ChemPhysChem

Supporting Information

Combined Crossed Molecular Beams and Ab Initio Study of the Bimolecular Reaction of Ground State Atomic Silicon (Si; ^3P) with Germane (GeH_4; X^1A_1)

Vladislav S. Krasnoukhov, Valeriy N. Azyazov, Alexander M. Mebel,* Srinivas Doddipatla, Zhenghai Yang, Shane Goettl, and Ralf I. Kaiser*

Supplemental Information

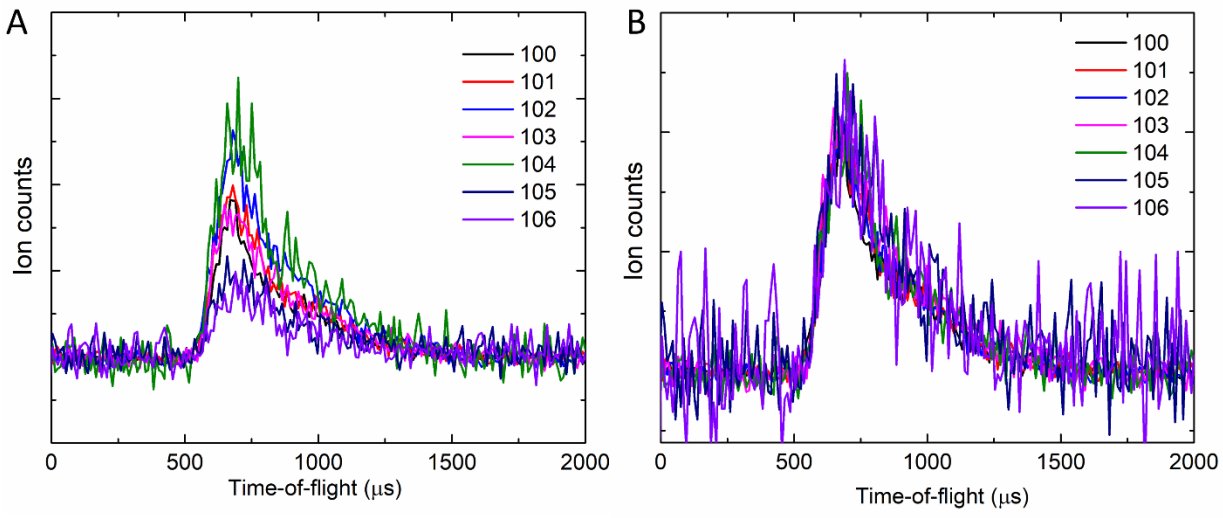

Figure S1. Time-of-flight spectra recorded at the CM angle for *m/z* = 100-106 for the reaction of ground state atomic silicon ($Si(^3P)$) with germane (GeH_4; X^1A_1)). The panels A and B depict raw and scaled TOF spectra, respectively.

Table S1. H_2 loss product mass combinations of silicon and germanium isotopes from the reaction of ground state atomic silicon and germane. Isotope abundance given in the parenthesis.

Si + GeH_4		$^{70}GeH_4$ (20.4%) 74	$^{72}GeH_4$ (27.3%) 76	$^{73}GeH_4$ (7.7%) 77	$^{74}GeH_4$ (36.7%) 78	$^{76}GeH_4$ (7.8%) 80
H_2 Loss	^{28}Si (92.2%) 28	$^{28}Si^{70}GeH_2$ 100	$^{28}Si^{72}GeH_2$ 102	$^{28}Si^{73}GeH_2$ 103	$^{28}Si^{74}GeH_2$ 104	$^{28}Si^{76}GeH_2$ 106
	^{29}Si (4.7%) 29	$^{29}Si^{70}GeH_2$ 101	$^{29}Si^{72}GeH_2$ 103	$^{29}Si^{73}GeH_2$ 104	$^{29}Si^{74}GeH_2$ 105	$^{29}Si^{76}GeH_2$ 107
	^{30}Si (3.1%) 30	$^{30}Si^{70}GeH_2$ 102	$^{30}Si^{72}GeH_2$ 104	$^{30}Si^{73}GeH_2$ 105	$^{30}Si^{74}GeH_2$ 106	$^{30}Si^{76}GeH_2$ 108

Table S2. Optimized Cartesian coordinates (Å) and vibrational frequencies (cm^{-1}) of the reactants, products, transition states, and MSX on the singlet and triplet potential energy surface involved in the reaction of ground state atomic silicon ($Si(^3P)$) with germane (GeH_4; X^1A_1).

