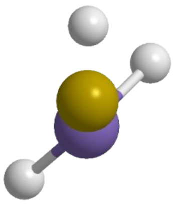
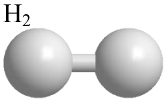
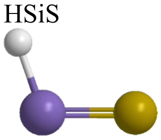
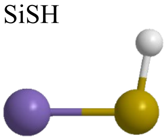
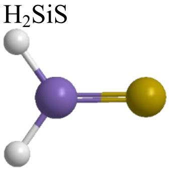
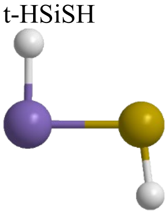
Table S1. Optimized Cartesian coordinates (Å) and vibrational frequencies (cm^{-1}) for all intermediates, transition states, reactants, and products involved in the SiH+H_2S reaction at the CCSD(T)/aug-cc-pV(T+d)Z level. The energies are given for all isotopic substitutions considered in this work at the CCSD(T)-F12/aug-cc-pV(T+d)Z//CCSD(T)/aug-cc-pV(T+d)Z+ZPE(M06-2X/cc-pV(T+d)Z) level in kJ mol^{-1}.

E(D0) – gives the energy of the non-deuterated case
E(D1) – gives the energy for one deuterium at the first position of the Cartesian coordinates
E(D2) – gives the energy for one deuterium at the second position of the Cartesian coordinates
E(D3) – gives the energy for one deuterium at the third position of the Cartesian coordinates
E(D1,D2,D3) – gives the energy of the fully deuterated case

Species	**Vibrational Frequencies (cm^{-1})**	**Relative Energy (kJ mol^{-1})**	**Cartesian Coordinates (Å)**			
			Atom	**X**	**Y**	**Z**
SiH  T1 diagnostic: 0.01362941	2027.38		H Si	0.0000000000 0.0000000000	0.0000000000 0.0000000000	-0.7626723064 0.7626723064
H_2S  T1 diagnostic: 0.01105045	1211.38 2715.39 2730.68		H H S	0.1196696836 1.2341510522 -0.0810267358	0.0000000000 0.0000000000 0.0000000000	1.2667032628 -0.3094033975 -0.0572948654
i1b: $HSiSH_2$  T1 diagnostic: 0.01489830	174.21 238.94 446.28 468.34 796.91 1208.04 1999.73 2652.97 2702.15	E(D0)=-55.8 E(D1)=-58.9 E(D2)=-57.1 E(D3)=-58.5 E(D1,D2,D3)=-58.7	H H H S Si	0.0003935060 0.2609873303 -0.3697756867 0.4981237979 -0.3915017593	1.0090222955 -1.3482916268 -0.8893485662 -0.1131821796 0.0288457448	-1.7724994770 1.1494632907 -1.9052899747 -1.2315483277 1.0390615819
i1a: $HSiSH_2$  T1 diagnostic: 0.01477086	163.46 225.90 432.76 436.28 722.54 1206.31 1997.86 2673.89 2679.92	E(D0)=-52.5 E(D1)=-53.8 E(D2)=-55.3 E(D3)=-55.3 E(D1,D2,D3)=-55.2	H H H S Si	-0.0015617101 0.9684244707 -0.9700785413 0.0001568099 0.0003314886	1.4809419224 0.7933280396 0.7912018574 -0.0785599453 -0.0422403169	1.2122198795 -1.4670774062 -1.4669068765 -1.1402225695 1.3297447969

