Supporting Information for

**Gas Phase Synthesis of the Elusive Trisilacyclopropyl Radical (Si3H5) via Unimolecular Decomposition of Che­mi­cally Activated Doublet Trisilapropyl Radicals (Si3H7)**

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**Figure S1.** Profile of the potential energy surface for the roaming pathway connecting intermediate **i1** with the **p1** product of the molecular hydrogen loss obtained via intrinsic reaction coordinate (IRC) calculations for the corresponding transition state at the B3LYP/6-311G\*\* level of theory followed by geometry optimization of the final IRC structures. The pathway involves loss of an H atom from the SiH3 group of **i1** accompanied with the three-member closure, ‘roaming’ of the leaving H atom around the cyclic Si3H6 fragment, and H abstraction from one of the SiH2 group by the leaving H atom leading to the formation of **p1** with elimination of H2.

**Table S1**. Optimized Cartesian coordinates (Å), and vibrational frequencies(cm-1) of reactants, H and H2 dissociation products, intermediates, transition states involved in the formation of 2p1 and 2p7 products from silylidyne radical (SiH) + disilane (Si2H6) reaction.

|  |  |  |
| --- | --- | --- |
| Species | Vibrational Frequencies (cm-1) | Cartesian Coordinates (Å)  Atom X Y Z |
| 2p1 | 259.69, 292.71, 355.39,  374.57, 375.72, 419.75  470.29, 514.04, 565.06  606.4, 695.19, 919.47  924.81, 2100.66, 2199.8  2202.95, 2221.71, 2229.17 | Si -0.025694 -0.597056 1.210574  Si -0.025694 1.391515 0.000000  Si -0.025694 -0.597056 -1.210574  H -1.298193 -1.181839 1.699925  H 1.442467 1.724551 0.000000  H 1.116538 -1.062254 -2.035539  H -1.298193 -1.181839 -1.699925  H 1.116538 -1.062254 2.035539 |
| 2p2 | 248.96, 268.98, 366.66  371.51, 437.56, 456.76  518.7, 544.07, 588.5  776.67, 918.59, 933.48  1168.86, 1567.84, 2201.5  2210.57, 2214.78, 2234.86 | Si 0.000000 1.252158 0.000000  Si -1.535243 -0.578857 0.000000  Si 1.238187 -0.686657 0.000000  H 0.197093 2.077856 1.217746  H -0.069383 -1.623449 0.000000  H 1.916990 -1.172640 -1.224641  H 1.916990 -1.172640 1.224641  H 0.197093 2.077856 -1.217746 |
| 2p3 | 91, 91.85, 268.85  360.19, 379.92, 445.08  457.87, 491.15, 538.32  875.62, 935.67, 952.4  955.64, 2174.52, 2185.11  2196.22, 2198.89, 2201.82 | Si 1.740224 -0.382963 0.026108  H 1.475008 -1.722209 -0.568249  Si -1.734674 -0.450559 0.038328  H -1.733226 -1.717483 -0.746630  H -3.142941 -0.159301 0.424116  Si -0.123691 1.116083 -0.053157  H 2.167352 -0.574885 1.438822  H 2.887774 0.218032 -0.705969 |
| 2p4 | 91.85, 92.35, 269.19  360.04, 380.18, 444.85  458.13, 490.99, 538.62  875.82, 935.43, 952.31  955.89, 2171.25, 2182.31  2194.19, 2197.17, 2198.89 | Si 1.734996 -0.450455 0.038269  H 1.733245 -1.717819 -0.746086  H 3.143300 -0.158839 0.423991  Si -1.740348 -0.382974 0.026055  H -1.477575 -1.723139 -0.567400  H -2.166538 -0.573476 1.439345  H -2.887785 0.218930 -0.705650  Si 0.123592 1.115882 -0.053196 |