Species	Vibrational Frequencies (cm^{-1})	Cartesian Coordinates (Å)			
		Atom	X	Y	Z
^{3}i1, ^{3}A"	109.7335, 349.6724, 410.5659,	Ge	-0.698135	-0.010468	0.000000
	486.2070, 625.5880, 812.5878,	Si	1.677847	0.108823	-0.000001
	891.1673, 895.9144, 2160.8011,	H	-1.233733	1.419909	0.000152
	2165.2007, 2187.3223, 2194.1329	H	-1.210336	-0.739730	1.245808
		H	-1.210378	-0.739473	-1.245941
		H	2.504896	-1.129260	-0.000006
MSX,	4.45978, 362.88067,	Ge	-0.026759	-0.953297	0.044637
^{3}A-^{1}A	375.83398,412.60776, 797.94562,	Si	0.024549	1.404057	0.079185
	875.09513, 886.23037,	H	-1.432191	-1.566046	0.077879
	2101.17514, 2137.18344,	H	0.786369	-1.436558	1.252563
	2142.97307, 2166.68199	H	0.695332	-1.360573	-1.243023
		H	1.201120	2.278230	-0.066729
^{1}i1, ^{1}A'	75.19, 323.44, 347.40,	Ge	-0.077962	-0.395785	-0.004384
	392.01, 704.45, 799.84,	Si	-0.195205	2.040693	0.060900
	891.31, 903.79, 2065.97,	H	-1.446692	-1.085047	0.029960
	2134.98, 2144.56, 2167.33	H	0.732579	-0.920155	1.191057
		H	0.640914	-0.861119	-1.280116
		H	1.322945	2.099672	0.002582
i2, ^{1}A'	328.58, 333.55, 416.32,	Ge	-0.708505	3.370585E-4	-0.025577
	489.48, 513.59, 584.53,	Si	1.506568	1.995357E-4	0.070822
	877.02, 949.56, 2169.74,	H	-1.451994	1.257987	0.421446
	2188.73, 2243.96, 2269.49	H	-1.452468	-1.257012	0.421483
		H	2.210407	1.221875	-0.376990
		H	2.210549	-1.221416	-0.376922
i3, ^{1}A'	171.13, 340.28, 420.84, 426.19,	H	-0.409234	1.777914	0.409502

	513.49, 616.95, 638.22, 883.65, 1299.76, 2136.70, 2162.76, 3156.06	H	-0.409292	1.777887	-0.409646
		Ge	1.461859	0.015759	-8.11828E-5
		H	2.289064	-1.275082	-4.99227E-5
		H	2.420503	1.212296	-1.64072E-4
		Si	-0.800546	0.0471086	8.6609E-6
i4, ^{1}A	208.63, 372.55, 389.44, 598.14, 655.39, 851.58, 904.32, 964.49, 1773.95, 1957.90, 2231.53, 2250.84	Ge	-1.459545	-0.301804	-0.638210
		Si	0.850939	-0.002639	-0.773741
		H	-1.528713	1.273108	-0.477739
		H	1.795413	-1.143421	-0.817321
		H	1.618462	1.264760	-0.755997
		H	0.157939	-0.122791	0.640317
i5, ^{1}A’	56.81, 311.85, 374.33, 394.42, 673.02, 874.99, 945.84, 968.61, 1952.39, 2204.11, 2215.17, 2234.16	Ge	-1.257091	0.736421	-0.398070
		Si	1.077382	0.130153	0.100143
		H	-1.665301	0.100837	0.996203
		H	1.508806	0.791795	1.360582
		H	2.035944	0.516729	-0.964418
		H	1.182688	-1.341090	0.292407
i6, ^{1}A’	263.99, 346.86, 651.95, 774.09, 841.88, 852.53, 1170.94, 1363.52, 1428.15, 1621.44, 1956.49, 2073.52	Si	0.019469	1.819783	0.000000
		H	-0.107064	0.557959	1.053321
		H	-0.107064	0.557959	-1.053321
		H	-1.567325	-0.851590	0.000000
		H	1.527343	1.661308	0.000000
		Ge	0.017675	-0.864579	0.000000
i7, ^{1}A’	320.94, 365.18, 598.64, 694.09, 834.47, 870.88, 1171.32, 1335.68, 1345.34, 1607.02, 1987.97, 2098.15	Si	-0.054130	1.833761	0.000000
		H	-0.117779	0.543981	1.047716
		H	-0.117779	0.543981	-1.047716
		H	1.525141	-0.892270	0.000000
		H	1.457388	1.840550	0.000000
		Ge	-0.051540	-0.881232	0.000000
i8, ^{1}A’	222.04, 309.14, 405.83, 413.92, 448.73, 484.47, 528.73, 941.75,	H	1.384561	1.659823	-0.391147
		H	1.384591	1.659788	0.391188

