ELECTRONIC SUPPLEMENTARY INFORMATION

for

Hydrogermylation initiated by trialkylborohydrides: a living anionic mechanism

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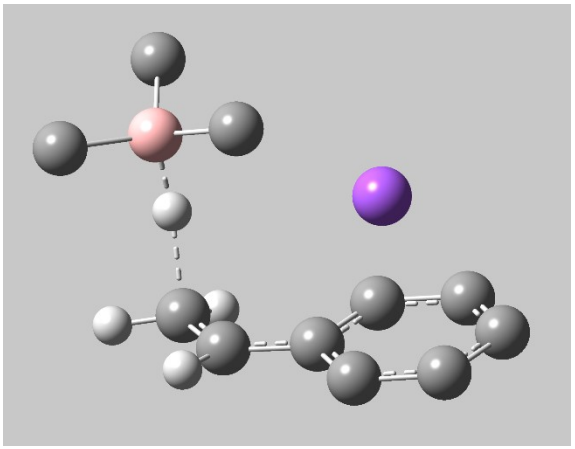
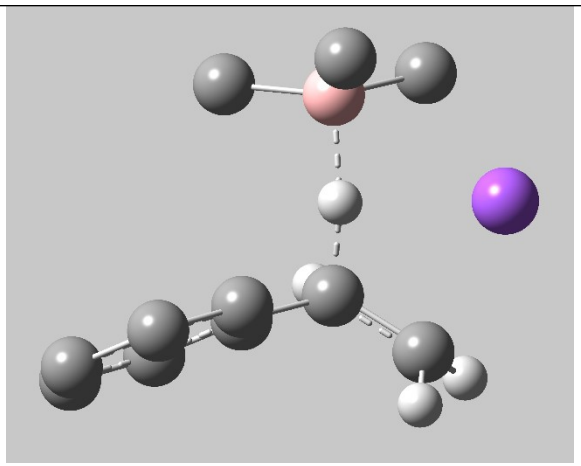
Geometric structures of calculated transition states

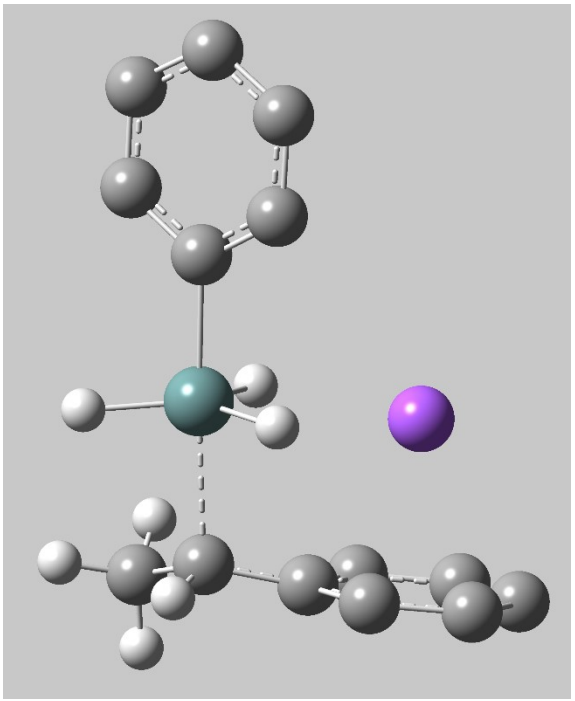
Most hydrogen atoms were omitted for clarity.



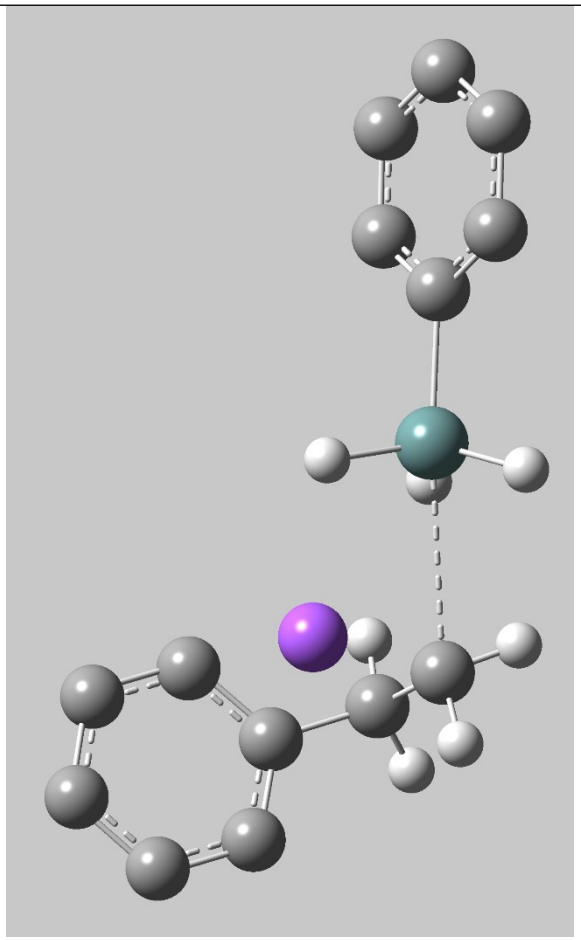
2M (phenylgermane)



