SUPPLEMENTAL INFORMATION

Directed Gas Phase Formation of the Germaniumsilylene Butterfly Molecule (Ge(μ−H_2)Si)

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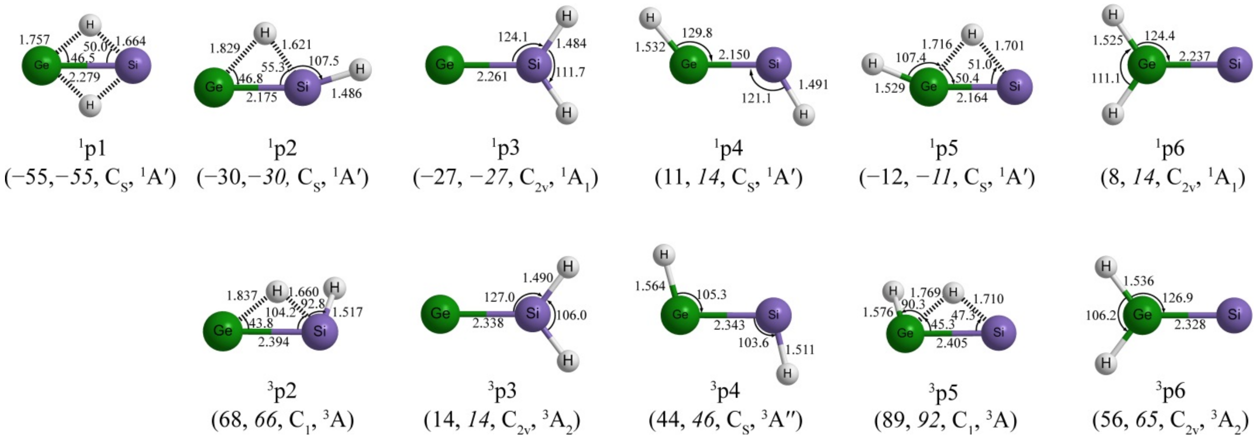


Fig. S1 Structural isomers of triplet and singlet $GeSiH_2$. Energies are given relative to the energies of the separated atomic germanium (Ge; $^3P_0$) and silane (SiH_4; X^1A_1) reactants in kJ mol^{-1} along with the point groups and electronic wave functions. Bond lengths and angles are given in angstroms (10^{-10} m) and degrees. Energies were computed at the CCSD(T)/CBS level; italicized energies were obtained by the mHEAT-345(Q) method. The ^{3}p1 structure does not represent a local minimum as it collapses to ^{3}p2 upon optimization.

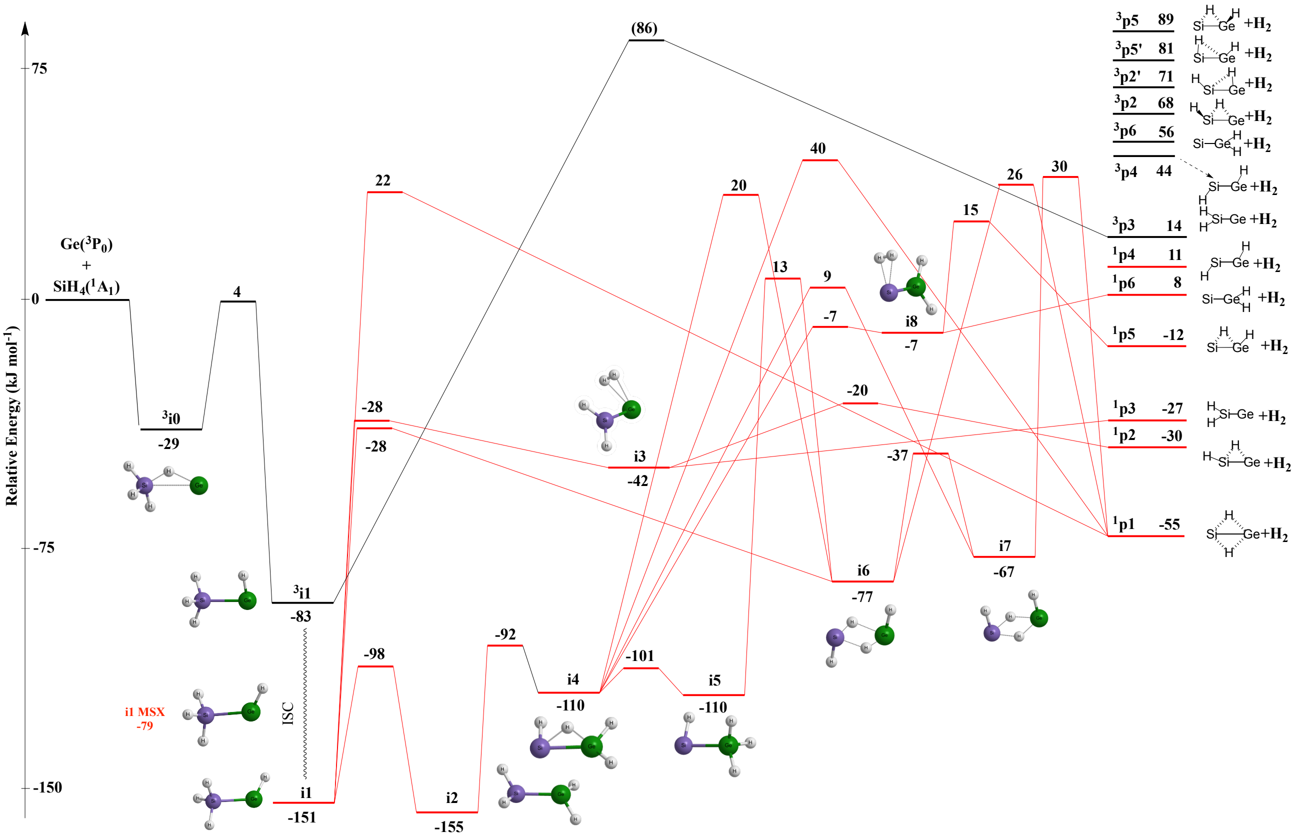


Fig. S2 Schematic of the $GeSiH_4$ potential energy surface accessed by the reaction of ground state atomic germanium (Ge) and silane (SiH_4) at the CCSD(T)/CBS level of theory. Energies are in units of kJ mol^{-1} and given relative to the $Ge(^3P_0)$ + SiH_4 bimolecular entrance channel. Black and red lines denote, respectively, triplet and singlet points on the surface.