	991.39, 2221.24, 2246.63, 3705.37	Si	-0.712455	-0.048577	1.96042E-5
		H	-1.648579	-1.199009	1.3439E-6
		H	-1.474963	1.222455	1.021812E-4
		Ge	1.5470301	-0.330465	-7.38971E-5
i9, ^{1}A	365.94, 367.65, 521.36, 603.93, 672.72, 834.72, 892.82, 1030.45, 1475.85, 2065.99, 2123.71, 2147.44	Si	-1.632004	-0.100185	-0.017449
		H	-0.428935	-0.061151	1.264458
		H	-1.601991	1.417141	0.038758
		H	1.543913	-1.234442	0.227175
		H	1.577471	1.235386	0.192567
		Ge	0.683535	0.008233	-0.058577
ts-i1-i2, ^{1}A	545.0425i, 141.8644, 372.4844 394.0490, 594.6061, 701.8991 863.4086, 972.9055, 1675.6756 1859.9538 , 2344.0006, 386.9025	H	-2.55844	1.08674	0.03865
		H	0.81125	1.37272	0.6579
		Ge	-1.51129	0.02345	-0.01985
		H	-2.27675	-1.25207	-0.05224
		H	0.19816	-0.8777	1.18013
		Si	0.78075	-0.02056	-0.04833
ts-i1-i6, ^{1}A	766.76i, 164.08, 258.45, 435.18, 480.36, 690.21, 809.91, 847.69, 2054.35, 2071.42, 2188.77, 2224.29	Ge	-1.707945	0.024689	-0.028380
		H	-1.2830043	0.796397	-1.268686
		H	-0.977340	0.601060	1.211834
		H	-1.731770	-1.4934904	-0.066257
		H	0.919714	1.461310	-0.057552
		Si	0.857982	-0.035691	0.209246
ts-i1-i9, ^{1}A	327.35i, 380.13, 382.69, 476.58, 697.02, 766.91, 844.13, 893.69, 1906.84, 2067.23, 2164.73, 2179.33	Si	-1.569210	-0.171879	-0.681901
		Ge	0.784643	-0.112682	-0.620995
		H	-1.563691	1.337173	-0.499285
		H	1.620053	-1.380350	-0.804006
		H	1.672233	1.122159	-0.783289
		H	0.303742	-0.131900	0.893444
ts-i2-i4,	587.95i, 276.08, 377.53, 465.47,	Ge	-1.747709	-0.173310	-0.740589