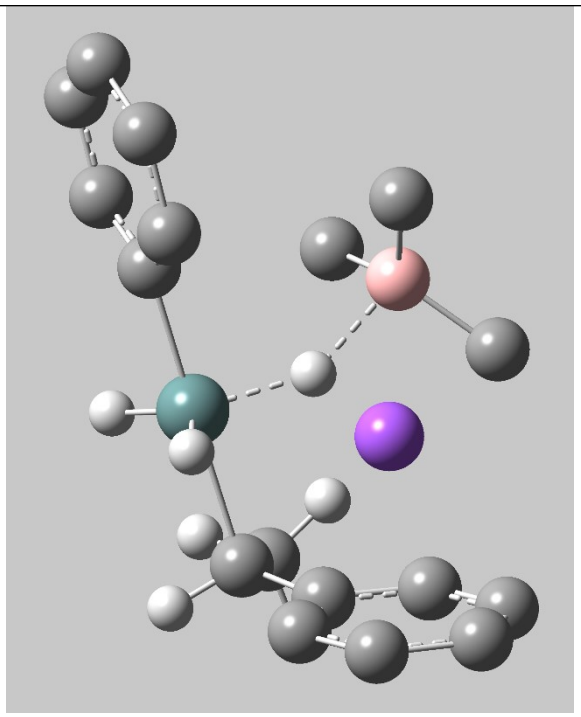
2aM (phenylgermane)



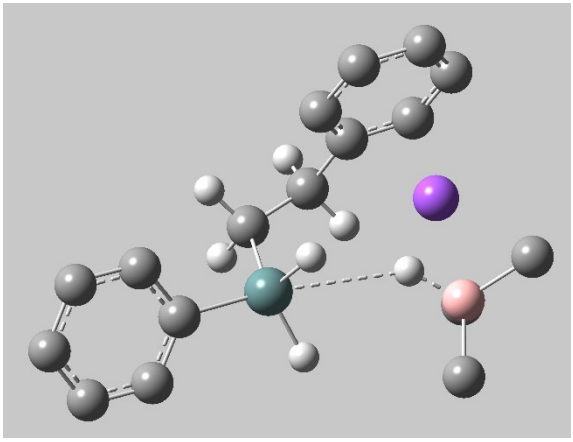
7M (phenylgermane)



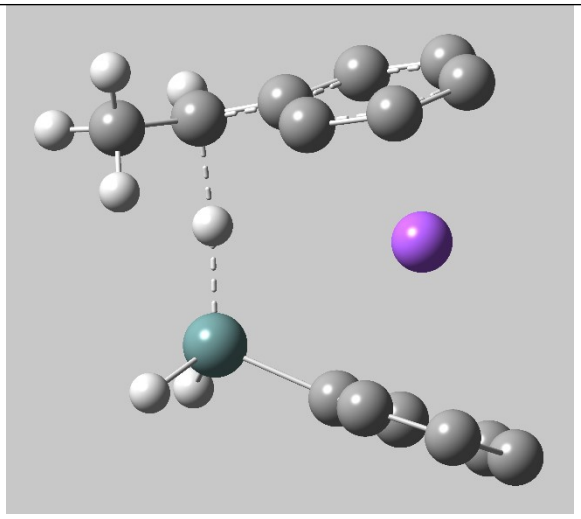
6aM (phenylgermane)



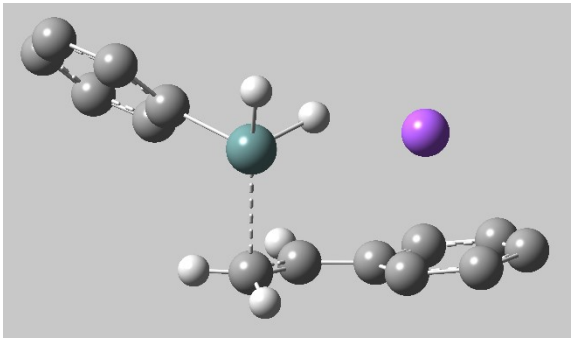
9M (phenylgermane)



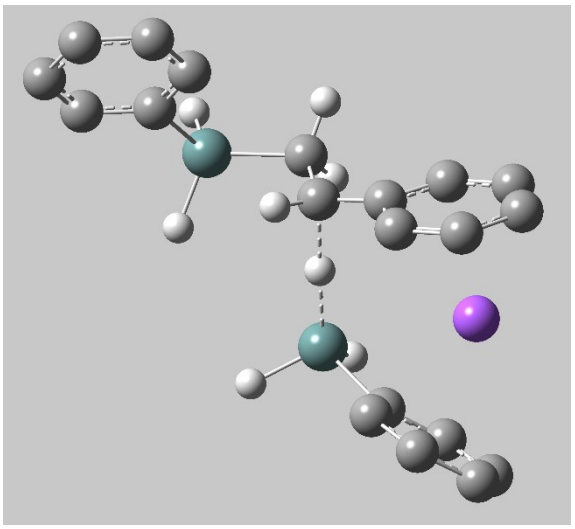
10aM (phenylgermane)