| 2p5 | 58.55, 118.77, 251.3  345.96, 385.72, 400.95  458.39, 480.74, 604.84  853.67, 930.52, 938.02  971.75, 2124.85, 2149.8  2155.05, 2214.88, 2231.87 | Si -1.042378 -1.022429 0.000000  H -2.278226 -0.171492 0.000000  H -1.125291 -1.850065 1.226233  H -1.125291 -1.850065 -1.226233  Si 0.000000 1.358619 0.000000  H -0.635376 2.006034 1.188037  H -0.635376 2.006034 -1.188037  Si 1.456633 -0.346221 0.000000 |
| 2p6 | 62.15, 84.92, 173.87  347.36, 427.33, 436.41  469.78, 487.57, 603.1  771.99, 876.66, 941.59  942.99, 2028.85, 2165.51  2198.64, 2206.83, 2230.95 | Si -1.973060 -0.302514 0.032065  H -1.863551 -1.761459 -0.210350  H -2.864386 0.295463 -0.997480  H -2.586662 -0.074318 1.366983  Si 2.210769 -0.320415 0.077392  H 1.700567 -1.585811 -0.599029  Si 0.161069 0.692769 -0.093528  H 0.031149 2.148379 0.216868 |
| 2p7 | 106, 193.17, 222.78  272.62, 376.32, 431.61  464.31, 496.1, 513.76  565.47, 728.54, 915.21  936.76, 2190.66, 2193.98  2198.88, 2223.24, 2225.4 | Si 0.021979 -0.366801 1.948842  H -0.949144 -1.483331 2.070243  H 0.022509 0.469977 3.175696  Si 0.021979 -0.366801 -1.948842  H -0.949144 -1.483331 -2.070243  H 0.022509 0.469977 -3.175696  Si 0.021979 0.741208 0.000000  H 0.930170 1.920239 0.000000 |
| 2p8 | 31.68, 72.08, 315.75  368.17, 394.8, 441.04  460.77, 644.03, 656.29  876.04, 932.32, 946.74  954.12, 2160.1, 2166.65  2204.67, 2216.43, 2217.66 | Si 0.196098 0.937883 0.000000  Si 2.000317 -0.605007 0.000000  Si -1.743970 -0.435621 0.000000  H 0.089655 1.817025 -1.201657  H -1.775932 -1.305129 -1.204185  H -1.775932 -1.305129 1.204185  H -2.962085 0.415234 0.000000  H 0.089655 1.817025 1.201657 |
| 2p9 | 73.64, 107.53, 267.65  363.88, 463.9, 475.69  497.07, 619.95, 725.25  856.94, 885.23, 943.82  945.94, 1635.27, 2139.34  2200.35, 2211.38, 2228.15 | Si 1.953618 -0.299254 0.002790  H 1.841835 -1.776080 0.081369  H 2.668224 0.065452 -1.248846  H 2.745853 0.196799 1.158066  Si -0.206063 0.667047 -0.070669  Si -2.190641 -0.423937 -0.030924  H -0.966014 0.155781 1.257113  H -0.086691 2.144063 0.135548 |
| 2p10 | 67.34, 102.63, 211.93  233.19, 360.51, 461.06  473.08, 486.28, 619.31  724.9, 880.41, 942.02  943.53, 2023.63, 2150.52  2199.9, 2208.09, 2226.28 | Si -1.987631 -0.291995 0.000045  H -1.890812 -1.745637 -0.281873  H -2.841064 0.344636 -1.037446  H -2.642036 -0.097000 1.321141  Si 2.144492 -0.485900 0.026643  H 2.935249 0.787495 -0.249112  Si 0.157435 0.676736 -0.031525  H 0.038524 2.126726 0.315003 |
| 2p11 | 68.71, 95.72, 318.7  363.84, 434.91, 481.52  529.38, 605.51, 694.41  872.86, 941.53, 947.64  1032.03, 1477.04, 2062.14  2196.23, 2207.68, 2211.77 | Si -1.892541 -0.535883 -0.066492  H -3.071068 0.332766 0.318793  Si -0.183893 0.932436 -0.050045  H -0.931278 0.085052 1.211824  Si 1.862905 -0.309919 0.007131  H 2.720887 0.187316 1.114936  H 1.699424 -1.778978 0.158680  H 2.571436 -0.039031 -1.272546 |
| 2p12 | 87, 115.16, 264.34  333.04, 397.04, 417.85  472.61, 540.12, 622.87  718.3, 860.68, 934.93  943, 2070.17, 2087.29  2152.35, 2214.44, 2234.38 | Si 1.464217 -0.232550 -0.011107  H 1.396205 -1.715596 -0.188101  H 2.206689 -0.004467 1.252549  H 2.220219 0.291323 -1.173204  Si -1.211484 -0.913080 -0.127689  H -1.019130 -1.518227 1.246007  Si -0.562177 1.225791 0.145803  H -0.471760 1.824714 -1.235354 |
