Directed Gas Phase Formation of the Elusive Silylgermylidyne Radical (H_3SiGe, X^2A'')

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Supplementary Information - Results

It should be noted that according to the isotopes of silicon and germanium (Table S2), the laboratory data can also be fit with reactions of ^{28}SiH plus $^{73}GeH_4$, ^{28}SiH plus $^{72}GeH_4$, and ^{29}SiH plus $^{70}GeH_4$ leading to $^{73}Ge^{28}SiH_3$ plus molecular hydrogen, $^{72}Ge^{28}SiH_3$ plus molecular hydrogen, and $^{70}Ge^{29}SiH_3$ plus molecular hydrogen. These fits are shown in Figures S2 and S3 for completeness. With the exception of the center-of-mass angular distribution of the ^{29}SiH plus $^{70}GeH_4$ system, the CM functions are essentially identical to those obtained for the ^{28}SiH plus $^{74}GeH_4$ system which accounts for the dominating naturally occurring isotopes of silicon and germanium.

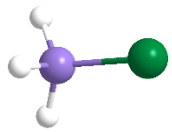
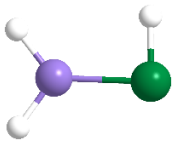
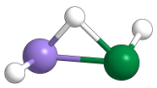
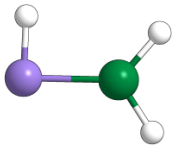
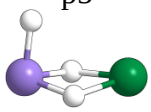
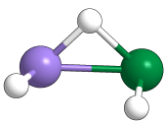
Table S1. Peak Velocity (v_p) and Speed Ratios (S) of the Silylidyne (SiH) and Germane (GeH_4) Beams along with the Corresponding Collision Energy (E_C) and Center-of-Mass Angle Θ_{CM}.

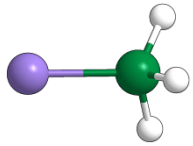
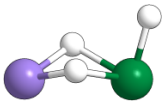
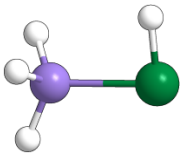
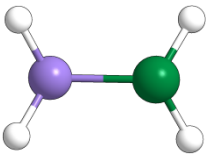
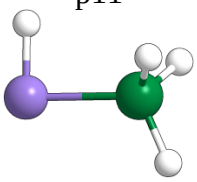
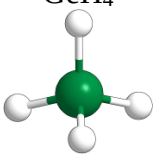
beam	v_p (m s^{-1})	S	E_c (kJ mol^{-1})	Θ_{CM} (deg)
SiH	1744 ± 11	16.7 ± 1.8		
GeH_4	529 ± 5	9.0 ± 0.7	35.0 ± 0.4	39.2 ± 0.2

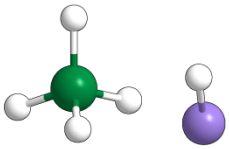
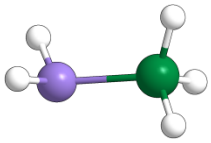
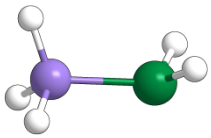
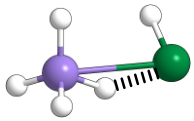
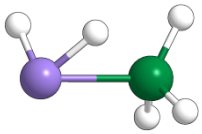
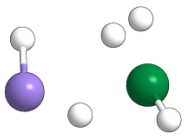
Table S2. H and H_2 dissociation products from silylidyne radical (SiH) + germane (GeH_4) reaction with isotopes of germanium and silicon.

