Supplementary Information for

**Chemical Dynamics Study on the Gas-Phase Reaction of the D1-Silylidyne Radical (SiD; X2Π) with Deuterium Sulfide (D2S) and Hydrogen Sulfide (H2S)**

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**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 (T0 = 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/D2S reaction, the PDG I outputs (+4 V, 50 Ω) AB (AI = T0 + 1859 µs, BI = AI + 80 µs) and CD (CI = AI − 22 µs, DI = CI + 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](#_ENREF_1" \o "Proch, 1989 #12) [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](#_ENREF_38)II = AI + 16654 µs, BII = AII + 5 µs) and CD (CII = AII + 186 µs, DII = CII + 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 (AIII = AI + 16666.66 µs, BIII = AIII + 5 µs) triggered the MCS. For the SiD/H2S reaction, the delay times were as follows: PDG I AB (AI = T0 + 1868 µs, BI = AI + 80 µs) and CD (CI = AI − 22 µs, DI = CI + 80 µs); PDG II AB (AII = AI + 16643 µs, BII = AII + 5 µs) and CD (CII = AII + 186 µs, DII = CII + 5); PDG III AB (AIII = AI + 16666.66 µs, BIII = AIII + 5 µs).



**Figure S1.** Pulse sequence for the crossed molecular beam reaction of the D1-silylidyne radical (SiD; X2Π) with deuterium sulfide (D2S) and hydrogen sulfide (H2S).

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**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 (H2S+SiH) case including transition states not accessible in our experiments.



**Figure S3.** Newton circle diagram for the reaction of ground state atomic silicon (Si(3P)) with deuterium sulfide (D2S) and of the D1-silylidyne radical (SiD; X2Π) with deuterium sulfide (D2S). 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(3P)) with hydrogen sulfide (H2S) and of D1-silylidyne radical (SiD; X2Π) with hydrogen sulfide (H2S). 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](#_ENREF_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+H2S 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 0.0000000000 0.0000000000 -0.7626723064  Si 0.0000000000 0.0000000000 0.7626723064 |
| H2S    T1 diagnostic: 0.01105045 | 1211.38  2715.39  2730.68 |  | H 0.1196696836 0.0000000000 1.2667032628  H 1.2341510522 0.0000000000 -0.3094033975  S -0.0810267358 0.0000000000 -0.0572948654 |
| i1b: HSiSH2    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 0.0003935060 1.0090222955 -1.7724994770  H 0.2609873303 -1.3482916268 1.1494632907  H -0.3697756867 -0.8893485662 -1.9052899747  S 0.4981237979 -0.1131821796 -1.2315483277  Si -0.3915017593 0.0288457448 1.0390615819 |
| i1a: HSiSH2    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 -0.0015617101 1.4809419224 1.2122198795  H 0.9684244707 0.7933280396 -1.4670774062  H -0.9700785413 0.7912018574 -1.4669068765  S 0.0001568099 -0.0785599453 -1.1402225695  Si 0.0003314886 -0.0422403169 1.3297447969 |

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| --- | --- | --- | --- |
| i2: H2SiSH    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: H3SiS    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 |

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| --- | --- | --- | --- | --- |
| 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 | |

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| --- | --- | --- | --- | --- |
| TS: i2 – H2SiS    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 | |
| H2    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+H2)=-133.9  E(DSiS+H2)=-134.8  E(HSiS+HD)=-134.0  E(DSiS+D2)=-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+H2)=-114.5  E(SiSD+H2)=-116.6  E(SiSH+HD)=-114.6  E(SiSD+D2)=-113.1 | H 0.0000000000 1.1799831517 -1.5695610837  S 0.0000000000 -0.1125267945 -1.1904889181  Si 0.0000000000 0.1293766784 0.9214577290 |
| H2SiS    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 |

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| --- | --- | --- | --- |
| 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(H2) cm−3 | 5 × 107 | 106 | 5 × 106 |
| T (K) | 225 | 125 | 200 |
| N(H2) cm−2 | 4.2 × 1023 | 2.1 × 1023 | 1023 |

**Table S3.** D and D2 loss product mass combinations of silicon and sulfur isotopes from the reaction of ground state atomic silicon (Si(3P)) and deuterium sulfide (D2S; X1A1). Isotope abundance given in parenthesis.

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| **Si + D2S** | | D232S (94.93%)  36 | D233S (0.76%)  37 | D234S (4.29%)  38 | D236S (0.02%)  40 |
| D Loss | 28Si (92.23%)  28 | 28Si32SD  62 | 28Si33SD  63 | 28Si34SD  64 | 28Si36SD  66 |
| 29Si (4.68%)  29 | 29Si32SD  63 | 29Si33SD  64 | 29Si34SD  65 | 29Si36SD  67 |
| 30Si (3.09%)  30 | 30Si32SD  64 | 30Si33SD  65 | 30Si34SD  66 | 30Si36SD  68 |
| D2 Loss | 28Si (92.23%)  28 | 28Si32S  60 | 28Si33S  61 | 28Si34S  62 | 28Si36S  64 |
| 29Si (4.68%)  29 | 29Si32S  61 | 29Si33S  62 | 29Si34S  63 | 29Si36S  65 |
| 30Si (3.09%)  30 | 30Si32S  62 | 30Si33S  63 | 30Si34S  64 | 30Si36S  66 |

**Table S4.** H and H2 loss product mass combinations of silicon and sulfur isotopes from the reaction of ground state atomic silicon (Si(3P)) and hydrogen sulfide (H2S; X1A1). Isotope abundance given in parenthesis.