| 2p13 | 212.78, 281.09, 298.51  370.95, 433.66, 451.05  514.11, 577.72, 643.33  655.67, 735.71, 941.47  1146.88, 1581.79, 2011.41  2142.37, 2217.97, 2239.63 | Si -1.229824 -0.817186 0.118152  Si 1.500374 -0.484512 -0.12022  Si -0.203395 1.247779 -0.024278  H 0.165733 -1.617442 0.191667  H 1.51973 -0.303267 1.394774  H -0.626258 2.008313 -1.225382  H -0.33624 2.077679 1.194149  H -1.663138 -1.410409 -1.186365 |
| 2p14 | 211, 280.75, 297.65  370.37, 433.2, 451.19  513.8, 576.59, 642.66  656.05, 735.78, 941.62  1143.32, 1580.44, 2017.5  2142.46, 2213.82, 2236.69 | Si -0.203425 1.247850 -0.024198  Si 1.500179 -0.484597 -0.120349  Si -1.229785 -0.817229 0.118091  H -0.625855 2.007700 -1.225916  H 1.521172 -0.302604 1.394549  H 0.165322 -1.617325 0.194737  H -1.661990 -1.410612 -1.186826  H -0.336222 2.078500 1.193844 |
| 2p15 | 246.29, 272.21, 319.07  358.04, 376.86, 417.86  494.98, 544.97, 616.36  644.68, 729.36, 942.9  1067.69, 1577.67, 2036.56  2111.18, 2202.02, 2225.81 | Si 0.481893 1.364131 -0.074835  Si 1.021679 -0.983384 -0.113923  Si -1.313618 -0.165027 0.037432  H 0.886605 1.260106 1.386026  H 1.137243 -1.728318 1.185387  H -0.446124 -1.627725 -0.454133  H -2.099260 -0.667126 1.193400  H -2.137811 -0.257006 -1.192109 |
| 2p16 | 249.13, 272.67, 352.37  370.58, 403.37, 442.53  511.37, 536.08, 626.25  674.67, 873.94, 925.58  1248.19, 1452.02, 2002.47  2152.42, 2215.8, 2237.93 | Si 0.101084 1.311957 -0.116969  Si 1.440663 -0.692583 -0.067628  Si -1.330106 -0.486172 0.010878  H -0.043968 2.221471 1.058397  H 1.246216 -0.659498 1.447408  H -0.098787 -1.545223 -0.156169  H -1.981211 -0.938195 1.262321  H -2.085229 -0.943377 -1.179895 |
| 2p17 | 85.26, 146.31, 332.57  363.61, 415.29, 483.55  497.31, 604.43, 668.87  877.45, 934.29, 951.79  979.13, 1490.91, 2054.48  2175.65, 2190.02, 2199.61 | Si 0.000000 0.000000 0.000000  Si 0.000000 0.000000 2.421319  Si 2.277871 0.000000 2.369901  H 1.270312 -0.222357 -0.740190  H 1.194761 -1.272122 2.419664  H 3.102687 -0.422643 1.176688  H -0.978063 -1.019420 -0.476044  H -0.525351 1.341438 -0.379442 |
| 2p18 | 66.21, 102.74, 252.9  330.71, 425.71, 467.43  504.61, 566, 816.64  863.63, 936.22, 941.94  955.17, 1494.9, 1977.17  2196.88, 2214.25, 2216.28 | Si -2.198278 -0.298282 -0.009290  H -1.351928 -1.520672 -0.382268  Si -0.161671 0.762330 -0.055745  H -0.946511 0.000494 1.194979  Si 1.996014 -0.258374 0.005682  H 2.704982 0.115449 1.256498  H 1.917695 -1.739575 -0.088671  H 2.770853 0.264874 -1.149592 |
| 2p19 | 94.74, 177.19, 280.16  334.91, 382.17, 392.94  424.78, 536.21, 610.42  623.11, 848.36, 929.71  943.43, 1971.69, 2072.83  2163.1, 2203.27, 2241.8 | Si 1.461718 0.007768 0.001381  Si -0.853439 -1.187462 -0.065569  Si -0.890885 1.093464 -0.126025  H 2.040932 -0.153746 -1.351273  H -1.049785 -0.916243 1.431704  H -0.940214 1.971668 1.100005  H 1.910170 1.323315 0.548100  H 1.995387 -1.017773 0.934452 |
| 2p20 | 109.9, 138.09, 247.63  358.87, 443.67, 459.08  479.98, 590.75, 620.02  775.1, 816.86, 918.85  1023.09, 1531.19, 2028.22  2176.81, 2183.64, 2209.78 | Si 2.155216 -0.301347 -0.038996  H 0.955368 0.129138 1.211073  Si 0.077422 0.649416 -0.077035  H -0.022532 2.105209 0.229162  H 1.461244 -1.657426 -0.072393  Si -2.036571 -0.296513 0.087915  H -3.053358 0.442498 -0.711774  H -2.085663 -1.741199 -0.262446 |