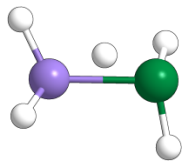
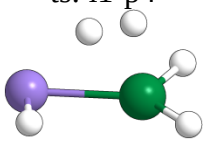
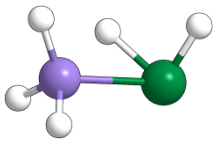
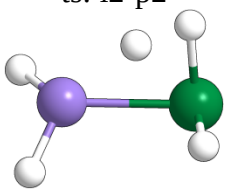
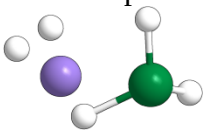
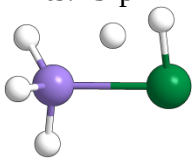
		$^{70}GeH_4$ (20.52%)	$^{72}GeH_4$ (27.45%)	$^{73}GeH_4$ (7.76%)	$^{74}GeH_4$ (36.7%)	$^{76}GeH_4$ (7.75%)
H loss	^{28}SiH (92.2%)	$^{28}Si^{70}GeH_4$ 102	$^{28}Si^{72}GeH_4$ 104	$^{28}Si^{73}GeH_4$ 105	$^{28}Si^{74}GeH_4$ 106	$^{28}Si^{76}GeH_4$ 108
	^{29}SiH (4.7%)	$^{29}Si^{70}GeH_4$ 103	$^{29}Si^{72}GeH_4$ 105	$^{29}Si^{73}GeH_4$ 106	$^{29}Si^{74}GeH_4$ 107	$^{29}Si^{76}GeH_4$ 109
	^{30}SiH (3.1%)	$^{30}Si^{70}GeH_4$ 104	$^{30}Si^{72}GeH_4$ 106	$^{30}Si^{73}GeH_4$ 107	$^{30}Si^{74}GeH_4$ 108	$^{30}Si^{76}GeH_4$ 110
H_2 loss	^{28}SiH (92.2%)	$^{28}Si^{70}GeH_3$ 101	$^{28}Si^{72}GeH_3$ 103	$^{28}Si^{73}GeH_3$ 104	$^{28}Si^{74}GeH_3$ 105	$^{28}Si^{76}GeH_3$ 107
	^{29}SiH (4.7%)	$^{29}Si^{70}GeH_3$ 102	$^{29}Si^{72}GeH_3$ 104	$^{29}Si^{73}GeH_3$ 105	$^{29}Si^{74}GeH_3$ 106	$^{29}Si^{76}GeH_3$ 108
	^{30}SiH (3.1%)	$^{30}Si^{70}GeH_3$ 103	$^{30}Si^{72}GeH_3$ 105	$^{30}Si^{73}GeH_3$ 106	$^{30}Si^{74}GeH_3$ 107	$^{30}Si^{76}GeH_3$ 109

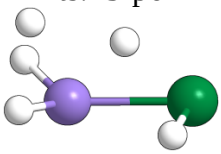
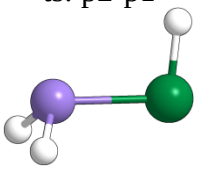
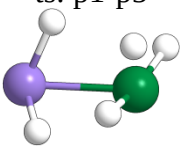
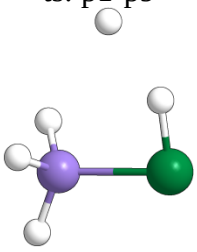
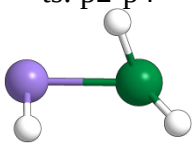
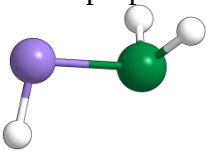
Table S3. Optimized Cartesian coordinates (Å), and vibrational frequencies(cm^{-1}) of reactants, H and H_2 dissociation products, intermediates, transition states from silylidyne radical (SiH) + germane (GeH_4) reaction.

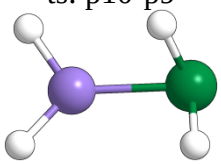
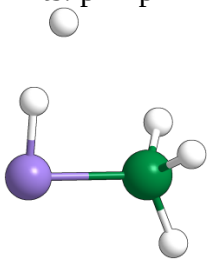
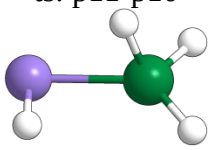
Species	Vibrational Frequencies (cm^{-1})	Cartesian Coordinates (Å)			
		Atom	X	Y	Z
p1 	275.77, 356.71, 376.69 873.58, 928.03, 964.71 2182.03, 2215.21, 2219.01	Ge Si H H H	-0.883917 1.569751 2.202675 2.202667 1.903503	0.000000 0.000000 1.199640 -1.199706 0.000072	-0.003735 -0.007234 -0.613371 -0.613250 1.447423
p2 	229.17, 358.79, 376.12 392.70, 661.71, 974.82 1945.71, 2207.50, 2230.78	Ge Si H H H	0.807081 -1.551397 0.764983 -2.392422 -2.479584	-0.046575 0.000963 1.538757 -1.223837 1.161996	0.000003 -0.000149 0.000483 0.001046 0.000467
p3 	317.30, 363.63, 617.66 652.58, 700.89, 984.56 1512.90, 1991.99, 2118.80	H Si Ge H H	-0.575022 -1.577961 0.738761 -2.085856 1.111988	0.172811 0.119898 -0.063911 -1.264444 1.458206	1.249557 -0.069943 -0.019293 0.236541 0.110481
p4 	164.74, 363.36, 372.30 376.83, 706.43, 900.00 2055.35, 2117.44, 2143.75	Ge Si H H H	0.680536 -1.663519 1.614265 1.586156 -1.688322	0.000790 -0.101911 1.224456 -1.242449 1.419463	0.000018 -0.000028 -0.000351 -0.000053 0.000228
p5 	243.54, 350.07, 804.53 822.80, 1123.54, 1277.36 1443.87, 1634.00, 2061.60	Si Ge H H H	1.803162 -0.876329 1.692058 0.553216 0.552989	-0.081276 0.004534 1.430950 -0.204561 -0.233621	0.001093 -0.000062 -0.019500 1.052955 -1.046781
p6 	333.37, 360.96, 517.75 596.55, 794.00, 901.61 1558.18, 1897.2, 2118.90	H Si Ge H H	0.624861 1.587996 -0.776519 2.398901 -0.407102	-0.006094 -0.124895 -0.027820 1.128267 1.516600	1.258019 -0.062314 -0.010669 0.112673 -0.156875