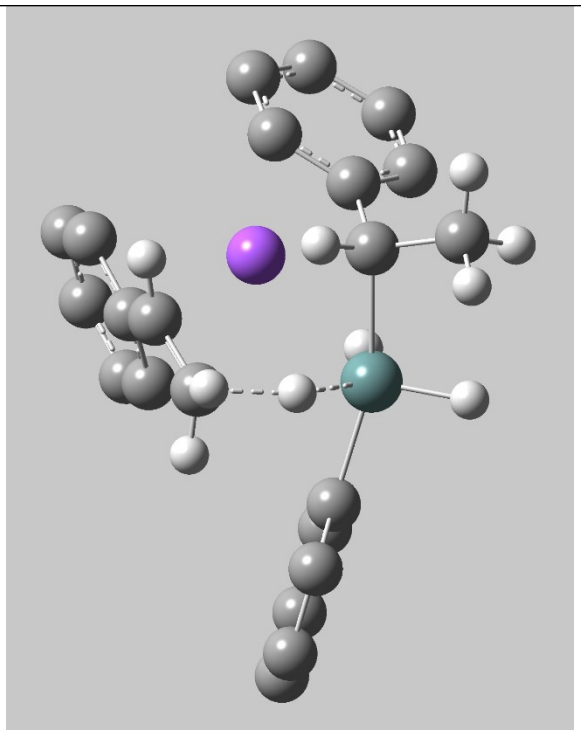
6L (phenylgermane)



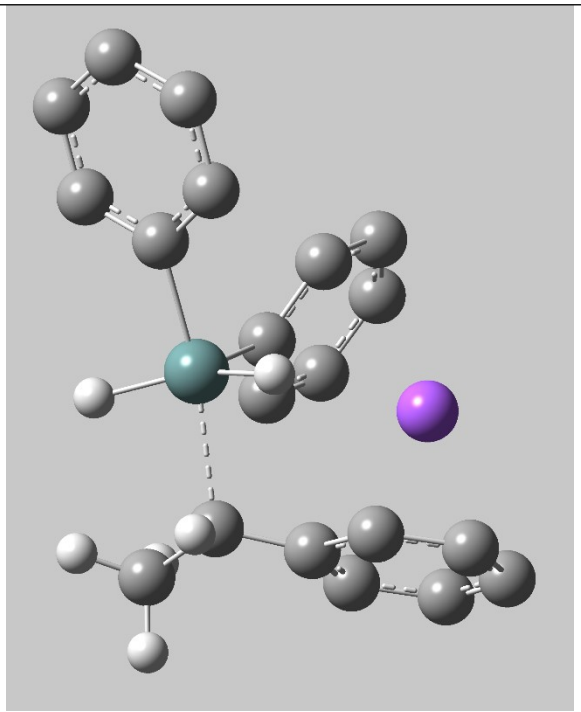
10L (phenylgermane)



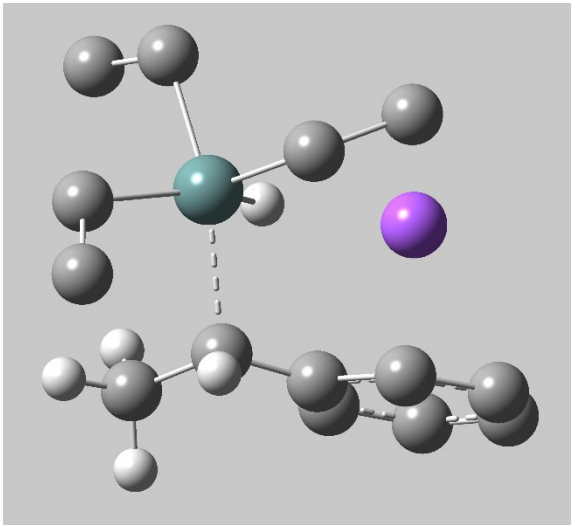
13L (phenylgermane)



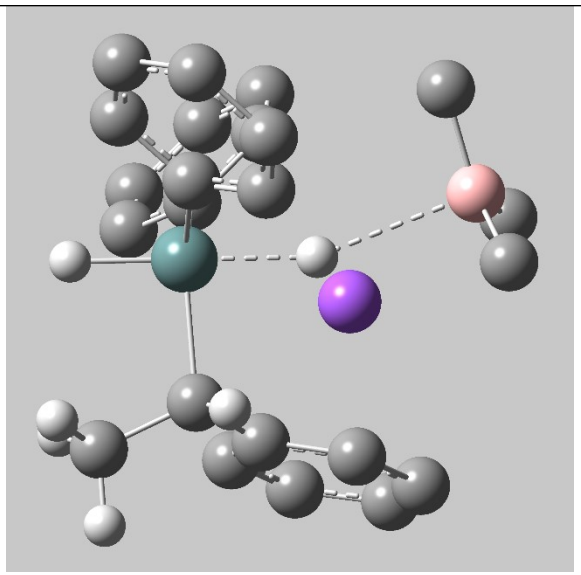
9S (phenylgermane)



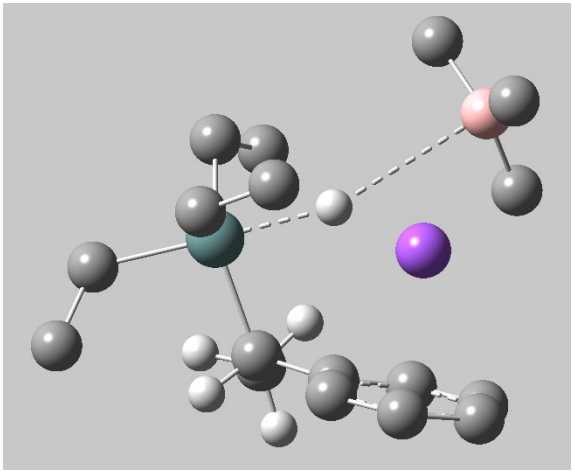
6M (diphenylgermane)