^{1}A	622.35, 655.31, 882.28, 1006.02, 1811.49, 2001.21, 2183.22, 2223.18	Si	0.547676	-0.200188	-0.864443
		H	-1.652521	1.233836	-0.052537
		H	1.285381	-1.490509	-0.919389
		H	1.613694	0.844259	-0.914009
		H	-1.113053	-1.0378453	0.4622280
ts-i2-i9, ^{1}A	571.47i, 323.14, 378.58, 493.46, 647.50, 673.82, 907.82, 955.38, 1832.09, 2081.03, 2090.39, 2131.52	Ge	-0.673197	0.008601	-0.021873
		H	1.620505	1.331045	0.510055
		H	-1.720811	1.1280358	0.196686
		H	0.984131	-0.780916	1.149206
		H	-1.496024	-1.296325	0.011276
		Si	1.620765	-0.057579	-0.090232
ts-i3-i9, ^{1}A	941.16i, 341.13, 401.57, 466.97, 481.49, 720.89, 821.45, 914.69, 1677.61, 1809.19, 2122.95, 2145.5885	Si	-1.595594	-0.160055	0.007243
		H	-0.923004	1.242329	0.608421
		H	-1.484175	1.441352	-0.244259
		Ge	0.682706	-0.012646	-0.027691
		H	1.608671	-1.178303	0.358093
		H	1.530159	1.2698579	0.007213
ts-i3-p4, ^{1}A	376.13i, 51.87, 154.11, 210.07, 234.28, 264.16, 437.97, 475.58, 769.78, 1943.67, 2179.63, 4353.23	H	-1.303836	-1.372206	6.77788E-5
		H	1.457288	2.369818	-0.373797
		H	1.456461	2.370648	0.371731
		H	-2.778516	0.734134	-0.003971
		Ge	-1.350838	0.209179	-0.001768
		Si	0.799054	-0.166450	0.001077
ts-i4-i5, ^{1}A	308.29i, 283.63, 374.59, 515.21, 604.66, 762.47, 890.02, 1052.11, 1836.69, 1931.87, 2117.44, 2200.32	Ge	-1.592828	-0.457344	-0.728177
		Si	0.656043	0.188980	-0.475314
		H	-2.292557	0.841821	-0.134514
		H	-0.071677	-0.226543	0.847586
		H	1.066573	-1.199033	-0.883692
		H	2.078524	0.597800	-0.315367
ts-i4-i8, ^{1}A	1169.07i, 369.01, 398.89, 482.94, 533.45, 715.53, 868.45, 986.82,	Ge	-1.689024	-0.234575	-0.810507
		Si	0.606498	-0.133787	-0.791693

	1548.78, 1690.69, 2208.47, 2228.51	H	-1.414592	1.440921	-0.926098
		H	-0.810147	1.110705	-0.101311
		H	1.472148	-1.285261	-0.425015
		H	1.454678	1.084746	-0.787471
ts-i4-p1, ^{1}A	449.50i, 272.48, 315.48, 450.68, 577.55, 685.73, 794.28, 870.97, 1470.80, 1927.65, 2065.41, 2939.04	Ge	-0.996764	-0.817047	-0.828713
		Si	0.884449	0.874466	-0.306203
		H	-1.467509	0.032318	-2.085817
		H	1.609062	-0.765889	-0.340738
		H	2.184151	-0.218854	-0.600023
		H	0.935409	0.482972	1.158834
ts-i5-i6, ^{1}A	747.78i, 100.90, 246.63, 456.80, 482.53, 667.49, 896.87, 917.80, 1938.85, 2183.70, 2203.71, 2271.84	Si	-1.726928	0.031524	0.004840
		H	-1.140041	0.687645	-1.197170
		H	-1.116202	0.620776	1.229513
		H	-1.737334	-1.443586	-0.035514
		H	0.930137	1.522366	0.020080
		Ge	0.868004	-0.064450	-0.021546
ts-i5-p1, ^{1}A	265.16i, 159.54, 327.96, 424.01, 474.16, 515.54, 577.37, 795.21, 1082.44, 1872.29, 2058.09, 3730.85	H	-1.540044	-0.233525	1.387399
		H	-2.211909	1.562495	-0.030687
		H	-1.499293	1.704443	0.256165
		H	0.606371	-1.493351	0.304375
		Si	-1.522183	-0.232971	-0.130810
		Ge	0.844966	0.066682	0.026812
ts-i6-i7, ^{1}A	522.38i, 266.19, 560.01, 609.09, 685.74, 923.34, 972.68, 1103.73, 1555.36, 1930.08, 1982.31, 2078.15	Si	1.822299	-0.012379	0.032098
		H	1.239944	1.173439	-0.710883
		H	1.007589	-1.059009	-0.737956
		H	-1.008468	1.529849	-0.009920
		H	0.569031	0.056175	1.077116
		Ge	-0.884174	-0.053678	-6.098979E-4
ts-i6-i9, ^{1}A	529.34i, 178.66, 452.19, 558.97, 676.78, 774.76, 889.13, 1252.81, 1862.42, 1908.44, 1962.36,	Si	-1.981880	0.057320	0.003874
		H	-0.642553	0.875261	0.006366
		H	-1.388575	-1.320664	-0.073134