i2: H_2SiSH  T1 diagnostic: 0.01852358	233.70 513.08 553.07 682.20 812.49 913.13 2184.91 2229.17 2698.40	E(D0)=-215.8 E(D1)=-217.8 E(D2)=-218.3 E(D3)=-217.8 E(D1,D2,D3)=-218.3	H -0.0725257577 1.2400496850 -1.7198885632 H 0.1391215870 -1.2863381361 1.1445888941 H -0.2081773596 -1.1918438291 -1.8938658389 S -0.2467688427 -0.0247930143 0.8992717405 Si 0.3865775612 -0.0500290377 -1.1509191393
i3: H_3SiS  T1 diagnostic: 0.01299818	429.05 495.46 560.88 920.45 922.13 972.38 2228.05 2245.06 2247.13	E(D0)=-215.4 E(D1)=-217.8 E(D2)=-217.8 E(D3)=-217.8 E(D1,D2,D3)=-218.5	H -0.7053306888 1.2064166061 -1.6057582649 H -0.7055177224 -1.2064663757 -1.6057202364 H 1.3978469431 0.0001254761 -1.5012968320 S 0.0476275678 -0.0000044712 1.0530729633 Si -0.0251973911 -0.0000712355 -1.0877839074
TS: i1a – i1b  T1 diagnostic: 0.01454585	167.91 i 220.82 418.86 457.26 716.51 1202.10 2003.06 2676.95 2711.73	E(D0)=-51.0 E(D1)=-53.8 E(D2)=-52.1 E(D3)=-53.8 E(D1,D2,D3)=-53.5	H -0.0123311133 -1.0289923027 -1.7210828235 H -0.4036145457 -1.3040386741 0.9045779622 H -0.4252254333 0.8680813375 -1.7419544033 S 0.5915338944 0.0987905737 -1.3200351844 Si 0.2478643861 0.0532047334 1.1576815421
TS: i1a – i2  T1 diagnostic: 0.01908338	704.89 i 349.94 402.62 536.41 744.64 930.92 1414.00 2043.09 2706.86	E(D0)=-23.9 E(D1)=-26.7 E(D2)=-24.1 E(D3)=-25.5 E(D1,D2,D3)=-24.2	H 1.0761229146 -0.1720676996 -0.9023103276 H -0.7688441944 -0.6486134386 -0.0888945962 H 0.8694153546 -0.7814042028 1.5894413571 S -0.0347175877 0.5575801979 -0.7267120551 Si -0.4993555372 -0.1230668568 1.5775944418
TS: i1b – i2  T1 diagnostic: 0.01915692	665.39 i 351.03 480.76 523.13 837.38 1039.69 1458.06 2039.71 2694.48	E(D0)=-30.3 E(D1)=-31.9 E(D2)=-33.3 E(D3)=-30.8 E(D1,D2,D3)=-31.1	H -0.1581234079 1.1760144278 -1.7294475338 H 0.2362076436 -1.4070535429 0.8917866757 H -0.5435573903 -0.8584828748 -0.8698758097 S -0.3825350130 -0.2739811602 0.5255274234 Si 0.8462353561 0.0505488177 -1.5388036623