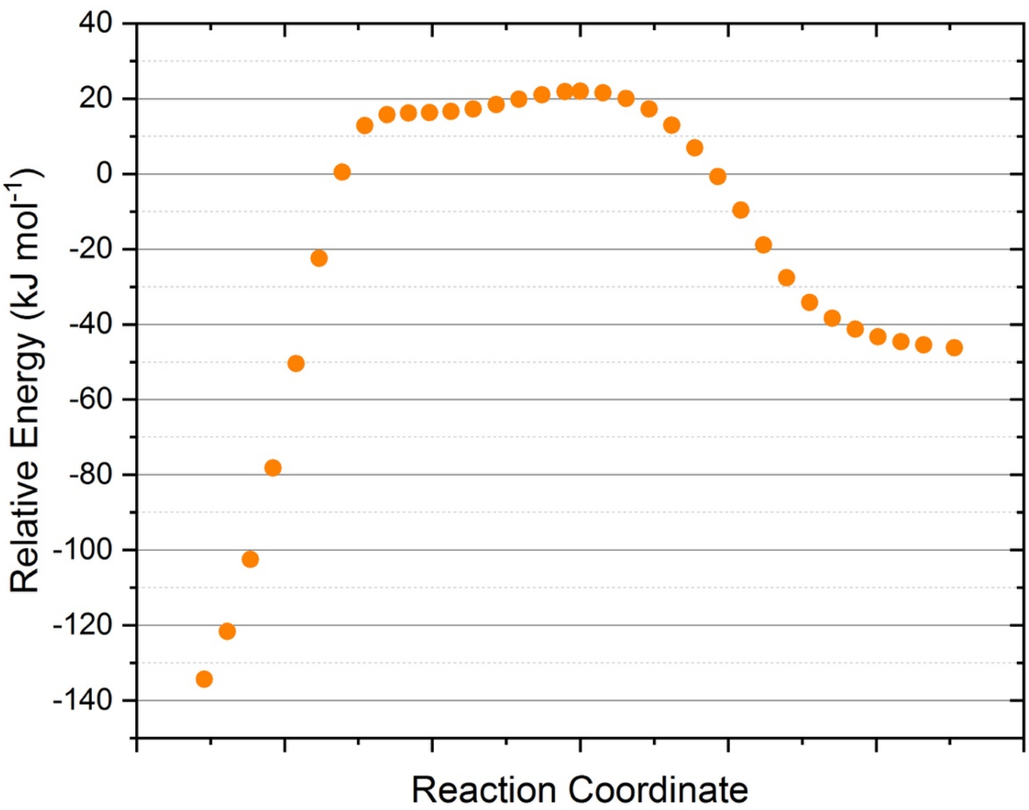


Fig. S3 Minimum energy path plot from the singlet isomer [1]i1 (H_3SiGeH) to [1]p1 (GeH_2Si) at the CCSD(T)/CBS level of theory with CCSD/cc-pVTZ zero point energy correction. Note that the energies computed along the intrinsic reaction coordinate are obtained over a finite distance, whereas the final energies reported throughout the manuscript text and in Figs. 6, S1, and S2 are obtained for an infinite separation of the $GeSiH_2$ and H_2 products. Energies are in units of kJ mol^{-1} and given relative to the Ge($^3P_0$) + SiH_4 bimolecular entrance channel.

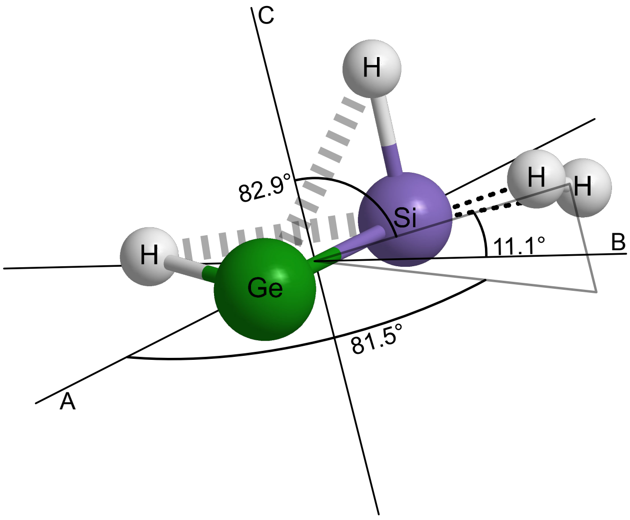


Fig. S4 Exit transition state leading to the dibridged germaniumsilylene (^{1}p1) plus molecular hydrogen.

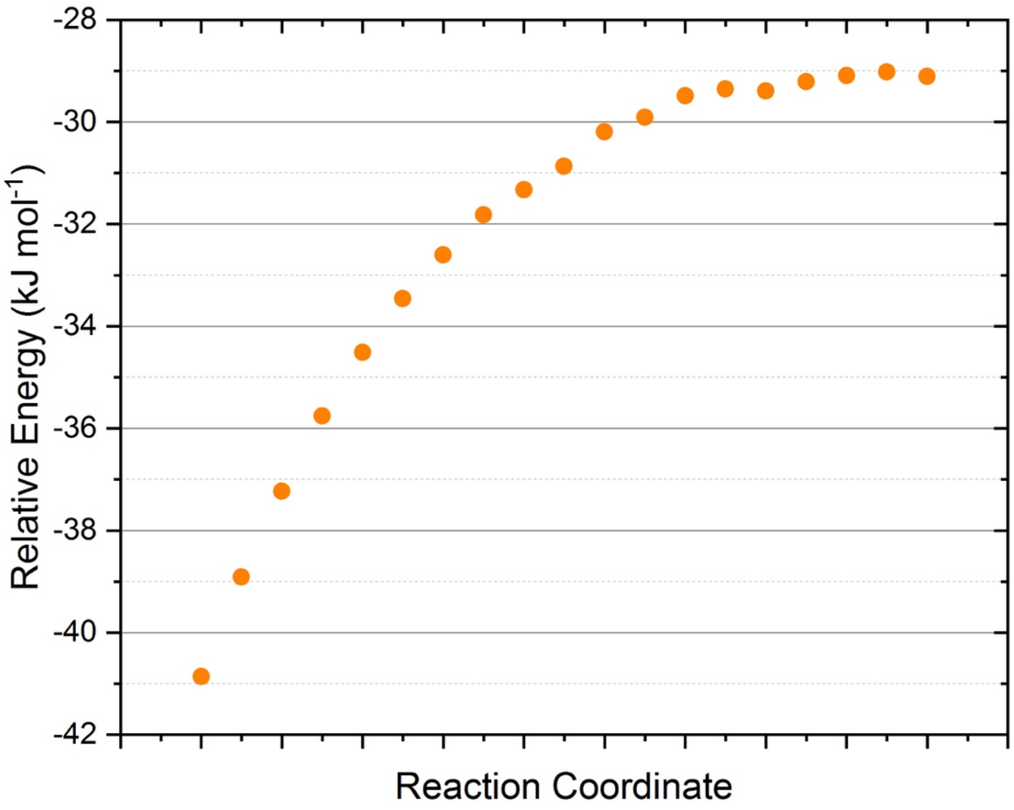


Fig. S5 Minimum energy path plot from the singlet isomer [1]i3 (H_2SiGeH_2) to [1]p3 (H_2SiGe) at the CCSD(T)/CBS level of theory with CCSD/cc-pVTZ zero point energy correction. Note that the energies computed along the intrinsic reaction coordinate are obtained over a finite distance, whereas the final energies reported throughout the manuscript text and in Figs. 6, S1, and S2 are obtained for an infinite separation of the $GeSiH_2$ and H_2 products. Energies are in units of kJ mol^{-1} and given relative to the Ge($^3P_0$) + SiH_4 bimolecular entrance channel.