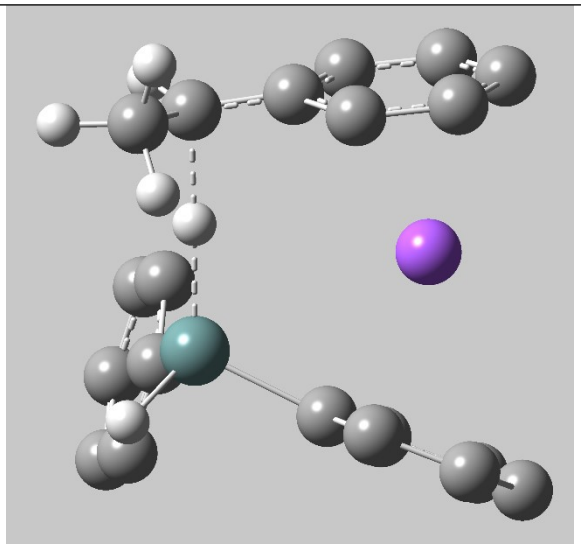
6M (triethylgermane)



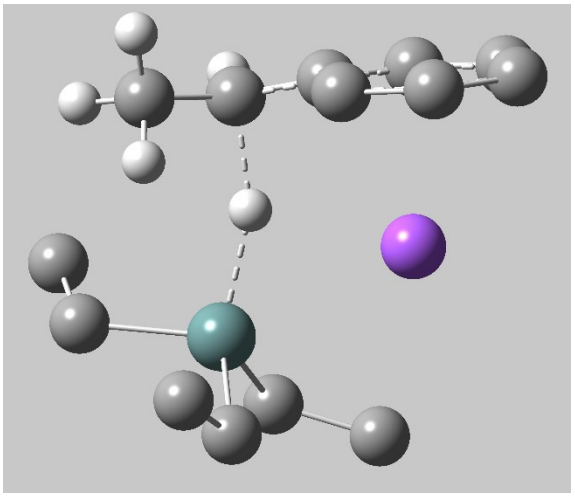
9M (diphenylgermane)



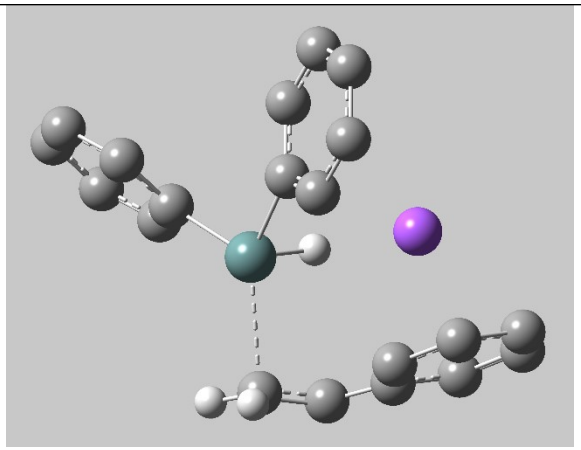
M (triethylgermane)



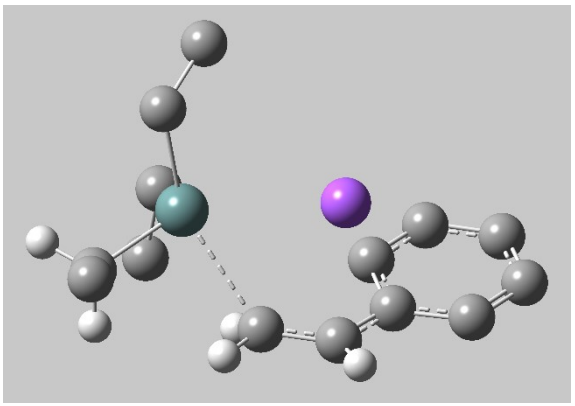
6L (diphenylgermane)



6L (triethylgermane)



10L (diphenylgermane)



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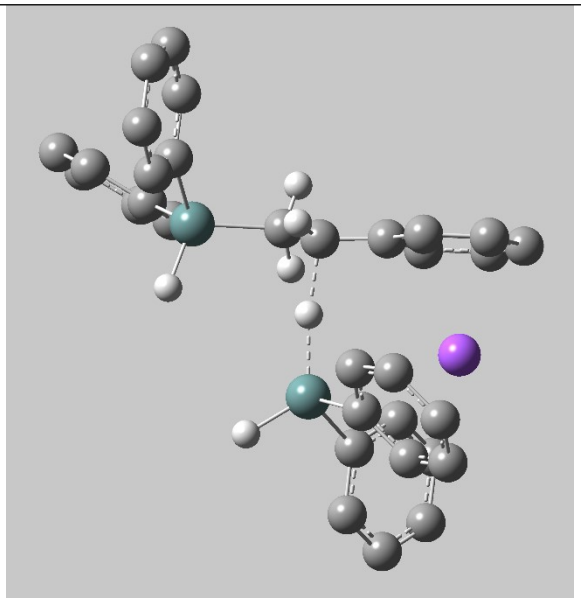
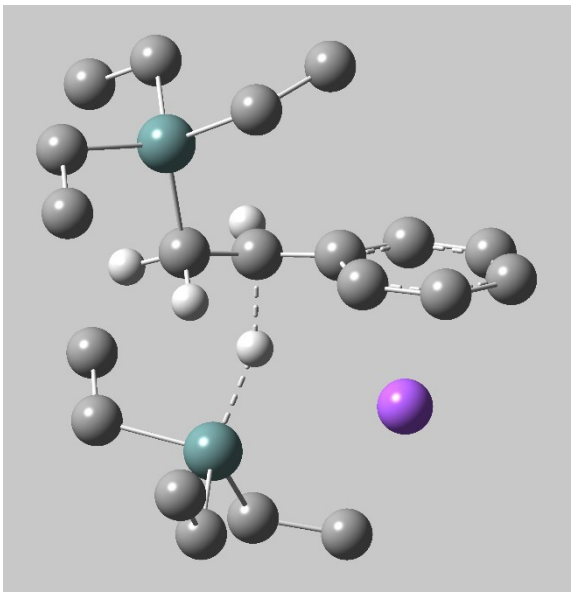