TS: i1a – SiSH  T1 diagnostic: 0.01532170	1174.19 i 332.28 361.24 618.28 987.42 1091.37 1453.78 1766.31 2674.03	E(D0)=-3.3 E(D1)=-6.0 E(D2)=-3.8 E(D3)=-4.9 E(D1,D2,D3)=-3.7	H -0.1627126861 0.4575626717 -2.0988434848 H 0.2137768879 -0.9266738266 -0.4886360802 H -0.3351369496 -1.4120897042 0.2937734088 S 0.8257018958 0.4269246957 -1.1896799672 Si -0.5434019598 0.1413218312 0.7625732166
TS: i1b – t-HSiSH  T1 diagnostic: 0.02953411	816.29 i 208.83 365.75 496.51 609.96 708.31 916.52 2051.05 2695.95	E(D0)=23.1 E(D1)=19.9 E(D2)=21.3 E(D3)=25.9 E(D1,D2,D3)=25.1	H -0.0016860697 0.9876538231 -1.5372396614 H 0.3354538983 -1.2327832020 1.3619182647 H -0.5264501878 -1.0174605390 -2.5129845076 S 0.4616446767 -0.1586981065 -1.0186298335 Si -0.2707351293 0.1083336920 0.9861228309
TS: i1a – c-HSiSH  T1 diagnostic: 0.02930655	835.11 i 224.29 345.35 485.56 585.34 715.16 801.20 2046.20 2705.70	E(D0)=33.7 E(D1)=32.0 E(D2)=30.7 E(D3)=36.5 E(D1,D2,D3)=35.9	H 0.2645467141 -1.2028860774 1.4591198480 H 0.8308947216 -1.1168827663 -1.0001363218 H 2.0303767102 0.7203788712 -1.5495965466 S 0.2557350098 0.0912969574 -0.9377358263 Si -0.3630780658 0.1421572551 1.1388969768
TS: i2 – i3  T1 diagnostic: 0.01427596	1341.90 i 515.82 566.72 595.20 628.29 930.80 1710.96 2235.65 2263.05	E(D0)=-119.9 E(D1)=-122.0 E(D2)=-122.0 E(D3)=-119.9 E(D1,D2,D3)=-120.0	H -0.8280755407 1.2332114783 -1.7675479778 H -0.8367543593 -1.2335779015 -1.7580963620 H 1.3454283731 -0.0037506674 -0.6965108041 S 0.5398447628 0.0044872355 0.7156201412 Si -0.2110145273 -0.0003701452 -1.2409512748
TS: i2 – SiSH  T1 diagnostic: 0.03228793	1212.81 i 388.72 477.73 500.79 662.48 836.70 1591.31 1691.91 2685.50	E(D0)=-34.2 E(D1)=-34.8 E(D2)=-37.0 E(D3)=-34.3 E(D1,D2,D3)=-33.5	H -0.2389002069 0.7887057229 -1.6180597204 H 0.3179559118 -1.0120199990 1.4521525533 H -0.3719666851 -0.4954450728 -2.1705816973 S -0.4747746828 -0.2376083375 0.6941427583 Si 0.7659128513 -0.3565866458 -1.0784668007

TS: i2 – H_2SiS  T1 diagnostic: 0.02249936	560.50 i 126.59 195.81 610.61 611.15 701.52 996.69 2241.15 2257.05	E(D0)=-36.3 E(D1)=-33.2 E(D2)=-38.5 E(D3)=-38.5 E(D1,D2,D3)=-33.3	H -0.0031480161 -1.9327522017 1.9285719718 H 1.2150637956 -0.1015826553 -1.8482330848 H -1.2155844270 -0.0977248266 -1.8474330501 S 0.0004609955 0.0988763472 0.9482859326 Si 0.0001085382 -0.0201381253 -1.0106728362
TS: i3 – HSiS  T1 diagnostic: 0.02758986	972.79 i 438.88 510.13 675.63 879.78 958.69 1519.46 1928.36 2287.49	E(D0)=-45.6 E(D1)=-46.3 E(D2)=-47.9 E(D3)=-46.7 E(D1,D2,D3)=-45.3	H 0.0134612112 1.0221655240 -1.7044330334 H -0.8773267545 -1.1131920597 -1.6882748693 H 0.8748438347 0.5007529830 -1.7582971504 S -0.0025648348 -0.0334602251 1.1721801991 Si 0.0010152520 -0.3762662225 -0.7686614234
H_2  T1 diagnostic: 0.00601239	4400.22		H 0.0000000000 0.0000000000 0.3715191784 H 0.0000000000 0.0000000000 -0.3715191784
HSiS  T1 diagnostic: 0.03565980	577.18 692.59 2029.11	E(HSiS+H_2)=-133.9 E(DSiS+H_2)=-134.8 E(HSiS+HD)=-134.0 E(DSiS+D_2)=-131.3	H 0.0000000000 1.2374246601 -1.7921712477 S 0.0000000000 0.0106422259 0.9596721427 Si 0.0000000000 -0.0512338506 -1.0060931678
SiSH  T1 diagnostic: 0.01827924	510.32 667.54 2630.06	E(SiSH+H_2)=-114.5 E(SiSD+H_2)=-116.6 E(SiSH+HD)=-114.6 E(SiSD+D_2)=-113.1	H 0.0000000000 1.1799831517 -1.5695610837 S 0.0000000000 -0.1125267945 -1.1904889181 Si 0.0000000000 0.1293766784 0.9214577290
H_2SiS  T1 diagnostic: 0.01747638	614.44 636.23 717.46 1005.81 2236.96 2249.80	E(D0)=-42.3 E(D1)=-44.4 E(D2)=-44.4 E(D1,D2)=-38.7	H -0.0022686497 1.2202515430 -1.8556186086 H 0.0054933914 -1.2015802377 -1.8408225640 S -0.0048384390 0.0264361371 0.9542773806 Si -0.0003070689 0.0145171489 -0.9990731088
t-HSiSH  T1 diagnostic: 0.01672500	516.99 626.36 634.15 912.17 2048.92 2683.39	E(D0)=6.0 E(D1)=3.0 E(D2)=4.2 E(D1,D2)=9.1	H -1.1009437415 0.0000000000 2.4062455267 H 1.2741902382 0.0000000000 -0.3788405158 S 0.1788465601 0.0000000000 1.9996623518 Si -0.2184420568 0.0000000000 -0.0951663628