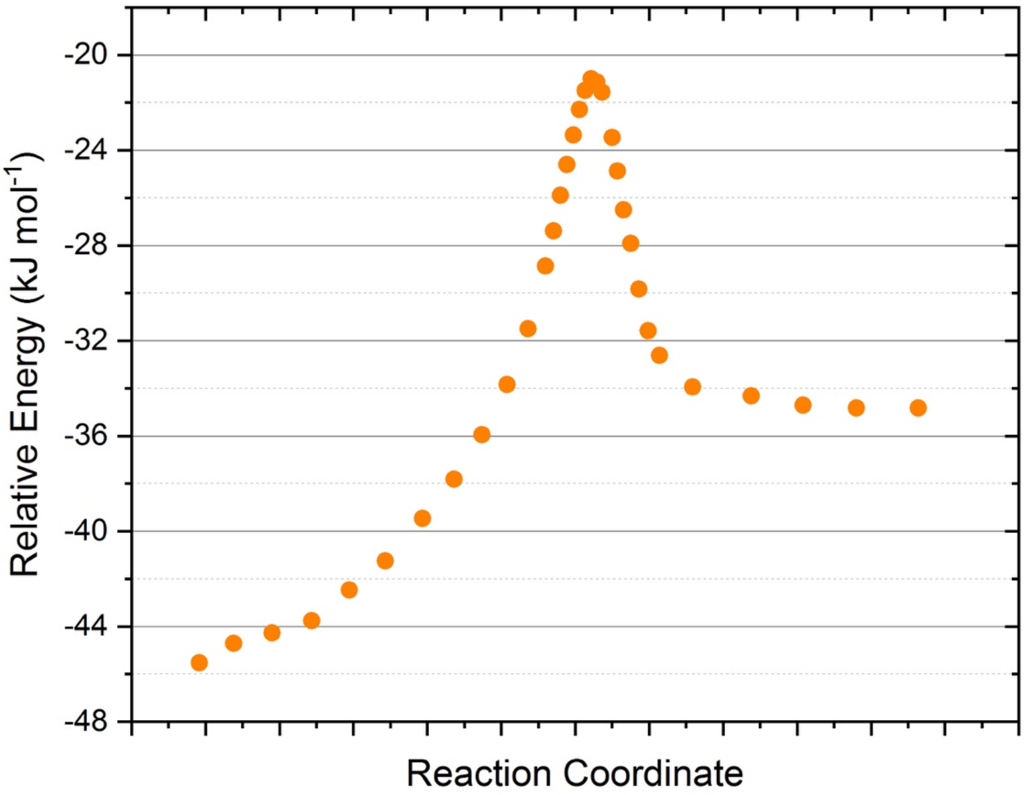
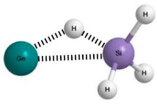
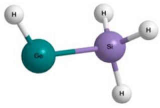
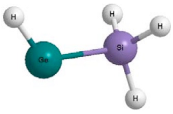
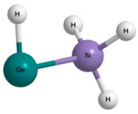
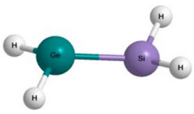
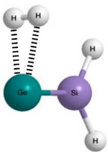
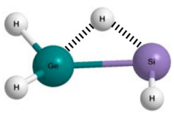
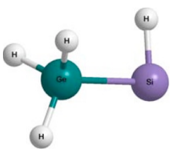
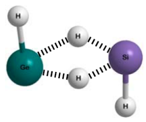
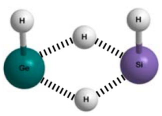
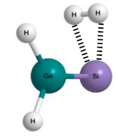
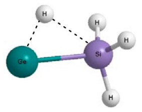
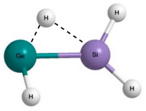
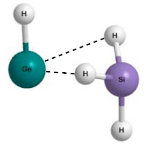
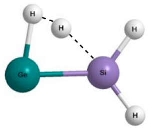
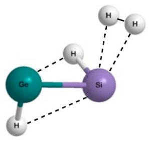
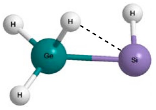
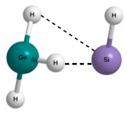
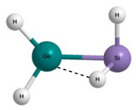
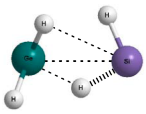
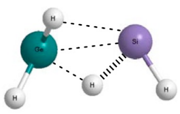
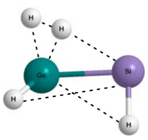
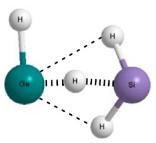
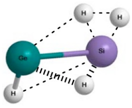
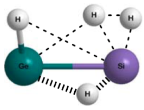
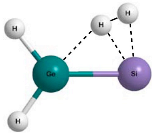
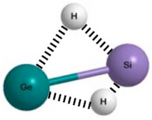
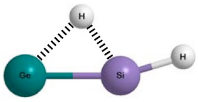
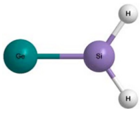
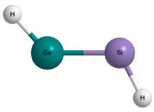
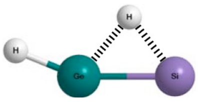
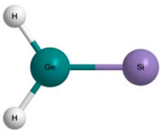
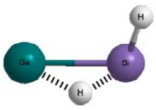
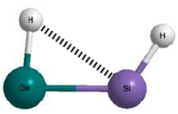
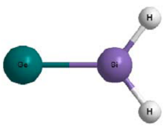


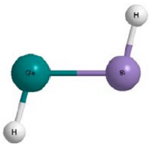
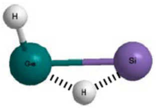
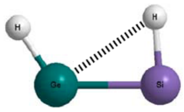
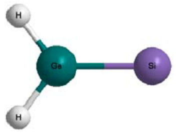
Fig. S6 Minimum energy path plot from the singlet isomer [1]i3 (H_2SiGeH_2) to [1]p2 (HSi(H)Ge) at the CCSD(T)/CBS level of theory with CCSD/cc-pVTZ zero point energy correction. Note that the energies computed along the intrinsic reaction coordinate are obtained over a finite distance, whereas the final energies reported throughout the manuscript text and in Figs. 6, S1, and S2 are obtained for an infinite separation of the $GeSiH_2$ and H_2 products. Energies are in units of kJ mol^{-1} and given relative to the Ge($^3P_0$) + SiH_4 bimolecular entrance channel.

Table S1 Structures and energies of species participating on the $GeSiH_4$ potential energy surface. Energies determined at the CCSD/cc-pVTZ//CCSD(T)/CBS level of theory with ZPE correction.

		CCSD/ cc-pVTZ + E_{zpc} [a]	E_{zpc} [b]	CCSD(T)/ CBS	E^c (kJ mol^{-1})
	Ge(^{3}P)	-2075.493248	0.000000	-2075.596899	
	SiH_4(T_d, $^1A_1$)	-291.401964	0.031561	-291.458201	
	Ge + SiH_4	-2366.895212	0.031561	-2367.055100	0
	**^{3}i0 (C_s, $^3A''$)**	-2366.902009	0.032161	-2367.066685	-29
	**^{3}i1 (C_s, $^3A''$)**	-2366.919738	0.031360	-2367.086639	-83
	**i1-MSX**		0.032082	-2367.085889	-79
	**i1 (C_s, $^1A'$)**	-2366.943699	0.030424	-2367.111638	-151
	**i2 (C_s, $^1A'$)**	-2366.939896	0.030772	-2367.113326	-155
	**i3 (C_1, ^1A)**	-2366.897006	0.029576	-2367.069011	-42
	**i4 (C_1, ^1A)**	-2366.925404	0.030426	-2367.095718	-110
	**i5 (C_s, $^1A'$)**	-2366.928048	0.030004	-2367.095268	-110
	**i6 (C_s, $^1A'$)**	-2366.914912	0.031160	-2367.084108	-77
	**i7 (C_s, $^1A'$)**	-2366.911470	0.030795	-2367.079940	-67

	**i8 (C_1, ^{1}A)**	-2366.884074	0.029613	-2367.055858	-7
	**^{3}tsi0-i1 (C_1, ^{1}A)**	-2366.885536	0.029477	-2367.051487	4
	**^{1}tsi1-i2 (C_1, ^{1}A)**	-2366.918443	0.028840	-2367.089662	-98
	**^{1}tsi1-i6 (C_1, ^{1}A)**	-2366.892161	0.028323	-2367.062580	-28
	**^{1}tsi1-i3 (C_1, ^{1}A)**	-2366.889615	0.027871	-2367.061936	-28
	**^{1}tsi1-p1 (C_1, ^{1}A)**	-2366.876028	0.027704	-2367.042843	22
	**^{1}tsi4-i5 (C_1, ^{1}A)**	-2366.923463	0.029542	-2367.091715	-101
	**^{1}tsi5-i6 (C_1, ^{1}A)**	-2366.876643	0.028212	-2367.046710	13
	**^{1}tsi2-i4 (C_1, ^{1}A)**	-2366.916735	0.028815	-2367.087277	-92
	**^{1}tsi4-i6 (C_1, ^{1}A)**	-2366.877998	0.029242	-2367.044975	20
	**^{1}tsi4-i7 (C_1, ^{1}A)**	-2366.880210	0.028697	-2367.048635	9
	**^{1}tsi4-p1 (C_1, ^{1}A)**	-2366.866096	0.027012	-2367.035281	40
	**^{1}tsi6-i7 (C_1, ^{1}A)**	-2366.897789	0.029581	-2367.067174	-37

	**^{1}tsi6-p1 (C_1, ^{1}A)**	-2366.870087	0.028283	-2367.041803	26
	**^{1}tsi7-p1 (C_1, ^{1}A)**	-2366.868810	0.027666	-2367.039925	30
	**^{1}tsi4-i8 (C_1, ^{1}A)**	-2366.881742	0.027666	-2367.053884	-7
	H	-0.499810	0.000000	-0.500019	
	H_2	-1.162291	0.010045	-1.174474	
	**^{1}p1 + H_2 (C_s, $^{1}A'$)**	-2366.904917	0.025277	-2367.069867	-55
	**^{1}p2 + H_2 (C_s, $^{1}A'$)**	-2366.892922	0.023760	-2367.058767	-30
	**^{1}p3 + H_2 (C_{2v}, $^{1}A_1$)**	-2366.895054	0.024692	-2367.058479	-27
	**^{1}p4 + H_2 (C_s, $^{1}A'$)**	-2366.875399	0.023633	-2367.043014	11
	**^{1}p5 + H_2 (C_s, $^{1}A'$)**	-2366.886118	0.023614	-2367.051639	-12
	**^{1}p6 + H_2 (C_{2v}, $^{1}A_1$)**	-2366.882156	0.024430	-2367.044965	8
	**^{3}p2 + H_2 (C_1, ^{3}A)**	-2366.863074	0.023595	-2367.021254	68
	**^{3}p2' + H_2 (C_s, $^{3}A''$)**	-2366.861967	0.023390	-2367.019758	71
	**^{3}p3 + H_2 (C_{2v}, $^{3}A_2$)**	-2366.884141	0.024844	-2367.043206	14

	**^{3}p4 + H_2 (C_s, $^3A''$)**	-2366.871173	0.023701	-2367.030593	44
	**^{3}p5 + H_2 (C_1, ^3A)**	-2366.855321	0.023257	-2367.012912	89
	**^{3}p5' + H_2 (C_s, $^3A''$)**	-2366.858736	0.025233	-2367.017738	81
	**^{3}p6 + H_2 (C_{2v}, $^3A_2$)**	-2366.869139	0.024405	-2367.026690	56

[a] CCSD/cc-pVTZ energy with zero-point energy correction in hartree.