13L (diphenylgermane)



13L (triethylgermane)

Cartesian coordinates, Mulliken and APT charges of all atoms, and absolute energies at all stationary points

All coordinates are given in ångströms.

All energies are given in hartrees.

All computations performed at M06-2X/6-31++G(d,p)/LANL2DZdp level of theory (LANL2DZdp basis set for Si and Ge atoms and 6-31++G(d,p) for other atoms) in toluene solvent (PCM).

Component molecules and ions

Styrene

Electronic energy: -309.52191

Electronic energy + zero-point energy: -309.38764

Electronic energy + thermal energy correction: -309.37844

Electronic energy + thermal enthalpy correction: -309.37725

Electronic energy + thermal free energy correction: -309.42718

Table S01. Cartesian coordinates, Mulliken and APT charges of all atoms at **styrene**.

Symbol	X	Y	Z	Mulliken	APT
C	1.780057	-1.042844	-0.000436	0.323588	-0.017353
C	0.406903	-1.281326	-0.000014	-0.816066	-0.080136
C	2.259356	0.265026	-0.000289	-0.515173	-0.069084
C	-0.511471	-0.223716	0.000408	1.297441	0.047501
C	-0.014625	1.088505	0.000562	-1.446540	-0.084226
C	1.354787	1.329411	0.000184	0.386121	-0.037724
H	2.473140	-1.878318	-0.000951	0.164729	0.038071
H	3.327586	0.456765	-0.000426	0.145247	0.042962
H	1.719887	2.351884	0.000276	0.177083	0.037016
H	-0.701104	1.929291	0.000821	0.043929	0.045572
H	0.036731	-2.303435	-0.000188	0.116777	0.042650
C	-1.954308	-0.535184	0.000724	-0.034288	0.127216
C	-2.964541	0.339188	-0.000908	-0.255580	-0.209170
H	-2.190259	-1.598490	0.002181	0.115982	0.015937
H	-2.810355	1.413956	-0.002530	0.134337	0.054622
H	-3.992581	-0.006024	-0.000577	0.162414	0.046145

Phenylsilane

Electronic energy: -237.22628

Electronic energy + zero-point energy: -237.10972

Electronic energy + thermal energy correction: -237.09922

Electronic energy + thermal enthalpy correction: -237.09804

Electronic energy + thermal free energy correction: -237.15192

Table S02. Cartesian coordinates, Mulliken and APT charges of all atoms at **phenylsilane**.

Symbol	X	Y	Z	Mulliken	APT
H	0.276323	-2.153142	-0.023532	0.118562	0.034573
H	2.842036	-1.208620	-0.676812	-0.049987	-0.303408
H	-2.187274	-2.148453	0.004437	0.159645	0.033678
C	-0.253008	-1.203120	-0.010754	-0.749798	-0.042113
C	-1.647515	-1.206425	0.003286	0.097640	-0.053995
H	2.852898	0.000254	1.392079	-0.076807	-0.323370
Si	2.341639	-0.000014	0.006405	0.148960	1.331140
C	0.469309	-0.000201	-0.014643	0.924133	-0.362202
C	-2.346589	0.000168	0.011356	-0.304125	-0.022797
H	-3.432224	0.000302	0.019762	0.156053	0.039806
H	2.841667	1.208558	-0.677123	-0.049993	-0.303396
C	-0.252719	1.202934	-0.010761	-0.750167	-0.042198
C	-1.647220	1.206597	0.003289	0.097730	-0.053967
H	0.276848	2.152823	-0.023566	0.118502	0.034575
H	-2.186759	2.148751	0.004448	0.159652	0.033674

Phenylgermane

Electronic energy: -237.09180

Electronic energy + zero-point energy: -236.97769

Electronic energy + thermal energy correction: -236.96785

Electronic energy + thermal enthalpy correction: -236.96667

Electronic energy + thermal free energy correction: -237.01933

Table S03. Cartesian coordinates, Mulliken and APT charges of all atoms at **phenylgermane**.