| 1p1 | 216.13, 216.13, 349.68  365.71, 365.71, 416.86  494.81, 600.34, 600.34  634.36, 634.36, 663.16  897.27, 898.19, 898.19  2204.85, 2204.85, 2206.38  2228.62, 2228.62, 2239.27 | Si 0.000000 1.355038 0.000000  Si -1.173497 -0.677519 0.000000  Si 1.173497 -0.677519 0.000000  H 0.000000 2.178912 1.232224  H -1.886993 -1.089456 -1.232224  H 1.886993 -1.089456 -1.232224  H 1.886993 -1.089456 1.232224  H 0.000000 2.178912 -1.232224  H -1.886993 -1.089456 1.232224 |
| 1p2 | 92.06, 99.37, 175.43  350.05, 405.34, 434.8  515.92, 538.29, 554.48  589.32, 729.38, 886.48  929.9, 937.76, 954.52  2203.45,2210.86, 2212.31  2225.59, 2227.11, 2253.26 | Si -1.946173 -0.314135 0.026235  H -1.736049 -1.752299 -0.271925  H -2.881949 0.256146 -0.976541  H -2.566880 -0.174570 1.368490  Si 1.948491 -0.377269 0.058815  H 3.286251 0.256942 0.055085  H 1.985231 -1.791406 -0.375268  Si 0.121513 0.764943 -0.096569  H 0.179766 2.175645 0.361425 |
| 1p3 | 250.98, 290.06, 362  366.35, 420.99, 454.12  521.25, 538.23, 594.81  685.73, 696.78, 886.31  917.81, 934.7, 1250.23  1498.36, 2028.02, 2217.45  2222.78, 2235.44, 2249.66 | Si 0.123064 -1.270875 -0.002509  Si 1.418692 0.747344 0.094724  Si -1.331002 0.514773 -0.001954  H -0.001261 -2.123117 1.203166  H 1.226202 0.867855 -1.412103  H -0.132837 1.586803 0.225858  H -1.982499 0.992990 -1.240988  H -2.112197 0.871699 1.205333  H 0.052033 -2.07363 -1.244935 |
| 1p4 | 254.76, 302.39, 340.96  358.38, 405.66, 418.5  419.65, 628.57, 668.96  712.68, 713.84, 897.85  938.32, 944.05, 1328.88  1427.02, 2008.64, 2196.28  2199.89, 2216.15, 2221.78 | Si -1.249090 -0.555310 -0.001199  Si -0.001353 1.461691 -0.103249  Si 1.250014 -0.553522 -0.001209  H -1.824296 -1.203070 -1.208426  H -0.001257 1.389693 1.422321  H 1.827452 -1.199520 -1.208289  H 1.913942 -1.108661 1.205194  H 0.001917 -1.705438 0.063634  H -1.911742 -1.113025 1.204764 |
| 1p5 | 102.67, 140.75, 315.14  374.17, 435.13, 466.91  477.34, 525.89, 569.09  738.81, 880.15, 938.63  942.77, 955.19, 982.03  1615.67, 2175.08, 2182.52  2188.63, 2193.87, 2205.61 | Si 1.701849 -0.392475 -0.002357  H 2.349726 -0.286030 1.335944  H 2.718094 0.008866 -1.013677  H 1.377930 -1.826989 -0.238885  Si -1.641930 -0.491291 0.066233  H -3.093162 -0.198101 -0.076721  H -0.992313 0.186788 -1.256628  H -1.451806 -1.962368 -0.063375  Si -0.124809 1.175041 0.029934 |
| 1p6 | 96.43, 98.57, 139.97  293.18, 321.06, 409.65  416.74, 486.85, 559.88  848.06, 879.09, 914.09  923.02, 956.96, 959.05  2152.13, 2152.69, 2186.11  2189.26, 2198.49, 2201.01 | Si 0.000000 1.728389 -0.439204  H 0.634092 1.427541 -1.752157  H 0.547610 3.020218 0.054227  H -1.464963 1.921541 -0.673549  Si 0.000000 -1.728389 -0.439204  H 1.464963 -1.921541 -0.673549  H -0.547610 -3.020218 0.054227  H -0.634092 -1.427541 -1.752157  Si 0.000000 0.000000 1.217191 |
| 1p7 | 55.65, 69.83, 159.75  364.21, 375.36, 404.16  442.52, 464.06, 634.72  651.53, 741.68, 878.03  935.63, 948.07, 954.84  2030.85, 2168.52, 2184.73  2201.12, 2211.23, 2217.76 | Si -0.131167 0.935342 0.017748  H -1.826508 -0.880275 1.367657  H -0.022412 1.857064 -1.148092  H -0.052773 1.761553 1.256942  Si 1.801716 -0.440917 -0.012341  H 3.026650 0.393221 -0.122049  H 1.881841 -1.247727 1.232006  H 1.768422 -1.373019 -1.169773  Si -2.011636 -0.530912 -0.106599 |