[b] zero-point energy by CCSD/cc-pVTZ in hartree.

[c] relative energy by CCSD(T)/CBS with CCSD/cc-pVTZ zero-point energy correction.

[d] geometries optimized by MP2/cc-pVTZ.

Table S2 Optimized cartesian coordinates of the seam of crossing from the triplet to singlet surface of **i1**.

i1-MSX			
H	-0.618435	2.326113	1.199899
H	-1.510413	-1.439618	-0.000005
Si	0.009181	1.742222	0.000001
H	1.451812	2.041524	0.000003
H	-0.618433	2.326113	-1.199898
Ge	-0.181730	-0.669419	0.000000

Table S3 Cartesian coordinates for singlet and triplet $GeSiH_4$ intermediates.

Atom	X	Y	Z	Atom	X	Y	Z
^{3}i0				**^{3}i1**			
Si	0.003855	2.011774	0.000000	H	-0.652386	2.086860	1.206886
H	0.823051	2.099527	1.223866	H	-1.255926	-1.664328	0.000000
H	-1.056391	3.044613	0.000000	Si	0.024315	1.551687	0.000000
H	-0.767063	0.702315	0.000000	H	1.442226	1.978538	0.000000
H	0.823051	2.099527	-1.223866	H	-0.652386	2.086860	-1.206886
Ge	0.003855	-1.128463	0.000000	Ge	0.024315	-0.819111	0.000000
i1				**i5**			
H	-0.682178	2.091061	1.205605	H	0.705243	-1.224489	1.235573
H	-1.545955	-0.840353	0.000000	H	1.489247	1.742932	0.000000
Si	0.032932	1.587841	0.000000	Ge	-0.031900	-0.697579	0.000000
H	1.395429	2.180268	0.000000	H	-1.432340	-1.311186	0.000000
H	-0.682178	2.091061	-1.205605	H	0.705243	-1.224489	-1.235573
Ge	0.032932	-0.867244	0.000000	Si	-0.031900	1.738554	0.000000
i2				**i3**			
Ge	-0.000002	-0.711841	0.000000	H	-0.426588	1.896073	0.388193
Si	-0.000002	1.518715	0.000000	H	-0.426505	1.896015	-0.388359
H	0.517835	-1.430902	1.257356	Si	1.492969	-0.033267	-0.000061
H	0.517835	-1.430902	-1.257356	H	2.317984	-1.267298	-0.000081
H	-0.517791	2.189357	-1.219182	H	2.367429	1.165117	-0.000161
H	-0.517791	2.189357	1.219182	Ge	-0.772934	-0.100755	0.000039
i8				**i6**			
Si	-1.569172	-0.212437	0.000066	Si	0.004931	1.805567	0.000000
H	-1.360903	1.613159	0.399747	H	-0.085814	0.537880	1.053310
H	-1.361040	1.613137	-0.399767	H	-0.085814	0.537880	-1.053310
H	1.628526	-1.203023	0.000046	H	-1.571151	-0.828272	0.000000
H	1.486177	1.283403	-0.000112	H	1.515952	1.677890	0.000000
Ge	0.674239	-0.010392	-0.000026	Ge	0.004931	-0.850104	0.000000
i7				**i4**			
Si	-0.060030	1.823087	0.000000	Si	-1.628959	-0.098023	-0.034009
H	-0.099904	0.532793	1.048844	H	-0.401905	-0.052404	1.269938
H	-0.099904	0.532793	-1.048844	H	-1.601839	1.419629	0.037325
H	1.509067	-0.889189	0.000000	H	1.540810	-1.238297	0.219137
H	1.452101	1.850221	0.000000	H	1.555351	1.233776	0.193407
Ge	-0.060030	-0.860933	0.000000	Ge	0.678531	0.000301	-0.038865

Table S4 Optimized Cartesian coordinates of transition states on the $GeSiH_4$ potential energy surface.

^{3}tsi0-i1				**^{3}tsi1-p3**			
Si	1.614644	-0.021538	0.000022	Ge	-0.077687	-0.843239	0.000000
H	2.036532	-1.443907	-0.000518	Si	-0.077687	1.620073	0.000000
H	2.072529	0.662938	1.225602	H	1.624237	-0.734293	0.000000
H	-0.152584	1.420846	-0.000227	H	1.318258	0.269760	0.000000
H	2.071709	0.663249	-1.225635	H	0.315553	2.383589	1.215607
Ge	-0.894788	-0.031300	0.000015	H	0.315553	2.383589	1.215607
^{1}tsi1-i2				**^{1}tsi1-i3**			
H	-2.558444	1.086739	0.038654	Ge	-0.790239	-0.066774	-0.003745
H	0.811247	1.372715	0.657895	H	0.121055	1.276889	0.624361
Si	-1.511293	0.023453	-0.019845	H	-0.472730	1.584715	-0.196230
H	-2.276753	-1.252072	-0.052239	Si	1.494491	-0.047021	-0.039082
H	0.198163	-0.877702	1.180131	H	2.338398	-1.212547	0.336531
Ge	0.780747	-0.020563	-0.048331	H	2.378043	1.146002	-0.097679
^{1}tsi1-i6				**^{1}tsi5-i6**			
Si	-1.732216	0.035465	0.002958	H	-0.380679	1.010743	-1.060838
H	-1.136832	0.688470	-1.199809	H	0.057808	0.272059	1.275254
H	-1.091153	0.610671	1.224909	H	-0.852462	-1.451431	-0.370940
H	-1.736919	-1.442520	-0.038698	Si	1.775251	-0.123482	-0.025800
H	0.921815	1.520750	0.012091	H	1.874882	1.389915	0.097583
Ge	0.852941	-0.058559	-0.001247	Ge	-0.798533	0.015858	0.013130
^{1}tsi1-p1				**^{1}tsi5-i4**			
H	-1.608392	-0.229662	1.398590	Ge	-0.678327	-0.000987	-0.021702
H	-2.185684	1.583901	-0.048929	H	1.672807	1.415185	0.033485
H	-1.489439	1.699656	0.282600	H	-1.537711	1.238777	-0.241742
H	0.693054	-1.497351	0.308309	H	-0.105907	0.086698	1.462693
Si	-1.555705	-0.238453	-0.118527	H	-1.546592	-1.253885	-0.057719
Ge	0.824073	0.055681	-0.008787	Si	1.658847	-0.103942	-0.035876
^{1}tsi4-i7				**^{1}tsi4-i8**			
Si	-1.778630	-0.116455	-0.014396	Si	-1.595015	-0.159881	-0.0038
H	-0.585232	0.971025	-0.001613	H	-0.907502	1.231699	0.60793
H	-2.579540	1.187220	0.025834	H	-1.464067	1.446236	-0.235446
H	0.199510	-0.700866	1.249663	Ge	0.674724	-0.016906	-0.021278
H	1.399505	1.271232	0.602403	H	1.607598	-1.170269	0.363706
Ge	0.827080	-0.034320	-0.052336	H	1.503024	1.271655	-0.00209