p7 	276.17, 348.26, 357.83 799.33, 876.80, 900.19 2113.90, 2144.30, 2145.02	Ge 0.004947 -0.660839 0.000000 Si 0.004947 1.772792 0.000000 H -1.490349 -1.034246 0.000000 H 0.631398 -1.318999 1.237402 H 0.631398 -1.318999 -1.237402
p8 	126.52, 379.15, 526.80 715.90, 1081.98, 1234.35 1500.80, 1624.09, 1909.87	Ge 0.773240 -0.067452 -0.000004 Si -1.767610 -0.020311 -0.000001 H 1.189937 1.466959 0.000107 H -0.593543 0.487840 1.029873 H -0.593519 0.488016 -1.029840
p9 	56.81, 311.85, 374.34 394.42, 673.02, 874.99 945.84, 968.61, 1952.39 2204.11, 2215.17, 2234.16	Ge -0.869630 -0.049326 -0.000002 Si 1.592780 -0.003613 -0.000004 H -0.847479 1.536268 0.000010 H 2.080444 0.721648 -1.203658 H 2.215968 -1.350168 -0.000172 H 2.080293 0.721268 1.203945
p10 	328.59, 333.56, 416.33 489.48, 513.60, 584.53 877.02, 949.56, 2169.74 2188.73, 2243.96, 2269.49	Ge -0.706756 -0.000006 -0.040265 Si 1.506832 -0.000010 0.085723 H -1.456228 1.257592 0.396806 H -1.456550 -1.257409 0.396793 H 2.216517 1.221716 -0.352624 H 2.216807 -1.221576 -0.352597
p11 	75.19, 323.44, 347.40 392.02, 704.46, 799.85 891.32, 903.79, 2065.97 2134.98, 2144.56, 2167.33	Ge 0.698763 -0.001463 -0.000034 Si -1.739076 -0.108116 -0.000079 H 1.380949 -1.374161 -0.002540 H 1.196531 0.758640 1.239118 H 1.199088 0.764499 -1.234452 H -1.789928 1.411449 0.000057
SiH 	2046.06	Si 0.000000 0.000000 0.101748 H 0.000000 0.000000 -1.424471
GeH_4 	844.05, 844.40, 844.50 945.58, 945.97, 2194.31 2199.85, 2199.97, 2200.01	Ge 0.000000 0.000017 0.000000 H 1.246688 0.880010 0.000000 H -1.245291 0.881987 0.000000 H -0.000699 -0.881278 1.245807 H -0.000699 -0.881278 -1.245807