Symbol	X	Y	Z	Mulliken	APT
H	-0.314632	-2.153341	-0.019914	0.130051	0.034491
H	2.344976	-1.188081	-0.829784	-0.105206	-0.338376
H	-2.777460	-2.149465	0.004000	0.161587	0.030602
C	-0.843645	-1.202922	-0.008718	-0.868897	-0.060151
C	-2.238432	-1.206933	0.002977	0.150012	-0.049331
H	2.361380	-0.137855	1.441988	-0.137127	-0.354530
Ge	1.829963	0.000121	0.002550	0.166384	1.453247

C	-0.125002	0.001046	-0.012454	1.045890	-0.344950
C	-2.938869	-0.000838	0.009655	-0.361311	-0.030262
H	-4.024500	-0.001595	0.016685	0.154389	0.038821
H	2.335925	1.326899	-0.591519	-0.091737	-0.335383
C	-0.844954	1.203611	-0.008815	-0.679760	-0.063124
C	-2.240346	1.205671	0.002863	0.136929	-0.046719
H	-0.316534	2.154164	-0.019923	0.137403	0.035064
H	-2.780495	2.147581	0.003810	0.161392	0.030603

Diphenylgermane

Electronic energy: -468.06503

Electronic energy + zero-point energy: -467.86681

Electronic energy + thermal energy correction: -467.84866

Electronic energy + thermal enthalpy correction: -467.84748

Electronic energy + thermal free energy correction: -467.92206

Table S04. Cartesian coordinates, Mulliken and APT charges of all atoms at **diphenylgermane**.

Symbol	X	Y	Z	Mulliken	APT
H	2.773853	-1.498622	1.250370	0.163772	0.035650
H	0.111032	-2.289677	1.250498	-0.112216	-0.381184
H	4.780349	-0.068587	1.139947	0.151059	0.028684
C	2.752133	-0.596851	0.642549	0.002170	-0.046974
C	3.889522	0.209975	0.585133	-0.226145	-0.052458
H	-0.111142	-2.289658	-1.250555	-0.112224	-0.381181
Ge	-0.000014	-1.393266	-0.000027	0.138440	1.697752
C	1.590301	-0.256949	-0.063635	0.561461	-0.398317
C	3.878784	1.374458	-0.181301	-0.103636	-0.028493
H	4.761553	2.004905	-0.225887	0.156532	0.037289
C	1.595574	0.920218	-0.826105	-0.667266	-0.066339
C	2.728970	1.730424	-0.886778	-0.296252	-0.049008
H	0.703331	1.216473	-1.374173	0.141990	0.040933
H	2.714654	2.638693	-1.481599	0.159317	0.031351
C	-1.590282	-0.256875	0.063612	0.561495	-0.398316
C	-1.595441	0.920443	0.825847	-0.667179	-0.066347
C	-2.752239	-0.596934	-0.642288	0.001951	-0.046975
C	-2.728837	1.730646	0.886560	-0.296212	-0.049009
H	-0.703105	1.216826	1.373694	0.141988	0.040933
C	-3.889630	0.209888	-0.584835	-0.226029	-0.052463
H	-2.774055	-1.498822	-1.249934	0.163753	0.035646
C	-3.878775	1.374523	0.181364	-0.103673	-0.028495
H	-2.714419	2.639036	1.481195	0.159316	0.031350
H	-4.780551	-0.068806	-1.139433	0.151058	0.028682
H	-4.761544	2.004971	0.225982	0.156530	0.037288

Triethylgermane

Electronic energy: -241.91660

Electronic energy + zero-point energy: -241.71164

Electronic energy + thermal energy correction: -241.69432

Electronic energy + thermal enthalpy correction: -241.69314

Electronic energy + thermal free energy correction: -241.76262

Table S05. Cartesian coordinates, Mulliken and APT charges of all atoms at **triethylgermane**.

Symbol	X	Y	Z	Mulliken	APT
Ge	0.000000	0.000000	0.263106	0.463025	1.503652
H	0.000000	0.000000	1.818604	-0.127670	-0.393442
C	-0.829189	1.670995	-0.363032	-0.267351	-0.314686
H	-1.831314	1.748549	0.073975	0.158520	-0.031990
H	-0.968685	1.597247	-1.448746	0.176755	-0.031538
C	1.861718	-0.117399	-0.363032	-0.267351	-0.314657
H	1.867599	0.040282	-1.448746	0.176755	-0.031471
H	2.429945	0.711690	0.073975	0.158520	-0.031800
C	-1.032530	-1.553596	-0.363032	-0.267351	-0.314399
H	-0.598631	-2.460239	0.073975	0.158520	-0.032011
H	-0.898914	-1.637529	-1.448746	0.176755	-0.031571
C	-0.000000	2.913580	-0.015154	-0.681287	0.098670
H	0.987422	2.877390	-0.486948	0.177008	-0.018272
H	-0.488804	3.835069	-0.347589	0.164918	-0.055317
H	0.156966	2.996264	1.065760	0.159651	-0.016935
C	2.523234	-1.456790	-0.015154	-0.681287	0.098600
H	1.998182	-2.293827	-0.486948	0.177008	-0.018320
H	3.565670	-1.494218	-0.347589	0.164918	-0.055447
H	2.516358	-1.634069	1.065760	0.159651	-0.016953
C	-2.523234	-1.456790	-0.015154	-0.681287	0.098190
H	-2.985604	-0.583563	-0.486948	0.177008	-0.018343
H	-3.076865	-2.340852	-0.347589	0.164918	-0.055139
H	-2.673324	-1.362195	1.065760	0.159651	-0.016825

Sodium trimethylborohydride

Electronic energy: -307.41659

Electronic energy + zero-point energy: -307.29249

Electronic energy + thermal energy correction: -307.28055

Electronic energy + thermal enthalpy correction: -307.27937

Electronic energy + thermal free energy correction: -307.33462

Table S06. Cartesian coordinates, Mulliken and APT charges of all atoms at **sodium trimethylborohydride**.