¹tsi4-p1				¹tsi4-i6			
Si	1.665773	0.081451	-0.022468	Si	-1.991974	0.065150	-0.004788
H	-1.389715	-0.614443	1.192876	H	-0.642691	0.856378	0.003414
H	-1.019258	1.529871	0.176316	H	-1.414638	-1.321579	-0.073781
H	-0.183474	1.317739	0.765549	H	0.421569	-0.715207	1.293458
H	1.765789	-1.346302	0.495160	H	1.299370	1.347849	0.571826
Ge	-0.702943	-0.063349	-0.072355	Ge	0.882001	-0.033735	-0.053996
¹tsi4-i2				¹tsi8-p6			
Ge	-0.684136	0.010004	-0.017700	Si	1.317395	-0.827534	-0.000073
H	1.622602	1.333327	0.523319	H	3.345379	2.832097	-0.371011
H	-1.726217	1.130863	0.171248	H	3.345019	2.832476	0.372028
H	1.022354	-0.802660	1.150398	H	-2.016367	-0.606841	0.001745
H	-1.504839	-1.289214	0.020656	H	-0.924283	1.659254	-0.001686
Si	1.605604	-0.049460	-0.092802	Ge	-0.693540	0.152140	-0.000002
¹tsi3-p3				¹tsi6-p1			
Ge	0.770143	-0.146286	-0.002175	H	0.870533	1.243483	-0.338754
H	0.522842	2.725988	-0.316638	H	0.591222	-0.058844	1.185888
H	0.554591	2.471842	0.388900	H	1.725967	1.453966	0.171371
H	-2.329211	-1.266718	0.045495	H	-0.734622	-1.535939	-0.100297
H	-2.362815	1.179028	-0.043134	Si	1.665709	-0.161108	-0.043798
Si	-1.502142	-0.030642	-0.000358	Ge	-0.805407	0.036026	-0.009532
¹tsi7-p1				¹tsi6-i7			
Si	1.655330	-0.165878	-0.040451	Si	1.823989	-0.008639	0.035934
H	-0.991286	1.504364	0.114666	H	1.217015	1.164033	-0.715453
H	0.640514	-0.000655	1.222723	H	1.003035	-1.053388	-0.734917
H	0.914603	1.283785	-0.316805	H	-0.990975	1.525047	-0.002185
H	1.803082	1.457137	0.074995	H	0.546646	0.056442	1.070240
Ge	-0.798173	-0.060073	-0.016540	Ge	-0.853486	-0.049099	-0.003774
¹tsi4-i8				¹tsi3-p2			
Si	-1.595015	-0.159881	-0.0038	H	-1.287599	-1.349673	-0.002601
H	-0.907502	1.231699	0.60793	H	1.646615	2.473969	-0.373741
H	-1.464067	1.446236	-0.235446	H	1.628779	2.486748	0.371218
Ge	0.674724	-0.016906	-0.021278	H	-2.906173	0.563568	-0.001799
H	1.607598	-1.170269	0.363706	Si	-1.476816	0.179499	0.000082
H	1.503024	1.271655	-0.00209	Ge	0.674806	-0.208987	0.000180

Table S5 Optimized Cartesian coordinates of singlet and triplet $GeSiH_2$ isomers.

^{1}p1				**^{1}p2**			
H	0.748325	0.494206	1.007738	Si	0.036907	1.439505	0.000000
H	0.748325	0.494206	-1.007738	H	-1.296005	0.516692	0.000000
Si	-0.032536	1.563668	0.000000	H	-0.401740	2.859415	0.000000
Ge	-0.032536	-0.714993	0.000000	Ge	0.036907	-0.735287	0.000000
^{1}p3				**^{1}p4**			
H	0.000000	1.228338	-2.305138	H	2.363056	-1.054599	-0.000225
H	0.000000	-1.228338	-2.305138	H	-1.752691	1.017379	-0.000244
Si	0.000000	0.000000	-1.472296	Ge	-0.664585	-0.061627	0.000009
Ge	0.000000	0.000000	0.788201	Si	1.475453	0.143521	0.000014
^{1}p5				**^{1}p6**			
H	-1.281845	0.469465	0.000000	H	0.000000	1.257578	1.479103
H	-0.537961	-2.040404	0.000000	H	0.000000	-1.257578	1.479103
Ge	0.039561	-0.624606	0.000000	Si	0.000000	0.000000	-1.620469
Si	0.039561	1.539880	0.000000	Ge	0.000000	0.000000	0.616511
^{3}p2				**^{3}p2'**			
H	0.564541	0.485478	1.131476	Si	0.058958	1.618521	0.000000
H	2.053945	1.254864	-0.448094	H	-1.521127	-0.621419	0.000000
Si	1.606176	-0.125989	-0.007605	H	-1.190960	2.454096	0.000000
Ge	-0.784530	0.000735	-0.018028	Ge	0.058958	-0.765374	0.000000
^{3}p3				**^{3}p4**			
H	0.000000	1.189641	-2.417513	H	2.083520	1.299230	-0.000013
H	0.000000	-1.189641	-2.417513	H	-1.265550	-1.406233	0.000005
Si	0.000000	0.000000	-1.520988	Ge	-0.728457	0.062345	0.000009
Ge	0.000000	0.000000	0.816527	Si	1.606617	-0.134859	-0.000019
^{3}p5				**^{3}p5'**			
H	0.532242	0.532113	1.098883	H	-1.465213	1.527332	0.000000
H	-1.065625	1.422233	-0.415554	H	-1.233544	-1.585212	0.000000
Si	1.683624	-0.005189	-0.045161	Ge	0.058669	-0.721165	0.000000
Ge	-0.719917	-0.058803	-0.001596	Si	0.058669	1.652510	0.000000
^{3}p6							
H	0.000000	1.228088	1.562916				
H	0.000000	-1.228088	1.562916				
Si	0.000000	0.000000	-1.687503				
Ge	0.000000	0.000000	0.640600				

Table S6 Vibrational frequencies and infrared intensities for intermediates and transition states on the $GeSiH_4$ potential energy surface.

^{3}i0			^{3}i1		
Normal modes	Frequency(cm^{-1})	IR Inten	Normal modes	Frequency(cm^{-1})	IR Inten
ν1	88.5329	0.1439	ν1	108.4758	0.0122
ν2	123.9691	0.092	ν2	354.789	3.1894
ν3	344.8639	36.1215	ν3	427.1758	16.2715
ν4	855.7807	49.2706	ν4	534.4745	6.9406
ν5	896.6555	432.2233	ν5	622.2915	12.3624
ν6	945.2195	76.7201	ν6	902.546	374.1409
ν7	962.3033	45.2833	ν7	953.9028	48.7959
ν8	1038.9291	62.6684	ν8	964.533	51.9019
ν9	1997.1713	456.3431	ν9	2149.865	105.3467
ν10	2268.9089	73.1122	ν10	2237.7138	79.0075
ν11	2291.7478	44.2233	ν11	2245.0519	83.078
ν12	2302.8652	63.9303	ν12	2264.663	82.0614
i1			i2		
Normal modes	Frequency(cm^{-1})	IR Inten			
ν1	100.2993	5.2743	ν1	327.1784	0.0711
ν2	321.1006	7.1257	ν2	333.05	16.7438
ν3	384.5733	27.3854	ν3	440.755	27.8825
ν4	402.6169	18.2771	ν4	494.2634	1.0557
ν5	682.2761	40.235	ν5	515.7432	0.1008
ν6	887.8983	280.1397	ν6	587.4619	0.0651
ν7	950.5216	58.4748	ν7	884.8144	120.1183
ν8	972.0197	40.2996	ν8	950.5633	63.1634
ν9	1989.8743	238.2734	ν9	2215.5047	72.5261
ν10	2209.1705	81.1528	ν10	2231.5996	71.5497
ν11	2218.0948	107.1126	ν11	2251.8542	60.6809
ν12	2236.1756	122.4834	ν12	2274.6104	91.7866