i0 	97.40, 151.77, 215.74 433.78, 627.01, 767.54 804.22, 883.40, 897.28 1245.82, 1613.76, 2022.48 2196.96, 2226.39, 2238.79	Si -2.080930 -0.071688 -0.010467 Ge 0.854969 -0.000458 -0.005075 H 0.822152 0.560150 -1.415086 H 1.270679 1.024457 1.037886 H 1.729156 -1.250621 0.065500 H -0.536314 -0.657506 0.516208 H -1.511669 1.341799 0.104439
i1 	116.95, 356.51, 376.11 399.92, 589.30, 603.72 811.00, 901.52, 901.69 935.24, 2154.65, 2181.85 2187.21, 2215.21, 2241.67	Ge 0.737911 -0.000014 0.006739 Si -1.638101 -0.000066 -0.091679 H 1.279838 1.252405 -0.683365 H 1.282757 -1.232512 -0.716127 H 1.255493 -0.018804 1.449718 H -2.248412 1.211801 0.508915 H -2.249413 -1.211518 0.508709
i2 	116.96, 343.90, 376.41 404.20, 572.33, 611.02 847.16, 910.80, 957.83 961.17, 2137.54, 2161.92 2227.15, 2252.19, 2260.69	Ge -0.797202 -0.000001 -0.044202 Si 1.581205 -0.000001 0.017019 H -1.445540 -1.249813 0.566304 H -1.445511 1.249832 0.566294 H 2.108252 -0.000079 1.403979 H 2.078210 -1.207093 -0.680259 H 2.078181 1.207189 -0.680113
i3 	82.05, 115.23, 193.09 415.83, 605.20, 847.68 883.22, 947.23, 958.73 1102.35, 1875.69, 1926.44 2266.25, 2295.02, 2314.47	Ge -1.066110 -0.043661 -0.002236 Si 1.946716 -0.005149 -0.012930 H 1.874745 0.974765 -1.106893 H 2.917045 0.422794 1.017004 H 2.255018 -1.364082 -0.491152 H 0.647861 -0.092964 0.801263 H -0.833169 1.528705 0.032340
ts: i0-i1 	-538.52, 167.63, 278.69 374.02, 545.58, 610.15 813.14, 872.94, 895.09 920.52, 1675.30, 2075.16 2104.12, 2184.05, 2213.30	Si -1.785107 -0.120944 -0.007713 H -2.083476 1.310135 -0.406403 Ge 0.754624 -0.001442 -0.010397 H 1.072448 -0.277762 -1.490615 H 1.430279 1.305453 0.404963 H 1.204648 -1.155871 0.876170 H -0.780358 0.557413 1.056570
ts: i0-p3 	-349.58, 113.17, 159.07 256.19, 457.10, 575.54 684.76, 707.87, 816.64 905.84, 1024.09, 1423.35 1984.27, 2017.75, 3430.45	Si 2.119840 -0.071382 -0.074544 H 1.821099 0.502291 1.310515 Ge -0.967774 -0.064457 0.052430 H 0.598151 -0.803138 0.004271 H -0.427825 1.845751 -0.100095 H -0.978775 -0.044006 -1.526224 H 0.278375 1.561062 -0.322598

ts: i1-i2 	-821.18, 133.69, 301.27 387.11, 461.83, 617.38 686.32, 804.37, 819.22 945.85, 1393.24, 2072.61 2144.64, 2211.84, 2238.00	Ge 0.796794 0.000017 0.039083 Si -1.615465 0.000086 -0.130949 H 1.159506 1.307645 -0.677116 H 1.158349 -1.308527 -0.675999 H -0.566562 -0.000324 1.196553 H -2.316266 1.209130 0.370252 H -2.315933 -1.209664 0.368941
ts: i1-p4 	-997.06, 260.21, 272.55 322.14, 453.67, 641.94 670.20, 724.25, 900.80 921.29, 1192.35, 1510.04 2035.90, 2084.08, 2139.13	Ge -0.714231 -0.038505 0.058856 Si 1.747195 0.046728 0.100100 H -1.552921 1.119426 0.632492 H -1.701947 -1.047566 -0.568451 H 1.678765 -1.206205 -0.764608 H 0.484703 0.874883 -1.459357 H 0.455478 0.837416 -1.124878
ts: i3-i2 	-600.56, 188.17, 303.80 393.80, 602.34, 694.67 847.16, 892.59, 950.13 987.98, 1620.28, 2005.35 2186.56, 2257.02, 2284.60	Ge -0.866362 -0.062645 0.003699 H -1.355015 1.312316 -0.569146 Si 1.613833 -0.001484 -0.023543 H 2.030330 -0.818554 -1.195977 H 2.231304 1.334694 -0.156977 H 2.046565 -0.682413 1.211185 H 0.176747 0.879352 0.922154
ts: i2-p2 	-1296.63, 254.62, 281.81 344.34, 408.77, 614.77 796.94, 851.03, 942.47 1009.25, 1361.40, 1716.24 1989.45, 2223.17, 2253.77	Ge 0.825351 -0.024754 -0.089328 Si -1.645551 0.009801 0.037533 H 0.668497 1.280188 0.980781 H 0.874138 -0.989270 1.155663 H -0.330064 0.910850 1.003538 H -2.323936 0.775039 -1.034364 H -2.262171 -1.321879 0.227428
ts: i2-p8 	-683.10, 136.45, 302.08 397.96, 509.48, 587.77 729.31, 827.90, 915.23 1036.42, 1302.63, 1588.58 2052.00, 2122.62, 2307.38	Ge -0.854888 -0.003076 -0.038187 Si 1.812496 -0.184945 0.048380 H -0.806346 -1.362189 0.685016 H 0.526661 -0.015753 -1.038151 H -0.958634 1.182457 0.942290 H 1.310660 1.423758 0.308992 H 1.909148 1.459398 -0.353484
ts: i3-p1 	-1162.97, 119.49, 245.73 369.59, 560.33, 649.53 751.29, 903.16, 956.41 969.43, 1619.63, 1748.77 2234.00, 2242.00, 2249.01	Ge -0.910430 -0.063819 -0.000016 Si 1.657575 -0.024403 0.000026 H 1.853802 -1.491442 -0.000037 H 2.314519 0.532463 -1.206254 H 2.314468 0.532357 1.206382 H 0.268058 1.210351 0.000037 H -0.823144 1.600104 0.000040