Symbol	X	Y	Z	Mulliken	APT
H	0.128001	0.001651	-1.355141	-0.068023	-0.441930
C	-0.047094	1.373227	0.610463	-0.669985	-0.162796
H	1.004722	1.546222	0.914825	0.087507	-0.136683
H	-0.347940	2.281109	0.070708	0.162214	-0.056161
H	-0.601461	1.373483	1.559923	0.153751	-0.045180
C	-0.031321	-1.363753	0.617789	-0.675930	-0.164145
H	-0.610353	-1.378479	1.552137	0.153876	-0.043951
H	-0.294791	-2.279345	0.071490	0.162590	-0.056470
H	1.015190	-1.508475	0.953499	0.088986	-0.137209
C	-2.046952	-0.010229	-0.515237	-0.788735	-0.154058
H	-2.380510	0.868669	-1.084082	0.148127	-0.067233
H	-2.369674	-0.897661	-1.077013	0.147970	-0.067095
H	-2.612985	-0.009830	0.429282	0.133532	-0.065778
B	-0.444083	0.000745	-0.230303	0.203570	0.706835
Na	2.003856	0.000315	-0.469291	0.760551	0.891855

Trimethylborane

Electronic energy: -144.53110

Electronic energy + zero-point energy: -144.41789

Electronic energy + thermal energy correction: -144.40771

Electronic energy + thermal enthalpy correction: -144.40653

Electronic energy + thermal free energy correction: -144.45969

Table S07. Cartesian coordinates, Mulliken and APT charges of all atoms at **sodium trimethylborane**.

Symbol	X	Y	Z	Mulliken	APT
C	0.838143	1.333921	0.003204	-0.732597	-0.304270
H	0.252828	2.251646	0.109042	0.164817	-0.019411
H	1.601051	1.308488	0.791880	0.178412	0.012106
H	1.401814	1.394030	-0.938537	0.181994	0.015997
C	-1.577069	0.057410	0.004558	-0.730231	-0.304672
H	-2.076001	-0.911001	0.101809	0.165933	-0.018223
H	-1.946672	0.729889	0.788343	0.177352	0.009244
H	-1.904031	0.511886	-0.942152	0.182307	0.019140
C	0.737943	-1.391652	-0.006728	-0.732049	-0.304998
H	1.815505	-1.341691	-0.187739	0.166089	-0.017155

H	0.586894	-1.853004	0.980771	0.183706	0.019009
H	0.284497	-2.087477	-0.722582	0.175995	0.007778
B	-0.001998	-0.000169	0.002593	0.618273	0.885455

Sodium borohydride

Electronic energy: -189.51705

Electronic energy + zero-point energy: -189.47939

Electronic energy + thermal energy correction: -189.47392

Electronic energy + thermal enthalpy correction: -189.47274

Electronic energy + thermal free energy correction: -189.51117

Table S08. Cartesian coordinates, Mulliken and APT charges of all atoms at **sodium borohydride**.

Symbol	X	Y	Z	Mulliken	APT
H	0.874099	0.236110	-1.132162	-0.125861	-0.338032
B	1.309670	-0.000153	0.000167	-0.247117	0.380545
Na	-1.064119	-0.000037	-0.000047	0.728122	0.898478
H	0.884468	0.866910	0.772971	-0.126868	-0.337712
H	2.517827	-0.001415	-0.007152	-0.102177	-0.263537
H	0.880565	-1.100433	0.366031	-0.126099	-0.339741

Borane

Electronic energy: -26.58896

Electronic energy + zero-point energy: -26.562303

Electronic energy + thermal energy correction: -26.558592

Electronic energy + thermal enthalpy correction: -26.55741

Electronic energy + thermal free energy correction: -26.587466

Table S09. Cartesian coordinates, Mulliken and APT charges of all atoms at **borane**.

Symbol	X	Y	Z	Mulliken	APT
B	0.000011	0.000017	-0.000009	0.092057	0.587587
H	1.156217	0.283169	0.000015	-0.030678	-0.196166
H	-0.332867	-1.142900	0.000015	-0.030692	-0.195947
H	-0.823407	0.859647	0.000015	-0.030687	-0.195474

Phenylsilane + styrene

1

Electronic energy: -616.94978

Electronic energy + zero-point energy: -616.68955

Electronic energy + thermal energy correction: -616.66523

Electronic energy + thermal enthalpy correction: -616.66404

Electronic energy + thermal free energy correction: -616.75062

BSSE correction: 0.002510

Table S10. Cartesian coordinates, Mulliken and APT charges of all atoms at **1** in the reaction between phenylsilane and styrene.