i3			i4		
Normal modes	Frequency(cm^{-1})	IR Inten	Normal modes	Frequency(cm^{-1})	IR Inten
ν1	234.6776	0.0082	ν1	375.6507	6.378
ν2	309.5452	13.7597	ν2	382.8358	3.4144
ν3	397.8346	0.9058	ν3	487.921	14.274
ν4	400.7122	26.2018	ν4	627.1465	4.2839
ν5	426.2251	5.1965	ν5	683.7536	23.3231
ν6	470.8608	4.9367	ν6	856.2638	89.8408
ν7	509.4474	1.3433	ν7	905.9532	79.4537
ν8	942.5742	89.8087	ν8	1032.8504	347.8229
ν9	965.5959	1.3643	ν9	1548.308	113.9592
ν10	2231.5821	90.6644	ν10	2071.5658	153.304
ν11	2253.6083	77.4458	ν11	2182.9325	171.6097
ν12	3839.5525	46.4027	ν12	2200.4929	142.0354

i5			i6		
Normal modes	Frequency(cm^{-1})	IR Inten	Normal modes	Frequency(cm^{-1})	IR Inten
ν1	106.5106	6.0046	ν1	270.7562	1.9997
ν2	331.496	3.7756	ν2	341.6229	0.0721
ν3	357.7195	23.5898	ν3	673.5245	12.3263
ν4	399.7581	16.9337	ν4	792.4411	43.1035
ν5	704.9804	50.8052	ν5	859.5441	3.7885
ν6	816.9836	228.5068	ν6	869.5972	116.8275
ν7	904.0274	35.9425	ν7	1254.3172	28.1777
ν8	916.3665	29.7165	ν8	1432.7155	970.0203
ν9	2067.3105	169.9447	ν9	1449.6728	10.5927
ν10	2175.8728	93.8744	ν10	1637.6428	127.2516
ν11	2185.0949	115.6872	ν11	2006.7015	209.3059
ν12	2203.8977	138.9905	ν12	2089.2154	214.5484

	i7			i8	
Normal modes	Frequency(cm^{-1})	IR Inten	Normal modes	Frequency(cm^{-1})	IR Inten
ν1	321.6816	1.8611	ν1	197.2229	0.0032
ν2	364.0318	0.0418	ν2	343.366	25.2087
ν3	612.9545	0.6145	ν3	417.1604	0.302
ν4	718.3987	72.4085	ν4	434.3649	0.2719
ν5	858.9592	16.8212	ν5	478.2319	15.1943
ν6	887.6794	37.9392	ν6	571.3735	0.5529
ν7	1240.4312	33.1283	ν7	573.521	31.8526
ν8	1367.1489	10.4389	ν8	891.1802	80.8711
ν9	1394.0907	1383.257	ν9	1211.8235	0.1479
ν10	1614.491	58.3571	ν10	2191.8863	94.4937
ν11	2029.6655	174.2235	ν11	2211.3123	99.9394
ν12	2107.7169	219.6778	ν12	3477.2524	155.1012

	^{3}tsi0-i1			^{1}tsi4-i8	
Normal modes	Frequency(cm^{-1})	IR Inten	Normal modes	Frequency(cm^{-1})	IR Inten
ν1	897.8683*i*	15.4559	ν1	948.3557*i*	299.9279
ν2	248.5548	15.4911	ν2	335.2996	24.7723
ν3	279.1445	0.0916	ν3	396.4907	2.0795
ν4	500.8451	10.0374	ν4	450.2450	20.9694
ν5	538.0741	2.9411	ν5	475.2115	3.9687
ν6	888.8106	341.2015	ν6	716.2571	96.3495
ν7	949.0133	78.8128	ν7	833.9033	3.8152
ν8	957.1087	50.5071	ν8	915.4912	169.9459
ν9	1777.1398	264.4795	ν9	1683.4222	88.5334
ν10	2235.4791	63.0624	ν10	1822.5210	119.1880
ν11	2275.706	61.1296	ν11	2105.5641	137.9249
ν12	2288.8162	65.7703	ν12	2129.9131	142.6454

^{1}tsi8-p6			^{1}tsi1-i2		
Normal modes	Frequency(cm^{-1})	IR Inten	Normal modes	Frequency(cm^{-1})	IR Inten
ν1	48.1613*i*	0.0338	ν1	639.2174*i*	8.2193
ν2	18.9973	0.001	ν2	288.5815	10.2264
ν3	23.6665	0.0066	ν3	380.8995	0.5312
ν4	44.8545	0.0016	ν4	473.3039	10.973
ν5	133.1055	0.4438	ν5	629.1034	1.3403
ν6	265.8317	23.565	ν6	661.4611	13.7573
ν7	341.3327	3.538	ν7	887.059	120.0655
ν8	448.4465	5.7686	ν8	1011.4793	179.1402
ν9	850.4633	53.8778	ν9	1854.0257	102.5782
ν10	2194.7775	60.094	ν10	2044.5161	165.5512
ν11	2214.741	77.4021	ν11	2195.5577	169.9123
ν12	4403.2281	0.3357	ν12	2233.3786	116.7173

^{1}tsi1-i6			^{1}tsi1-i3		
Normal modes	Frequency(cm^{-1})	IR Inten	Normal modes	Frequency(cm^{-1})	IR Inten
ν1	772.072*i*	267.8143	ν1	1255.9279*i*	261.0567
ν2	89.4438	4.7043	ν2	371.8315	12.9652
ν3	253.2881	6.9219	ν3	409.5917	8.4729
ν4	456.4632	1.7899	ν4	484.5688	10.3691
ν5	496.3963	2.949	ν5	539.0406	1.9148
ν6	676.3926	12.7899	ν6	722.3905	67.5552
ν7	899.2764	56.3754	ν7	873.2762	34.7732
ν8	922.8251	52.6035	ν8	991.3911	185.1649
ν9	1982.1146	275.6465	ν9	1627.3565	84.1146
ν10	2182.1182	7.9315	ν10	1753.4091	115.3969
ν11	2203.2097	30.4066	ν11	2222.2287	116.4553
ν12	2271.0462	58.7677	ν12	2238.9948	96.6778

	¹tsi1-p1			¹tsi5-i6	
Normal modes	Frequency(cm^{-1})	IR Inten	Normal modes	Frequency(cm^{-1})	IR Inten
ν1	196.0791*i*	18.4028	ν1	783.8542*i*	198.9906
ν2	232.4585	9.7509	ν2	151.316	20.4089
ν3	327.6738	4.5233	ν3	258.5528	4.3125
ν4	387.9323	18.1035	ν4	441.5004	3.1917
ν5	460.7338	5.9704	ν5	493.1415	3.9195
ν6	497.5473	18.3106	ν6	696.4869	20.7807
ν7	570.1917	15.7552	ν7	832.1806	55.0832
ν8	790.3593	15.0133	ν8	870.4607	48.385
ν9	1095.0863	13.0764	ν9	2062.5635	204.5799
ν10	1938.5043	211.1755	ν10	2109.6707	26.5916
ν11	2071.7009	125.83	ν11	2216.0737	24.0538
ν12	3788.3919	32.8787	ν12	2251.6592	57.8948

	¹tsi4-i5			¹tsi2-i4	
Normal modes	Frequency(cm^{-1})	IR Inten	Normal modes	Frequency(cm^{-1})	IR Inten
ν1	350.0858*i*	44.3439	ν1	622.0056*i*	5.187
ν2	386.4372	11.3558	ν2	320.8406	8.8187
ν3	396.0269	4.149	ν3	381.9466	2.2976
ν4	528.1065	1.1787	ν4	485.2037	10.0495
ν5	697.5853	36.2963	ν5	644.3224	9.7002
ν6	784.3743	194.0426	ν6	670.8897	12.4264
ν7	856.295	25.2262	ν7	920.3636	23.3982
ν8	905.7688	68.4179	ν8	959.2906	240.5259
ν9	1905.4249	88.0021	ν9	1858.669	83.0411
ν10	2069.3203	163.3038	ν10	2090.8935	127.7667
ν11	2213.1277	129.9502	ν11	2138.9517	190.716
ν12	2225.0539	123.8164	ν12	2177.0042	154.0041