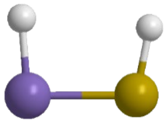
c-HSiSH  T1 diagnostic: 0.01699851	507.66 536.78 662.19 807.13 2045.24 2696.53	E(D0)=15.7 E(D1)=13.0 E(D2)=14.1 E(D1,D2)=19.1	H -0.0000960212 1.2924313596 -1.2088926370 H 0.0004095851 1.4406316565 1.3034694552 S -0.0003580214 -0.0310749324 -0.9922990305 Si 0.0000265565 -0.0702965394 1.1528746985

Table S2. Physical parameters adopted for the Orion sources.

	Orion Hot Core	Orion Plateau	Orion 15.5 km s^{-1} component
$n(H_2)$ cm^{-3}	5×10^7	10^6	5×10^6
T (K)	225	125	200
$N(H_2)$ cm^{-2}	4.2×10^{23}	2.1×10^{23}	10^{23}

Table S3. D and D_2 loss product mass combinations of silicon and sulfur isotopes from the reaction of ground state atomic silicon (Si(^{3}P)) and deuterium sulfide (D_2S; X^1A_1). Isotope abundance given in parenthesis.

Si + D_2S		$D_2{}^{32}S$ (94.93%) 36	$D_2{}^{33}S$ (0.76%) 37	$D_2{}^{34}S$ (4.29%) 38	$D_2{}^{36}S$ (0.02%) 40
D Loss	^{28}Si (92.23%) 28	$^{28}Si^{32}SD$ 62	$^{28}Si^{33}SD$ 63	$^{28}Si^{34}SD$ 64	$^{28}Si^{36}SD$ 66
	^{29}Si (4.68%) 29	$^{29}Si^{32}SD$ 63	$^{29}Si^{33}SD$ 64	$^{29}Si^{34}SD$ 65	$^{29}Si^{36}SD$ 67
	^{30}Si (3.09%) 30	$^{30}Si^{32}SD$ 64	$^{30}Si^{33}SD$ 65	$^{30}Si^{34}SD$ 66	$^{30}Si^{36}SD$ 68
D_2 Loss	^{28}Si (92.23%) 28	$^{28}Si^{32}S$ 60	$^{28}Si^{33}S$ 61	$^{28}Si^{34}S$ 62	$^{28}Si^{36}S$ 64
	^{29}Si (4.68%) 29	$^{29}Si^{32}S$ 61	$^{29}Si^{33}S$ 62	$^{29}Si^{34}S$ 63	$^{29}Si^{36}S$ 65
	^{30}Si (3.09%) 30	$^{30}Si^{32}S$ 62	$^{30}Si^{33}S$ 63	$^{30}Si^{34}S$ 64	$^{30}Si^{36}S$ 66

Table S4. H and H_2 loss product mass combinations of silicon and sulfur isotopes from the reaction of ground state atomic silicon (Si(^{3}P)) and hydrogen sulfide (H_2S; X^1A_1). Isotope abundance given in parenthesis.