| 1p8 | 77.39, 115.28, 226.06  358.12, 458.76, 481.44  501.27, 593.36, 623.79  769.18, 806.51, 880.78  941.03, 946.16, 975.52  1602.6, 2030.96, 2174.21  2202.07, 2212.47, 2230.94 | Si 2.208124 -0.316487 -0.025237  Si 0.154321 0.658826 -0.078371  Si -2.011295 -0.284200 0.005803  H 0.964195 0.161129 1.236592  H 0.070760 2.127798 0.170442  H -2.752493 0.152841 -1.206372  H -1.912352 -1.763664 0.007423  H -2.765309 0.163320 1.205195  H 1.479102 -1.655384 -0.044013 |
| 1p9 | 89.56, 111.09,247.4  367.2,457.01,480.76  494.53,574.56,634.87  740.58,831.8, 864.42  911.77, 944.71, 948.27  1603.03, 2032.29, 2161.73  2203.65, 2212.86, 2224.87 | Si 0.152924 0.691662 0.081868  Si 2.090308 -0.507219 0.037015  Si -1.986971 -0.296293 -0.008625  H 2.812266 0.822044 -0.150825  H -2.728257 0.081757 1.222938  H 0.045415 2.163403 -0.144834  H 0.906683 0.108300 -1.230307  H -1.854593 -1.773565 -0.055889  H -2.769173 0.163943 -1.184699 |
| 1p10 | 83.85, 105.48, 321.71  344.87, 366.89, 396.43  523.03, 563.91, 773.03  813.98, 879.6, 943.07  946, 1275.46, 1389.23  1389.89, 1618.81, 2046.21  2179.39, 2192.08, 2193.56 | Si -1.776881 -0.465102 0.000000  H -2.629348 -0.228150 1.198864  H -1.368148 -1.896902 0.000000  H -2.629348 -0.228150 -1.198864  Si 1.916027 -0.616580 0.000000  H 0.905976 0.217611 1.033707  H 0.905976 0.217611 -1.033707  H 2.866845 0.570448 0.000000  Si 0.000000 1.177934 0.000000 |
| 1p11 | 70.28, 114.79, 328.89  363.11, 392.92, 438.95  487.04, 538.66, 752.76  809.94, 874.98, 935.1  955.5, 1269.89, 1328.2  1345.77, 1620.77, 2044.82  2181.97, 2192.8, 2201.78 | Si 1.747649 -0.457643 0.000000  H 1.676737 -1.323087 1.208060  H 3.084166 0.202280 0.000000  H 1.676737 -1.323087 -1.208060  Si -1.987620 -0.519433 0.000000  H -1.020791 0.376247 -1.030414  H -1.020791 0.376247 1.030414  H -1.036465 -1.704914 0.000000  Si 0.000000 1.219671 0.000000 |
| 1p12 | 210.55, 255.4, 293.15  323.39, 332.85, 342.71  447.92, 612.87, 621.59  686.56, 858.6, 876.12  921.44, 923.46, 1369.39  1415.18, 2077.46, 2096.17  2135.87, 2140.07, 2256.12 | Si -1.368186 0.005812 -0.000507  Si 0.757275 1.333541 -0.095579  Si 0.745638 -1.339864 -0.095541  H -2.055666 0.007543 -1.308060  H 1.044837 1.345229 1.388600  H 1.691098 -0.007230 -0.398018  H 1.034116 -1.353844 1.388492  H -1.804548 -1.177965 0.806444  H -1.796010 1.193417 0.805314 |
| 1p13 | 221.21, 236.02, 306.41  394.42, 400.52, 440.28  579.96, 617.88, 650.48  688.25, 879.85, 899.29  954.23, 1120.73, 1275.71  1310.17, 1526.17, 2055.92  2108.32, 2200.04, 2220.94 | Si 1.173777 -1.098112 -0.083048  Si -1.726567 -0.282228 -0.069938  Si 0.590813 1.193245 0.007423  H 0.982181 -1.226226 1.416361  H -1.476497 -0.103459 1.407064  H -1.023009 1.173317 -0.421805  H 0.559401 2.030449 1.231868  H 0.892126 2.073482 -1.152483  H -0.466513 -1.328239 -0.443127 |