ts: i3-p6 	-1106.79, 260.40, 284.91 352.88, 435.81, 565.35 790.75, 817.21, 922.39 979.74, 1258.89, 1409.38 1907.76, 1994.31, 2242.65	Ge -0.891882 -0.045809 -0.015300 H -0.573839 1.450643 0.431540 Si 1.526982 0.107793 -0.142831 H 2.442810 1.102081 0.462392 H 2.366056 -1.051560 0.800358 H 2.428993 -1.146645 -0.287522 H 0.498457 -0.397748 1.082458
ts: p2-p1 	-738.49, 290.06, 361.38 438.32, 727.50, 910.25 1966.38, 2142.28, 2161.17	Si -1.631789 -0.121838 -0.018896 Ge 0.812940 0.060128 0.006797 H -2.119705 0.449137 1.277025 H 1.101296 -1.485610 -0.168160 H -2.150631 0.818102 -1.061834
ts: p1-p5 	-200.10, 267.83, 307.04 340.94, 417.10, 461.81 503.61, 639.64, 653.95 916.46, 974.42, 1945.29 2175.42, 2203.14, 3894.99	Ge 0.74278 -0.249 0.18235 Si -1.63323 -0.24906 0.08393 H 1.44682 0.57998 -0.95214 H 0.06201 -0.68875 1.45376 H -1.16695 1.14749 0.68779 H -1.41812 -1.14749 1.27713 H 0.79984 0.5318 -1.45376
ts: p1-p9 	-126.85, 52.06, 85.06 141.44, 311.67, 374.73 389.20, 664.54, 872.55 944.68, 967.69, 1884.33 2206.16, 2217.89, 2235.52	Ge -0.872560 -0.108433 -0.000005 Si 1.589897 -0.079347 -0.000015 H -0.833850 1.482221 -0.000083 H 2.079812 0.643611 -1.203532 H 2.199491 -1.431849 -0.000631 H 2.079267 0.642232 1.204569 H 0.138648 3.244490 0.000055
ts: p2-p4 	-504.25, 338.63, 379.67 406.84, 621.54, 806.14 1870.78, 2025.85, 2059.93	Ge -0.715919 -0.039781 -0.045969 Si 1.661332 -0.059442 -0.032179 H -1.595521 1.212382 0.202764 H -0.317998 -0.536048 1.418361 H 1.564276 1.428838 0.300374
ts: p7-p4 	-1138.85, 287.76, 305.93 384.84, 706.81, 846.72 2044.59, 2060.96, 2073.74	Ge -0.727045 -0.063226 -0.003361 Si 1.694313 0.131518 0.005042 H -1.217828 0.703453 1.256398 H 1.996577 -1.355084 -0.053284 H -1.233687 0.833608 -1.166143