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| **Si + H2S** | | H232S (94.93%)  34 | H233S (0.76%)  35 | H234S (4.29%)  36 | H236S (0.02%)  38 |
| H Loss | 28Si (92.23%)  28 | 28Si32SH  61 | 28Si33SH  62 | 28Si34SH  63 | 28Si36SH  65 |
| 29Si (4.68%)  29 | 29Si32SH  62 | 29Si33SH  63 | 29Si34SH  64 | 29Si36SH  66 |
| 30Si (3.09%)  30 | 30Si32SH  63 | 30Si33SH  64 | 30Si34SH  65 | 30Si36SH  67 |
| H2 Loss | 28Si (92.23%)  28 | 28Si32S  60 | 28Si33S  61 | 28Si34S  62 | 28Si36S  64 |
| 29Si (4.68%)  29 | 29Si32S  61 | 29Si33S  62 | 29Si34S  63 | 29Si36S  65 |
| 30Si (3.09%)  30 | 30Si32S  62 | 30Si33S  63 | 30Si34S  64 | 30Si36S  66 |

**Table S5.** D and D2 loss product mass combinations of silicon and sulfur isotopes from the reaction of the D1-silylidyne radical (SiD; X2Π) and deuterium sulfide (D2S; X1A1). Isotope abundance given in parenthesis.

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| **SiD + D2S** | | D232S (94.93%)  36 | D233S (0.76%)  37 | D234S (4.29%)  38 | D236S (0.02%)  40 |
| D Loss | 28SiD (92.23%)  30 | 28Si32SD2  64 | 28Si33SD2  65 | 28Si34SD2  66 | 28Si36SD2  68 |
| 29SiD (4.68%)  31 | 29Si32SD2  65 | 29Si33SD2  66 | 29Si34SD2  67 | 29Si36SD2  69 |
| 30SiD (3.09%)  32 | 30Si32SD2  66 | 30Si33SD2  67 | 30Si34SD2  68 | 30Si36SD2  70 |
| D2 Loss | 28SiD (92.23%)  30 | 28Si32SD  62 | 28Si33SD  63 | 28Si34SD  64 | 28Si36SD  66 |
| 29SiD (4.68%)  31 | 29Si32SD  63 | 29Si33SD  64 | 29Si34SD  65 | 29Si36SD  67 |
| 30SiD (3.09%)  32 | 30Si32SD  64 | 30Si33SD  65 | 30Si34SD  66 | 30Si36SD  68 |

**Table S6.** H, D, H2, and HD loss product mass combinations of silicon and sulfur isotopes from the reaction of the D1-silylidyne radical (SiD; X2Π) and hydrogen sulfide (H2S; X1A1). Isotope abundance given in parenthesis.

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| **SiD + H2S** | | H232S (94.93%)  34 | H233S (0.76%)  35 | H234S (4.29%)  36 | H236S (0.02%)  38 |
| H Loss | 28SiD (92.23%)  30 | 28Si32SHD  63 | 28Si33SHD  64 | 28Si34SHD  65 | 28Si36SHD  67 |
| 29SiD (4.68%)  31 | 29Si32SHD  64 | 29Si33SHD  65 | 29Si34SHD  66 | 29Si36SHD  68 |
| 30SiD (3.09%)  32 | 30Si32SHD  65 | 30Si33SHD  66 | 30Si34SHD  67 | 30Si36SHD  69 |
| D Loss | 28SiD (92.23%)  30 | 28Si32SH2  62 | 28Si33SH2  63 | 28Si34SH2  64 | 28Si36SH2  66 |
| 29SiD (4.68%)  31 | 29Si32SH2  63 | 29Si33SH2  64 | 29Si34SH2  65 | 29Si36SH2  67 |
| 30SiD (3.09%)  32 | 30Si32SH2  64 | 30Si33SH2  65 | 30Si34SH2  66 | 30Si36SH2  68 |
| H2 Loss | 28SiD (92.23%)  30 | 28Si32SD  62 | 28Si33SD  63 | 28Si34SD  64 | 28Si36SD  66 |
| 29SiD (4.68%)  31 | 29Si32SD  63 | 29Si33SD  64 | 29Si34SD  65 | 29Si36SD  67 |
| 30SiD (3.09%)  32 | 30Si32SD  64 | 30Si33SD  65 | 30Si34SD  66 | 30Si36SD  68 |
| HD Loss | 28SiD (92.23%)  30 | 28Si32SH  61 | 28Si33SH  62 | 28Si34SH  63 | 28Si36SH  65 |
| 29SiD (4.68%)  31 | 29Si32SH  62 | 29Si33SH  63 | 29Si34SH  64 | 29Si36SH  66 |
| 30SiD (3.09%)  32 | 30Si32SH  63 | 30Si33SH  64 | 30Si34SH  65 | 30Si36SH  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) × 10−10 | (5.4−8.8) × 10−10 | (8.8−26.4) × 10−10 |
| Orion Plateau | (0.43−1.29) × 10−9 | (1.29−2.05) × 10−9 | (2.05−6.14) × 10−9 |
| Orion 15.5 km s−1 | (1.76−5.3) × 10−9 | (5.3−8.7) × 10−9 | (8.7−26.1) × 10−9 |

**References**

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