Si + H_2S		$H_2{}^{32}S$ (94.93%) 34	$H_2{}^{33}S$ (0.76%) 35	$H_2{}^{34}S$ (4.29%) 36	$H_2{}^{36}S$ (0.02%) 38
H Loss	^{28}Si (92.23%) 28	$^{28}Si^{32}SH$ 61	$^{28}Si^{33}SH$ 62	$^{28}Si^{34}SH$ 63	$^{28}Si^{36}SH$ 65
	^{29}Si (4.68%) 29	$^{29}Si^{32}SH$ 62	$^{29}Si^{33}SH$ 63	$^{29}Si^{34}SH$ 64	$^{29}Si^{36}SH$ 66
	^{30}Si (3.09%) 30	$^{30}Si^{32}SH$ 63	$^{30}Si^{33}SH$ 64	$^{30}Si^{34}SH$ 65	$^{30}Si^{36}SH$ 67
H_2 Loss	^{28}Si (92.23%) 28	$^{28}Si^{32}S$ 60	$^{28}Si^{33}S$ 61	$^{28}Si^{34}S$ 62	$^{28}Si^{36}S$ 64
	^{29}Si (4.68%) 29	$^{29}Si^{32}S$ 61	$^{29}Si^{33}S$ 62	$^{29}Si^{34}S$ 63	$^{29}Si^{36}S$ 65
	^{30}Si (3.09%) 30	$^{30}Si^{32}S$ 62	$^{30}Si^{33}S$ 63	$^{30}Si^{34}S$ 64	$^{30}Si^{36}S$ 66

Table S5. D and D_2 loss product mass combinations of silicon and sulfur isotopes from the reaction of the D1-silylidyne radical (SiD; $X^2\Pi$) and deuterium sulfide (D_2S; X^1A_1). Isotope abundance given in parenthesis.

SiD + D_2S		$D_2{}^{32}S$ (94.93%) 36	$D_2{}^{33}S$ (0.76%) 37	$D_2{}^{34}S$ (4.29%) 38	$D_2{}^{36}S$ (0.02%) 40
D Loss	^{28}SiD (92.23%) 30	$^{28}Si^{32}SD_2$ 64	$^{28}Si^{33}SD_2$ 65	$^{28}Si^{34}SD_2$ 66	$^{28}Si^{36}SD_2$ 68
	^{29}SiD (4.68%) 31	$^{29}Si^{32}SD_2$ 65	$^{29}Si^{33}SD_2$ 66	$^{29}Si^{34}SD_2$ 67	$^{29}Si^{36}SD_2$ 69
	^{30}SiD (3.09%) 32	$^{30}Si^{32}SD_2$ 66	$^{30}Si^{33}SD_2$ 67	$^{30}Si^{34}SD_2$ 68	$^{30}Si^{36}SD_2$ 70
D_2 Loss	^{28}SiD (92.23%) 30	$^{28}Si^{32}SD$ 62	$^{28}Si^{33}SD$ 63	$^{28}Si^{34}SD$ 64	$^{28}Si^{36}SD$ 66
	^{29}SiD (4.68%) 31	$^{29}Si^{32}SD$ 63	$^{29}Si^{33}SD$ 64	$^{29}Si^{34}SD$ 65	$^{29}Si^{36}SD$ 67
	^{30}SiD (3.09%) 32	$^{30}Si^{32}SD$ 64	$^{30}Si^{33}SD$ 65	$^{30}Si^{34}SD$ 66	$^{30}Si^{36}SD$ 68

Table S6. H, D, H_2, and HD loss product mass combinations of silicon and sulfur isotopes from the reaction of the D1-silylidyne radical (SiD; $X^2\Pi$) and hydrogen sulfide (H_2S; X^1A_1). Isotope abundance given in parenthesis.