ts: p10-p9 	-587.49, 276.12, 377.54 465.56, 622.37, 655.32 882.36, 1006.01, 1810.32 2001.26, 2183.22, 2223.19	Ge -0.783447 -0.019511 -0.048727 Si 1.514884 0.021352 -0.018877 H -0.776346 1.371655 0.677295 H -0.204677 -0.896562 1.173432 H 2.550329 1.096261 0.027488 H 2.292617 -1.245930 -0.054678
ts: p11-p7 	-304.33, 52.06, 96.54 301.70, 324.27, 394.33 451.35, 696.96, 797.78 890.22, 903.12, 1827.77 2132.88, 2143.83, 2165.53	Si -1.695180 -0.295835 0.000001 Ge 0.727292 -0.007475 0.000000 H -1.849036 1.235726 -0.000004 H 1.162339 0.790951 -1.237734 H 1.506406 -1.327142 0.000025 H 1.162350 0.791005 1.237695 H -1.522866 2.890339 0.000001
ts: p11-p10 	-327.34, 380.13, 382.69 476.58, 697.02, 766.91 844.13, 893.69, 1906.81 2067.23, 2164.73, 2179.34	Ge -0.681057 -0.000791 -0.020159 Si 1.672037 -0.103870 -0.033121 H -1.536008 -1.265329 -0.111729 H -1.543403 1.230618 -0.301192 H -0.225966 0.099127 1.499081 H 1.690669 1.415065 0.022617

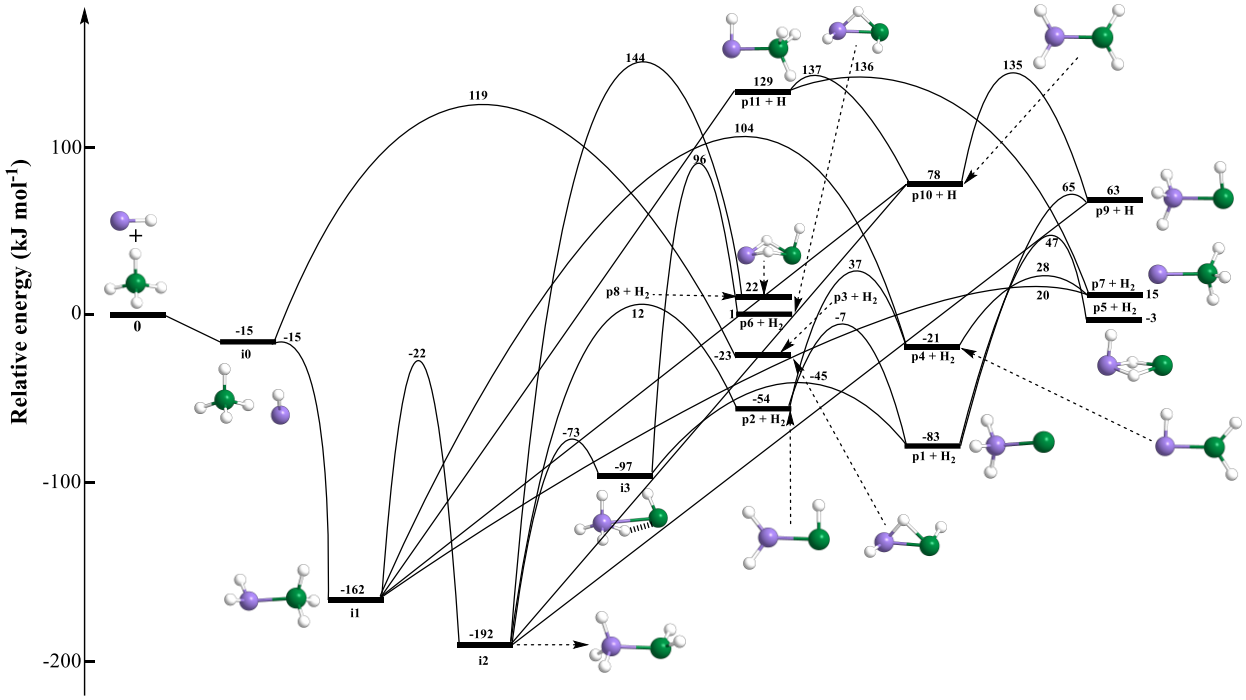


Figure S1. Potential energy surface for the reaction of the silylidyne radical with germane involving atomic and molecular hydrogen loss pathways. Optimized Cartesian coordinates of the atoms and vibrational frequencies are compiled in Table S3. Germanium, silicon, and hydrogen are color coded in green, purple, and white, respectively.