| 1p14 | 156.2, 250.39, 306.62  344.21, 354.88, 394.16  440.08, 474.25, 504.64  587.08, 614.74, 653.27  735.4, 899.65, 910.74  1374.66, 2206.64, 2208.45  2229.48, 2237.09, 3024.94 | Si -1.480230 0.187859 -0.198939  Si 0.507390 -1.230730 0.012604  Si 0.853444 1.025141 -0.020495  H -1.514622 0.055322 1.571673  H 0.802480 -1.945755 -1.251215  H 1.284021 1.692206 -1.270946  H 1.312769 1.757019 1.184051  H -1.041691 0.727889 1.449501  H 0.828598 -2.038448 1.212562 |
| 1p15 | 155.85, 249.85, 306.52  343.69, 354.51, 394.02  439.95, 473.96, 504.35  586.64, 614.26, 652.94  733.13, 899.64, 910.61  1371.15, 2206.65, 2208.45  2229.5, 2237.12, 3032.62 | Si 1.480381 0.186625 -0.199202  Si -0.852468 1.025943 -0.020481  Si -0.508590 -1.230215 0.012637  H 1.513624 0.053027 1.572867  H -1.284095 1.692944 -1.270582  H -0.803659 -1.944756 -1.251480  H -0.829785 -2.038655 1.212101  H 1.043691 0.727007 1.450901  H -1.3103 1.757486 1.184826 |
| 1p16 | 75.6, 114.05, 136.8  182.27, 363.34, 405.34  503.48, 520.84, 534.08  581.47, 614.99, 744.73  885.34, 939.08, 949.53  1189.87, 2174.24, 2197.52  2205.86, 2211.79, 3301.75 | Si -0.160817 0.693247 -0.008599  H -1.196460 -1.766523 -0.380921  H -0.096209 2.182778 0.051620  H -1.069064 -1.677314 0.413857  Si 1.983146 -0.257715 0.000622  H 2.740483 0.120804 1.222379  H 1.844812 -1.736843 -0.035512  H 2.769690 0.176866 -1.183437  Si -2.178990 -0.242658 0.001692 |
| 1p17 | 83.13, 94.11, 148.31  327.18, 366.86, 401.05  438.59, 487.61, 523.36  535.1, 596.77, 718.66  885.46, 939.92, 948.96  1163.19, 2173.59, 2199.61  2206.2, 2214.29, 3373.08 | Si -1.996771 -0.256348 0.016590  H -1.884319 -1.735272 -0.068276  H -2.817547 0.223857 -1.126063  H -2.707996 0.095187 1.273650  Si 1.967434 -0.614874 -0.003130  H 2.574617 1.086191 0.518882  H 2.946393 0.965038 -0.184837  Si 0.154447 0.671617 -0.046052  H 0.137316 2.159466 0.042945 |
| 1p18 | 35.81, 169.06, 245.88  263.04, 380.66, 462.17  633.13, 702.42, 729.02  749.83, 771.56, 876.72  1021.92, 1038.61, 1098.44  1526.49, 1692.13, 1714.71  2065.78, 2071.33, 2087.09 | Si 0.035680 -0.861689 1.544689  Si 0.035680 -0.861689 -1.544689  Si 0.035680 1.770461 0.000000  H -1.435629 -1.131856 1.299620  H -1.435629 -1.131856 -1.299620  H -0.324359 0.747367 -1.215770  H -0.324359 0.747367 1.215770  H 1.492354 1.352729 0.000000  H 0.529081 -1.242911 0.000000 |
| 1p19 | 225.26, 225.26, 248.36  366.35, 366.35, 535.23  589.15, 643.87, 643.87  786.04, 786.04, 957.31  1058.52, 1058.52, 1112.7  1507.22, 1507.22, 1580.12  2104.94, 2104.94, 2127.7 | Si 0.000000 1.780833 -0.069029  Si 1.542247 -0.890417 -0.069029  Si -1.542247 -0.890417 -0.069029  H 0.000000 1.518170 1.415924  H 1.314774 -0.759085 1.415924  H 0.000000 -1.393586 -0.449513  H -1.206881 0.696793 -0.449513  H -1.314774 -0.759085 1.415924  H 1.206881 0.696793 -0.449513 |
| 1p20 | 16.33, 23.85, 28.54  132.56, 380.28, 380.31  417.99, 630.13, 630.3  839.41, 917.1, 927.18  927.3, 951.33, 951.34  2198.99, 2204.42, 2204.51  2212.55, 2212.58, 2213.47 | Si 0.000000 0.000000 -2.856079  H 1.390230 0.000837 -3.383628  H -0.695840 1.203556 -3.383628  H -0.694390 -1.204394 -3.383628  Si 0.000000 0.000000 -0.498319  H -1.396768 0.000812 0.003902  H 0.697681 -1.210043 0.003902  H 0.699087 1.209231 0.003902  Si 0.000000 0.000000 4.078625 |