SiD + H_2S		$H_2{}^{32}S$ (94.93%) 34	$H_2{}^{33}S$ (0.76%) 35	$H_2{}^{34}S$ (4.29%) 36	$H_2{}^{36}S$ (0.02%) 38
H Loss	^{28}SiD (92.23%) 30	$^{28}Si^{32}SHD$ 63	$^{28}Si^{33}SHD$ 64	$^{28}Si^{34}SHD$ 65	$^{28}Si^{36}SHD$ 67
	^{29}SiD (4.68%) 31	$^{29}Si^{32}SHD$ 64	$^{29}Si^{33}SHD$ 65	$^{29}Si^{34}SHD$ 66	$^{29}Si^{36}SHD$ 68
	^{30}SiD (3.09%) 32	$^{30}Si^{32}SHD$ 65	$^{30}Si^{33}SHD$ 66	$^{30}Si^{34}SHD$ 67	$^{30}Si^{36}SHD$ 69
D Loss	^{28}SiD (92.23%) 30	$^{28}Si^{32}SH_2$ 62	$^{28}Si^{33}SH_2$ 63	$^{28}Si^{34}SH_2$ 64	$^{28}Si^{36}SH_2$ 66
	^{29}SiD (4.68%) 31	$^{29}Si^{32}SH_2$ 63	$^{29}Si^{33}SH_2$ 64	$^{29}Si^{34}SH_2$ 65	$^{29}Si^{36}SH_2$ 67
	^{30}SiD (3.09%) 32	$^{30}Si^{32}SH_2$ 64	$^{30}Si^{33}SH_2$ 65	$^{30}Si^{34}SH_2$ 66	$^{30}Si^{36}SH_2$ 68
H_2 Loss	^{28}SiD (92.23%) 30	$^{28}Si^{32}SD$ 62	$^{28}Si^{33}SD$ 63	$^{28}Si^{34}SD$ 64	$^{28}Si^{36}SD$ 66
	^{29}SiD (4.68%) 31	$^{29}Si^{32}SD$ 63	$^{29}Si^{33}SD$ 64	$^{29}Si^{34}SD$ 65	$^{29}Si^{36}SD$ 67
	^{30}SiD (3.09%) 32	$^{30}Si^{32}SD$ 64	$^{30}Si^{33}SD$ 65	$^{30}Si^{34}SD$ 66	$^{30}Si^{36}SD$ 68
HD Loss	^{28}SiD (92.23%) 30	$^{28}Si^{32}SH$ 61	$^{28}Si^{33}SH$ 62	$^{28}Si^{34}SH$ 63	$^{28}Si^{36}SH$ 65
	^{29}SiD (4.68%) 31	$^{29}Si^{32}SH$ 62	$^{29}Si^{33}SH$ 63	$^{29}Si^{34}SH$ 64	$^{29}Si^{36}SH$ 66
	^{30}SiD (3.09%) 32	$^{30}Si^{32}SH$ 63	$^{30}Si^{33}SH$ 64	$^{30}Si^{34}SH$ 65	$^{30}Si^{36}SH$ 67

Table S7. Fractional abundance ranges for SiS in the Orion Sources shown in Figure 13.

Source	Light Grey	Dark Grey	Light Grey
Orion Hot Core	$(1.8-5.4) \times 10^{-10}$	$(5.4-8.8) \times 10^{-10}$	$(8.8-26.4) \times 10^{-10}$
Orion Plateau	$(0.43-1.29) \times 10^{-9}$	$(1.29-2.05) \times 10^{-9}$	$(2.05-6.14) \times 10^{-9}$
Orion 15.5 km s^{-1}	$(1.76-5.3) \times 10^{-9}$	$(5.3-8.7) \times 10^{-9}$	$(8.7-26.1) \times 10^{-9}$

References

1. D. Proch and T. Trickl, *Review of Scientific Instruments*, 1989, **60**, 713-716.
2. T. Shiozaki, G. Knizia and H.-J. Werner, *The Journal of Chemical Physics*, 2011, **134**, 034113.