^{1}tsi4-i6			^{1}tsi4-i7		
Normal modes	Frequency(cm^{-1})	IR Inten	Normal modes	Frequency(cm^{-1})	IR Inten
ν1	515.225*i*	28.0376	ν1	573.8469*i*	2.9802
ν2	160.8496	7.593	ν2	179.9187	13.2418
ν3	437.4086	3.0951	ν3	426.2898	8.361
ν4	572.464	2.3521	ν4	557.7322	5.2826
ν5	680.3748	10.2202	ν5	642.634	46.5469
ν6	787.3064	88.4886	ν6	828.7775	39.8638
ν7	902.0784	143.9014	ν7	887.9074	225.1965
ν8	1242.7938	110.9944	ν8	1421.2253	39.1623
ν9	1920.9954	510.7832	ν9	1707.9065	273.1255
ν10	1962.2591	188.8736	ν10	1906.8979	98.6462
ν11	2007.7595	230.2912	ν11	2011.2177	231.3702
ν12	2161.5992	103.1927	ν12	2026.2133	283.9492

^{1}tsi4-i8			^{1}tsi4-p1		
Normal modes	Frequency(cm^{-1})	IR Inten	Normal modes	Frequency(cm^{-1})	IR Inten
ν1	-1069.7605	334.6727	ν1	1186.7131*i*	340.829
ν2	352.6502	24.0425	ν2	223.2778	2.4442
ν3	414.2086	2.1795	ν3	383.6753	8.9794
ν4	477.8425	15.7505	ν4	393.9392	28.9538
ν5	498.0375	8.0878	ν5	501.2732	2.2298
ν6	738.3318	83.2244	ν6	684.1972	18.3326
ν7	832.8722	10.6747	ν7	824.2284	91.4607
ν8	926.8019	169.0173	ν8	1004.1401	4.835
ν9	1704.1056	84.4056	ν9	1741.1441	133.2642
ν10	1831.291	99.1154	ν10	1908.177	51.2137
ν11	2176.0301	120.9505	ν11	2060.1151	187.8063
ν12	2191.7211	128.3982	ν12	2132.7568	153.6505

	[1]tsi6-i7			[1]tsi6-p1	
Normal modes	Frequency(cm^{-1})	IR Inten	Normal modes	Frequency(cm^{-1})	IR Inten
ν1	578.6014*i*	15.3067	ν1	1023.5036*i*	283.6149
ν2	272.4395	24.4869	ν2	334.7603	3.0401
ν3	592.2332	4.5011	ν3	533.0467	34.7752
ν4	639.383	77.3493	ν4	634.2275	12.1358
ν5	707.7029	9.7959	ν5	746.1538	6.9007
ν6	962.9721	54.735	ν6	816.0274	22.8049
ν7	994.2154	32.7851	ν7	953.5765	36.5187
ν8	1200.4529	216.2624	ν8	1136.8712	277.9588
ν9	1558.1897	89.3089	ν9	1587.9825	82.771
ν10	1972.1372	142.6101	ν10	1827.8286	57.5316
ν11	1999.9151	219.6758	ν11	1855.7799	164.8704
ν12	2084.8233	114.7142	ν12	1988.7422	244.7242

	[1]tsi7-p1			[1]tsi3-p3	
Normal modes	Frequency(cm^{-1})	IR Inten	Normal modes	Frequency(cm^{-1})	IR Inten
ν1	858.6787*i*	358.4967	ν1	150.6998	0.7364
ν2	322.5287	4.113	ν2	150.6998	0.7364
ν3	550.7957	4.5701	ν3	203.5471	0.3656
ν4	601.6044	8.2431	ν4	265.6548	0.3034
ν5	662.7536	9.2036	ν5	302.697	19.6607
ν6	796.1927	171.7308	ν6	350.9548	1.5787
ν7	908.018	183.6593	ν7	370.274	4.4637
ν8	1037.1706	134.2706	ν8	414.9665	9.5097
ν9	1615.7017	114.4255	ν9	903.1745	72.3248
ν10	1789.888	53.4623	ν10	2185.9627	71.4929
ν11	1897.0296	342.5702	ν11	2217.9365	71.3373
ν12	1962.4111	255.9812	ν12	4073.0344	5.2024

[1]tsi2-p3			[1]tsi2-p6		
Normal modes	Frequency(cm^{-1})	IR Inten	Normal modes	Frequency(cm^{-1})	IR Inten
ν1	248.1389	0.197	ν1	234.5356	0.5608
ν2	248.1389	0.197	ν2	234.5356	0.5608
ν3	308.6449	17.1208	ν3	309.5838	14.0144
ν4	383.5444	1.1283	ν4	366.7626	1.1264
ν5	413.9514	4.5904	ν5	383.0897	6.2805
ν6	446.8379	7.6674	ν6	426.3445	1.6112
ν7	469.2685	1.7128	ν7	457.1131	3.7025
ν8	632.0797	9.3874	ν8	573.8512	10.3488
ν9	937.0827	86.0658	ν9	872.6517	66.5968
ν10	2231.5197	87.6945	ν10	2196.7311	81.9783
ν11	2254.3549	75.1637	ν11	2216.564	87.7769
ν12	3927.9499	18.6958	ν12	3999.6251	9.4842

[1]tsi3-p2		
Normal modes	Frequency(cm^{-1})	IR Inten
ν1	-321.2236	21.1019
ν2	41.6942	0.0236
ν3	102.1843	0.2704
ν4	192.3322	1.4226
ν5	215.8936	2.7195
ν6	229.2047	24.5132
ν7	363.267	0.1838
ν8	475.3189	17.7907
ν9	846.9806	62.3061
ν10	1970.3894	37.4572
ν11	2254.6814	70.0887
ν12	4367.4533	5.15

Table S7 Vibrational frequencies and infrared intensities for singlet and triplet $GeSiH_2$ isomers.

$^{1}p1$			$^{1}p2$		
Normal modes	Frequency(cm^{-1})	IR Inten	Normal modes	Frequency(cm^{-1})	IR Inten
ν1	428.8308	1.123	ν1	161.791	40.9649
ν2	886.1585	41.8767	ν2	418.3026	9.5222
ν3	1057.8819	0.0644	ν3	502.902	16.6426
ν4	1157.0873	408.603	ν4	1036.6607	136.1689
ν5	1539.9872	22.2627	ν5	1681.187	57.9134
ν6	1616.1935	14.8875	ν6	2219.4472	86.3138

$^{1}p3$			$^{1}p4$		
Normal modes	Frequency(cm^{-1})	IR Inten	Normal modes	Frequency(cm^{-1})	IR Inten
ν1	269.4228	27.5913	ν1	254.3528	37.2934
ν2	346.2989	4.2418	ν2	272.0364	42.0012
ν3	427.3502	11.3393	ν3	468.3098	0.3608
ν4	908.1521	70.8488	ν4	603.4817	0.2239
ν5	2226.275	65.1248	ν5	2163.9268	67.3288
ν6			ν6	2202.4786	80.544

$^{1}p5$			$^{1}p6$		
Normal modes	Frequency(cm^{-1})	IR Inten	Normal modes	Frequency(cm^{-1})	IR Inten
ν1	121.0555	38.5037	ν1	265.2054	23.3913
ν2	430.2667	6.4697	ν2	341.7188	3.6047
ν3	544.4562	4.0504	ν3	448.2659	5.8761
ν4	1078.8756	132.3389	ν4	850.7026	53.9826
ν5	1617.9979	77.0469	ν5	2194.3645	59.9746
ν6	2163.4326	113.3209	ν6	2214.1777	77.1223

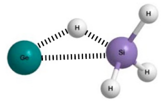
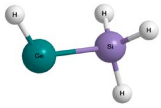
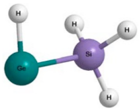
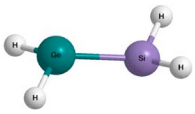
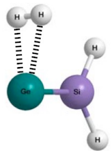
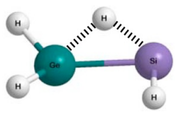
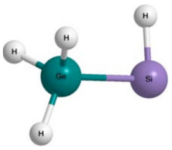
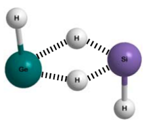
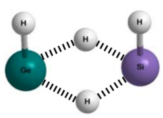
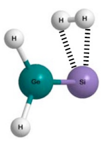
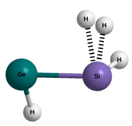
$^{3}p2$			$^{3}p2'$		
Normal modes	Frequency(cm^{-1})	IR Inten	Normal modes	Frequency(cm^{-1})	IR Inten
ν1	311.9393	3.9191	ν1	348.4722	10.9227
ν2	411.3717	6.6213	ν2	398.1668	6.5274
ν3	671.924	45.5495	ν3	413.7354	1.2663
ν4	988.5165	203.0177	ν4	618.1099	29.1263
ν5	1498.9486	120.0511	ν5	1950.421	208.7265
ν6	2064.8541	205.7534	ν6	2128.6624	138.3514