| SiH | 2008.4928 | Si 0.000000 0.000000 -0.051479  H 0.000000 0.000000 1.481479 |
| Si2H6 | 132.01, 373.05, 374.22  422.63, 630.15, 630.82  850.22, 923.26, 942.16  942.21, 956.09, 956.25,  2201.75, 2210.01, 2211.68,  2211.92, 2221.40, 2221.70 | Si -1.176702 0.000453 0.000000  Si 1.176702 -0.000453 0.000000  H -1.696138 -1.391640 0.000000  H -1.695366 0.696891 1.205744  H -1.695366 0.696891 -1.205744  H 1.696138 1.391640 0.000000  H 1.695366 -0.696891 -1.205744  H 1.695366 -0.696891 1.205744 |
| i0 | 82.53, 109.09, 130.43,  181.58, 275.90, 392.96  400.99, 497.56, 585.53  698.11, 739.05, 865.49  897.92, 925.02, 938.45  942.43, 1135.84, 1514.19  2014.79, 2167.86, 2199.63  2218.31, 2230.26, 2243.54 | Si -1.306892 -0.395740 0.126396  Si 1.050076 -0.235962 0.187569  H -1.722183 -1.693885 -0.479891  H -1.854509 0.713464 -0.688190  H -1.827418 -0.320142 1.511308  H 1.639750 -0.498390 -1.151177  H 1.620638 -1.198209 1.163250  H 2.058173 1.039690 0.569264  Si 1.002021 2.196621 1.121215  H 0.735481 2.502559 -0.352001 |
| i1 | 97.88, 103.77, 114.95  315.46, 376.57, 429.69  443.58, 453.55, 553.42  593.43, 715.08, 724.14  880.70, 921.33, 928.74  948.20, 949.98, 2175.96  2186.85, 2194.87, 2198.95  2205.34, 2212.67, 2219.31 | Si -0.693572 -0.301432 -0.203317  Si 1.088641 -1.818106 -0.144565  Si -0.066986 1.892695 0.408684  H -1.755743 -0.783783 0.720341  H -1.255231 -0.284788 -1.581097  H 1.675033 -1.997354 1.212513  H 2.179190 -1.494731 -1.105699  H -1.232058 2.815268 0.355353  H 0.478602 1.895561 1.790058  H 0.980232 2.395705 -0.516617 |
| i2 | 68.53, 75.66, 95.65  309.28, 366.07, 439.22  464.45, 485.50, 546.09,  577.21, 723.12, 872.36  902.02, 939.88, 944.54  946.43, 947.87, 2169.81  2186.89, 2190.75, 2209.64  2211.65, 2218.38, 2220.99 | Si -1.930348 -0.733499 0.087746  Si 0.410473 -0.713090 0.195186  Si 1.516659 1.347498 0.047764  H -2.438389 -2.079094 0.458119  H -2.468687 0.264827 1.046123  H -2.439664 -0.401298 -1.270851  H 1.027506 -1.751945 -0.678614  H 2.950110 1.174018 0.395659  H 1.436815 1.938936 -1.315824  H 0.900251 2.298723 1.007017 |
| i3 | 91.01, 97.60, 138.76  286.94, 340.45, 355.10  431.93, 446.74, 502.68  566.77, 573.61, 669.40  702.08, 753.91, 820.42  918.28, 928.22, 1292.70  2077.33, 2151.85, 2172.88  2177.46, 2189.52, 3379.99 | Si -0.689999 -0.326598 -0.381787  Si 1.033859 -1.745153 0.308208  H -1.974916 -0.809093 0.195916  H -0.817174 -0.407041 -1.865640  H 1.181213 -1.733845 1.795253  H 2.351681 -1.360839 -0.276458  Si -0.455198 2.042717 0.014911  H 0.988864 2.135217 -0.430236  H 0.066069 1.959968 1.723214  H 0.501292 1.331500 1.466902 |
| ts: i0→i1 | 830.11i, 92.44, 99.40 143.96, 287.05, 363.29  388.40, 423.87, 470.95  504.06, 641.56, 661.28  851.84, 887.10, 930.09  948.08, 950.35, 1977.05  2056.99, 2152.09, 2172.49  2200.01, 2211.92, 2216.75 | Si -2.207327 -0.435967 0.000000  H -1.353517 -0.779079 -1.206977  Si -0.036895 0.864434 0.000006  H -0.060062 1.742359 -1.206519  H -0.060044 1.742349 1.206538  H -1.353504 -0.779200 1.206930  Si 1.938480 -0.415736 -0.000002  H 3.141016 0.458434 -0.000269  H 1.983374 -1.281366 1.206381  H 1.983121 -1.281742 -1.206127 |