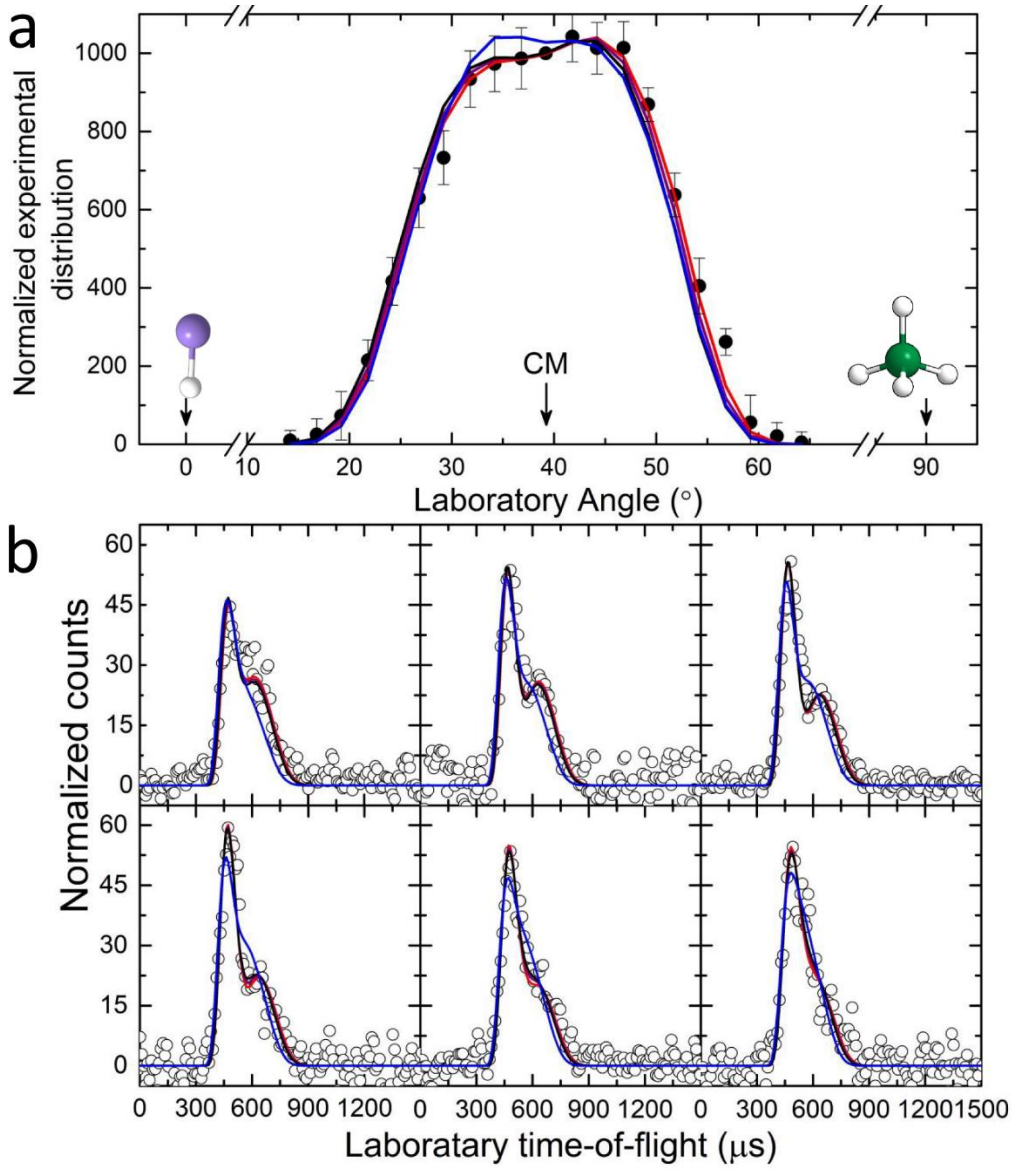


Figure S2. Laboratory angular distribution and the associated time-of-flight spectra. Laboratory angular distribution at mass-to-charge ratio (m/z) of m/z = 102 recorded in the reaction of the silylidyne radical with germane (a) (^{28}SiH + ^{74}GeH$_4$ (red), ^{28}SiH + ^{73}GeH$_4$ (purple), ^{28}SiH + ^{72}GeH$_4$ (black) and ^{29}SiH + ^{70}GeH$_4$ (blue)), and the time-of-flight spectra recorded at distinct laboratory angles overlaid with the best fits (b). The solid circles with their error bars represent the normalized experimental distribution with ±1σ uncertainty; the open circles indicate the experimental data points of the time-of-flight spectra. Silicon, germanium, and hydrogen are color coded in purple, green, and white, respectively.