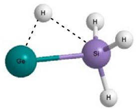
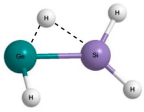
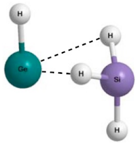
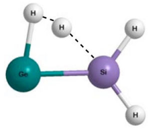
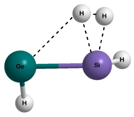
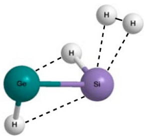
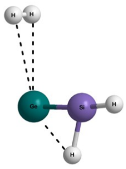
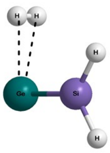
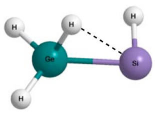
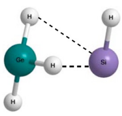
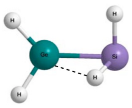
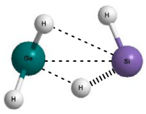
^{3}p3			^{3}p4		
Normal modes	Frequency(cm^{-1})	IR Inten	Normal modes	Frequency(cm^{-1})	IR Inten
ν1	320.099	2.8532	ν1	254.3528	37.2934
ν2	378.5321	11.2089	ν2	272.0364	42.0012
ν3	403.6427	8.0625	ν3	468.3098	0.3608
ν4	974.9797	114.2199	ν4	603.4817	0.2239
ν5	2203.1935	123.9045	ν5	2163.9268	67.3288
ν6	2215.3477	106.4332	ν6	2202.4786	80.544

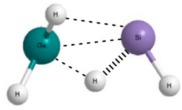
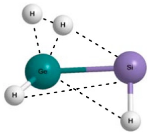
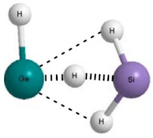
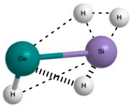
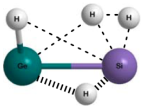
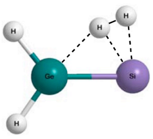
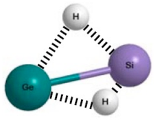
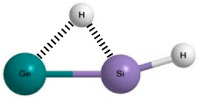
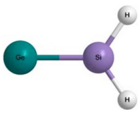
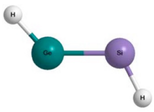
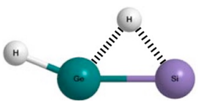
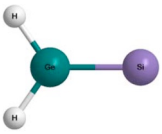
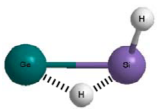
^{3}p5			^{3}p5'		
Normal modes	Frequency(cm^{-1})	IR Inten	Normal modes	Frequency(cm^{-1})	IR Inten
ν1	302.3422	1.1082	ν1	346.0575	6.968
ν2	398.9538	3.6748	ν2	397.3013	6.2707
ν3	647.3822	21.504	ν3	639.942	32.7738
ν4	1060.9088	312.3437	ν4	1204.0167	39.7483
ν5	1410.5127	90.6221	ν5	2023.8734	127.5141
ν6	1979.505	260.4835	ν6	2055.7875	206.3461

^{3}p6		
Normal modes	Frequency(cm^{-1})	IR Inten
ν1	297.4433	2.8464
ν2	386.7002	9.8147
ν3	391.848	7.6901
ν4	907.7259	94.9262
ν5	2155.408	126.9477
ν6	2164.0259	134.7064

Table S8 Rotational constants and dipole moments of singlet and triplet species on the $GeSiH_4$ potential energy surface calculated at the CCSD/cc-pVTZ//CCSD(T)/CBS level of theory.

		Dipole Moment (Debye)	Rotational Constants (GHz)		
			A	B	C
	^{3}**i0**	1.666642	82.81214	2.23962	2.23899
	^{3}**i1**	0.344962	67.45812	3.77325	3.72816
	**i1**	0.338612	60.82464	3.57142	3.51066
	**i2**	0.007009	72.89117	4.41314	4.21179
	**i3**	0.732032	45.63842	4.31777	3.96338
	**i4**	1.228708	70.8561	4.30446	4.17977
	**i5**	0.340602	60.20896	3.85028	3.78569
	**i6**	0.522114	72.6267	3.36793	3.31305
	**i7**	0.664295	73.23399	3.28654	3.23467
	**i8**	0.916982	52.39189	4.54191	4.20196
	**i9**	1.28278	49.34322	3.88007	3.72463

	**^{3}tsi0-i1**	1.365896	62.31978	3.46351	3.41543
	**^{1}tsi1-i2**	1.932421	67.83238	4.13544	4.02005
	**^{1}tsi1-i6**	0.5109	59.84166	3.46411	3.40539
	**^{1}tsi1-i3**	0.530436	64.43605	4.23644	4.01231
	**^{1}tsi1-i9**	0.860056	56.0453	3.92597	3.79437
	**^{1}tsi9-p1**	1.221838	43.62492	3.90386	3.71239
	**^{1}tsi3p2**	0.905717	28.5475	4.55731	3.94711
	**^{1}tsi3p3-V**	0.621296	39.40287	4.32437	3.91428
	**^{1}tsi4-i5**	0.733988	65.99955	4.18751	4.08213
	**^{1}tsi5-i6**	0.229708	59.78456	3.55713	3.49404
	**^{1}tsi2-i4**	2.01782	69.20688	4.31105	4.18183
	**^{1}tsi4-i6**	1.805519	70.55276	2.89975	2.85354

	**^{1}tsi4-i7**	1.088718	72.91728	3.3838	3.32233
	**^{1}tsi4-p1**	0.649032	54.68173	4.11947	3.98691
	**^{1}tsi6-i7**	1.043194	70.21205	3.32511	3.26681
	**^{1}tsi6-p1**	0.656955	60.87899	3.85691	3.71338
	**^{1}tsi7-p1**	0.895551	59.22088	3.8877	3.73862
	**^{1}tsi4-i8**	0.807668	64.88432	4.47055	4.22329
	**^{1}p1**	0.60838	155.7688	4.71175	4.67473
	**^{1}p2**	0.564125	264.67163	4.79511	4.70978
	**^{1}p3**	0.0146	166.17511	4.36451	4.25281
	**^{1}p4**	0.194435	180.24987	4.95528	4.8227
	**^{1}p5**	0.997306	245.52735	5.08487	4.9817
	**^{1}p6**	0.1033	158.53753	4.77351	4.63398
	**^{3}p2**	0.093416	137.52377	4.11588	4.09406

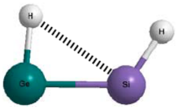
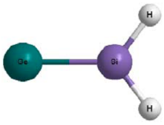
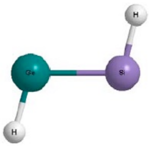
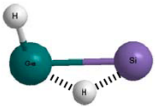
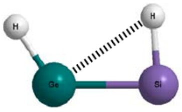
	**^{3}p2'**	0.412243	127.45083	4.13437	4.00447
	**^{3}p3**	0.9113	177.16197	4.06983	3.97844
	**^{3}p4**	0.097236	118.1625	4.3191	4.16679
	**^{3}p5**	0.497789	128.45133	4.20863	4.1716
	**^{3}p5'**	0.575122	128.14564	4.23835	4.10266
	**^{3}p6**	1.0739	166.24279	4.40137	4.28784

Table S9 Rotational constants (GHz) of singlet and triplet $GeSiH_2$ isomers calculated at the fc-CCSD(T)/cc-pVTZ level of theory.

	A	B	C
^{1}p1	156.8393205	4.6562251	4.6191175
^{1}p2	262.6009484	4.7362681	4.6523582
^{1}p3	165.5441822	4.3217001	4.2117482
^{1}p4	177.7806127	4.9080743	4.7762151
^{1}p5	244.1216288	5.0208403	4.9196579
^{1}p6	158.1929293	4.7294949	4.5922019
^{3}p2	136.8443462	4.1325387	4.1108545
^{3}p3	176.9804804	4.0518040	3.9611179
^{3}p4	117.8986827	4.3092548	4.1573034
^{3}p5	127.8109516	4.2298253	4.1927233