	2157.51	H	0.392638	-0.724464	1.292738
		H	1.305990	1.349126	0.561579
		Ge	0.868018	0.037723	-0.055291
ts-i6-p1, ^{1}A	941.90i, 312.28, 525.81, 609.52, 714.53, 793.09, 923.85, 1095.56, 1542.80, 1758.33, 1803.64, 1936.60	H	0.866309	1.245111	-0.341069
		H	0.598119	-0.062369	1.196160
		H	1.739684	1.455342	0.166471
		H	-0.727856	-1.539542	-0.105142
		Si	1.667223	-0.160412	-0.038246
		Ge	-0.830077	0.039454	-0.013295
ts-i7-i9, ^{1}A	576.89i, 193.21, 453.64, 547.09, 631.78, 821.79, 862.06, 1385.49, 1611.47, 1832.30, 1960.33, 2001.56	Si	-1.758539	-0.131483	-0.013717
		H	-0.589962	0.999349	0.019983
		H	-2.564788	1.171171	0.023646
		H	0.165181	-0.701320	1.248205
		H	1.415792	1.273980	0.587678
		Ge	0.815009	-0.033861	-0.056241
ts-i7-p1, ^{1}A	702.31i, 305.22, 523.14, 583.23, 656.76, 781.59, 894.57, 1010.92, 1579.29, 1701.05, 1861.87, 1910.79	Si	1.653752	-0.168837	-0.044162
		H	-1.006028	1.511900	0.089396
		H	0.664152	-0.018745	1.2383412
		H	0.914456	1.300171	-0.299377
		H	1.815104	1.458372	0.067483
		Ge	-0.817367	-0.064182	-0.013093
ts-i8-p2, ^{1}A	319.19i, 37.33, 128.78, 226.32, 237.28, 252.46, 409.93, 463.63, 842.43, 1978.94, 2237.95, 4376.04	H	-1.273681	-1.319420	1.257065E-4
		H	1.547464	2.410215	-0.373231
		H	1.546692	2.411057	0.371067
		H	-2.848938	0.614961	-0.003838
		Si	-1.425314	0.209151	-0.001801
		Ge	0.733389	-0.180841	0.001016
ts-i9-p1, ^{1}A	1115.25i, 223.03, 377.16, 404.78, 508.34, 679.14, 818.26, 1005.71, 1687.41, 1829.43, 2054.37, 2083.8440	Si	1.663206	0.095942	-0.024619
		H	-1.403668	-0.622236	1.193323
		H	-1.013348	1.529647	0.193245
		H	-0.149797	1.305483	0.749055

		H	1.753176	-1.327661	0.504921
		Ge	-0.713396	-0.076209	-0.080849
p1, ^{1}A’	264.54, 385.43, 463.87, 607.59, 2123.88, 2192.52	Ge	1.198529	-0.000975	-0.372920
		Si	-1.096245	-0.001123	-0.409575
		H	-0.051688	1.012970	0.389703
		H	-0.050597	-1.010872	0.392793
p2, ^{1}A’	197.69, 413.86, 490.26, 1009.145, 1661.79, 2199.36	Ge	-1.554095	-0.318411	-0.246229
		Si	0.565621	-0.363210	0.277420
		H	1.949529	0.050255	0.631156
		H	-0.302664	0.992515	0.101476
p3, ^{1}A$_1$	247.50, 348.35, 416.03, 902.91, 2216.59, 2245.18	Ge	-1.538525	-0.211969	-2.97335E-5
		Si	0.727920	-0.211677	-1.6786E-6
		H	1.559918	0.048664	1.199302
		H	1.560389	-0.470934	-1.199209
p4, ^{1}A’	178.31, 424.19, 535.22, 1050.66, 1584.03, 2112.07	Si	-1.512459	-0.258208	-0.255207
		Ge	0.589120	-0.416498	0.270384
		H	2.000515	0.049966	0.6572194
		H	-0.418785	0.985889	0.091428
p5, ^{1}A$_1$	231.09, 335.28, 437.44, 833.12, 2141.37, 2164.87	Si	-1.536326	-0.212021	-3.06504E-5
		Ge	0.703407	-0.211458	-4.73005E-5
		H	1.571079	0.055345	1.230550
		H	1.571544	-0.477782	-1.230410
p6, ^{1}A’	256.25, 384.27, 463.92, 604.96, 2128.25, 2190.12	Ge	-1.281922	0.483410	-0.313480
		Si	0.853815	0.751796	-0.231654
		H	-2.395756	1.430770	0.162895
		H	1.777689	-0.296089	-0.751507