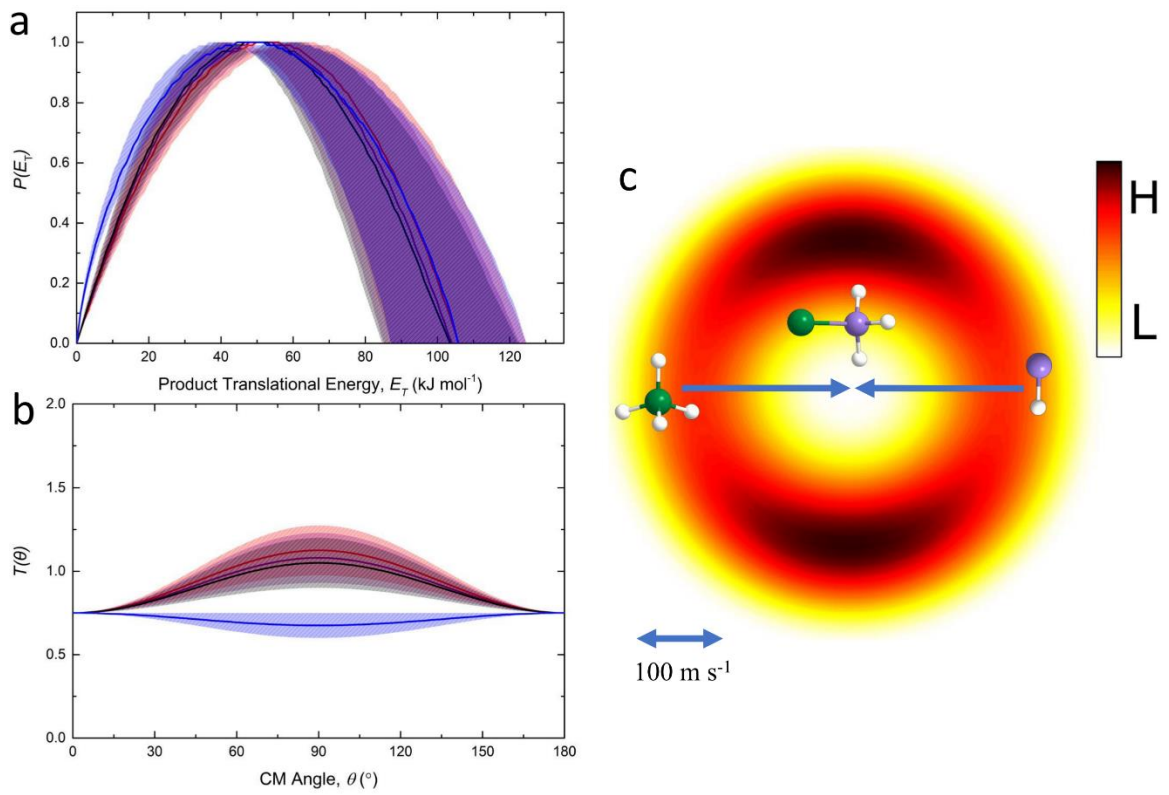


Figure S3. Center-of-Mass (CM) distributions and the associated flux contour map. CM translational energy flux distribution (a), CM angular flux distribution (b), and the top view of their corresponding flux contour map (c) leading to the formation of H_3SiGe plus molecular hydrogen in the reaction of silylidyne with germane (^{28}SiH + $^{74}GeH_4$ (red), ^{28}SiH + $^{73}GeH_4$ (purple), ^{28}SiH + $^{72}GeH_4$ (black) and ^{29}SiH + $^{70}GeH_4$ (blue)). Shaded areas indicate the error limits of the best fits accounting for the uncertainties of the laboratory angular distribution and TOF spectra. The flux contour map represents the flux intensity of the reactive scattering products as a function of the CM scattering angle (θ) and product velocity (u). The color bar indicates the flux gradient from high (H) intensity to low (L) intensity. Silicon, germanium, and hydrogen are color coded in purple, green, and white, respectively.