| ts: i0→i0’  (inflection point) | 298.28i, 83.31, 110.01  226.06, 265.43, 319.99  400.79, 421.37, 509.67  604.97, 671.49, 719.61  884.27, 945.03, 945.13  952.42, 968.22, 1892.31  1895.85, 2154.27, 2169.27  2203.28, 2216.50, 2221.55 | Si -2.220291 -0.472481 0.000148  H -1.105339 -0.475607 -1.087428  Si -0.049983 0.857363 -0.000005  H -0.069062 1.746922 -1.196884  H -0.068732 1.747271 1.196612  H -1.105040 -0.474833 1.087535  Si 1.931628 -0.418665 -0.000104  H 3.108556 0.489196 -0.000232  H 1.990416 -1.279935 1.207935  H 1.990231 -1.280043 -1.208073 |
| ts: i1→i2 | 1284.01i, 65.06, 99.04  137.36, 311.28, 354.69  419.07, 466.55, 504.54  532.96, 560.51, 727.68  877.28, 897.32, 938.89  943.83, 976.38, 1469.70  2146.19, 2185.47, 2212.67  2216.50, 2226.90, 2250.07 | Si -2.084575 -0.322752 0.038667  Si -0.062811 0.660830 -0.044432  Si 2.088388 -0.298889 0.040726  H -1.350149 0.697557 -1.190492  H -2.144135 -1.598141 -0.706174  H -3.181354 -0.175364 1.037435  H -0.180352 2.058805 0.437565  H 3.073574 0.611411 -0.596151  H 2.522158 -0.578438 1.437055  H 2.050084 -1.579105 -0.707739 |
| ts: i1→2p1 | 291.70i, 91.39, 96.77  233.03, 238.52, 361.05  365.10, 367.99, 427.97  493.54, 600.23, 604.24  633.13, 646.73, 666.26  893.84, 897.47, 898.41  1929.61, 2205.20, 2206.12,  2212.34, 2229.11, 2236.80 | Si 0.745622 -1.174543 0.067301  Si 0.745622 1.174543 0.067301  Si -1.259441 0.000000 -0.255001  H 0.960166 -1.873157 1.356823  H 1.344238 -1.901336 -1.077485  H 0.960166 1.873157 1.356823  H 1.344238 1.901336 -1.077485  H -1.871258 0.000000 -1.606118  H -2.295515 0.000000 0.835733  H -3.582746 0.000000 1.903952 |
| ts: i1→i3 | 1094.54i, 90.86, 105.21  138.08, 313.77, 364.72  372.84, 440.74, 457.38  543.43, 601.45, 716.41,  752.29, 801.08, 919.00  928.51, 991.47, 1682.30  2027.95, 2167.11, 2170.98  2188.70, 2191.53, 2202.82 | Si -0.689911 -0.326643 -0.381831  Si 1.033876 -1.745233 0.308249  H -1.974859 -0.808697 0.196177  H -0.817409 -0.407292 -1.865639  H 1.181416 -1.733394 1.795273  H 2.351629 -1.361158 -0.276725  Si -0.454929 2.042700 0.014726  H 0.989295 2.135269 -0.429859  H 0.065682 1.959918 1.723072  H 0.500903 1.331363 1.466841 |
| ts: i2→2p7 | 444.28i, 59.51, 89.69  134.02, 166.12, 220.24  354.07, 407.28, 449.49  512.15, 540.94, 567.08  593.29, 722.32, 889.95  930.74, 936.88, 945.72  1724.76, 2200.72, 2210.04  2211.37, 2226.90, 2254.15 | Si 1.956908 0.403342 -0.066127  Si 0.192121 -0.830168 0.120990  Si -1.918835 0.149574 -0.069005  H 3.324860 -0.161890 -0.032871  H -1.735875 3.113021 0.383765  H 1.917283 1.828230 0.3300297  H 0.321852 -2.245284 -0.309186  H -2.847042 -0.388178 0.959034  H -2.529493 -0.063416 -1.406800  H -1.764521 1.647470 0.165367 |
| ts: i3→2p1 | 213.57i, 60.70, 113.80  163.91, 228.88, 236.26  333.24, 367.99, 395.56  423.26, 463.01, 482.81  531.95, 628.73, 649.58  732.12, 926.89, 929.54  2046.42, 2156.85, 2173.13  2181.24, 2198.30, 4257.78 | Si -0.992152 -0.579408 -0.522646  Si 0.724849 -1.806901 0.475994  Si -0.915242 1.667203 0.323442  H -2.286104 -1.249560 -0.222681  H -0.791521 -0.590928 -1.999346  H 0.562899 -1.910547 1.956067  H 2.073873 -1.224225 0.215929  H 0.366741 1.970434 -0.439051  H 0.507737 1.529856 2.281187  H 1.082607 1.192549 1.933750 |