Symbol	X	Y	Z	Mulliken	APT
Na	-1.140463	0.708601	1.322676	0.652824	0.867742
H	-4.547177	-1.450244	-1.199776	0.128366	-0.073911
H	-2.555301	1.144248	-1.606625	0.168201	-0.059593
C	-3.465721	-1.624740	-1.089273	-0.826919	-0.151095
H	-3.185932	-0.013343	2.243769	0.099426	-0.124267
H	-3.031322	-1.558588	-2.097124	0.126274	-0.066195
C	-3.016900	0.982968	-0.621372	-0.854374	-0.189241
H	-3.345495	-2.665519	-0.757410	0.149379	-0.065498
B	-2.803154	-0.557732	-0.051170	0.543073	0.708177
C	-3.492407	-0.717183	1.444790	-0.611514	-0.167700
H	-2.683985	1.830206	0.009232	0.145583	-0.111279
H	-4.095100	1.153095	-0.752997	0.133487	-0.047485
H	-4.577334	-0.561406	1.355097	0.168232	-0.053103
H	-3.353471	-1.723729	1.862209	0.169282	-0.057144
H	-1.576887	-0.836538	0.014629	-0.252629	-0.451246
C	2.610137	-1.862639	-0.204319	-0.179143	-0.028207
H	2.509320	-2.936444	-0.325009	0.170624	0.045641
C	3.778509	-1.323846	0.331128	-0.111384	-0.042687
C	1.567609	-1.022306	-0.590848	0.019864	-0.071014
H	4.594086	-1.975663	0.627616	0.152477	0.045586
H	0.652572	-1.439711	-1.003096	0.185837	0.075023
C	3.902410	0.060315	0.472511	-0.224579	-0.062809
C	1.675260	0.367061	-0.438824	0.310745	-0.031279
C	2.861625	0.899396	0.088750	-0.300804	-0.056591
C	0.534545	1.215217	-0.841260	-0.595707	0.156345
H	4.817798	0.485617	0.871810	0.164584	0.039369
H	-0.208996	0.725348	-1.469514	0.143359	0.054058
C	0.326675	2.488958	-0.478259	-0.126641	-0.258114
H	2.980711	1.975331	0.177863	0.098734	0.050418
H	-0.541688	3.028999	-0.842267	0.177766	0.066917
H	1.018616	3.033173	0.159859	0.175577	0.059183

2M

Electronic energy: -616.91416

Electronic energy + zero-point energy: -616.65674

Electronic energy + thermal energy correction: -616.63345

Electronic energy + thermal enthalpy correction: -616.63227

Electronic energy + thermal free energy correction: -616.71435

BSSE correction: 0.003299

Table S11. Cartesian coordinates, Mulliken and APT charges of all atoms at **2M** in the reaction between phenylsilane and styrene.

Symbol	X	Y	Z	Mulliken	APT
C	-3.617260	0.567409	-1.065151	-0.831534	-0.245113
H	-2.106422	0.589106	0.728421	-0.229390	-0.914503
C	-3.642373	-1.199872	1.029142	-0.723519	-0.268072
C	-1.534395	-1.116983	-0.710184	-0.887931	-0.305088
H	-4.394525	1.179198	-0.586994	0.158601	-0.061692
H	-4.131322	-0.084664	-1.788742	0.146339	-0.086355
H	-2.982241	1.248736	-1.651754	0.162503	-0.043508
H	-4.395127	-0.607944	1.566192	0.168905	-0.055255
H	-3.033397	-1.715154	1.785254	0.154705	-0.052949
H	-4.193669	-1.981465	0.481745	0.149023	-0.121907
H	-0.878036	-0.371703	-1.190413	0.267909	-0.041698
H	-1.896577	-1.803967	-1.488965	0.129932	-0.016295
H	-0.984737	-1.703451	0.044169	0.206316	-0.065366
C	-1.142013	1.828683	0.887154	-0.405289	1.167321
C	-0.083269	1.829726	0.001541	-0.119821	-1.101605
C	1.089977	1.012730	0.156490	-0.186456	0.816253
C	1.252882	0.081165	1.218429	-0.188609	-0.280697
H	0.471159	-0.018589	1.965024	0.150084	0.058315
C	2.387339	-0.721800	1.316074	-0.047203	0.173446
H	2.475430	-1.412932	2.149856	0.188752	0.044197
C	3.403398	-0.661802	0.352784	-0.289464	-0.370254
H	4.286870	-1.284836	0.438053	0.165129	0.051764
C	3.262008	0.243653	-0.708366	-0.172224	0.196373
H	4.040994	0.320360	-1.461777	0.169850	0.037202
C	2.134820	1.054975	-0.806185	0.055316	-0.388541
H	2.047123	1.753334	-1.634680	0.169294	0.043638
Na	1.050461	-1.502924	-1.010205	0.503851	0.761716
H	-1.954648	2.531235	0.729313	0.198015	-0.013886
H	-0.995563	1.536927	1.924003	0.184047	-0.052103
H	-0.183742	2.366921	-0.937884	0.121489	0.011898
B	-2.762666	-0.303252	0.002210	0.631377	1.122765

3M

Electronic energy: -616.93541

Electronic energy + zero-point energy: -616.67580

Electronic energy + thermal energy correction: -616.65027

Electronic energy + thermal enthalpy correction: -616.64909

Electronic energy + thermal free energy correction: -616.73962

BSSE correction: 0.003438

Table S12. Cartesian coordinates, Mulliken and APT charges of all atoms at **3M** in the reaction between phenylsilane and styrene.

Symbol	X	Y	Z	Mulliken	APT
C	-3.811334	1.008263	-0.216396	-0.738439	-0.319406
H	-1.085133	1.719601	0.975946	0.159069	-0.087638
C	-4.408419	-1.629795	0.156099	-0.721156	-0.321808
C	-1.816199	-0.864030	-0.180849	-0.917420	-0.371229
H	-4.871873	1.131718	-0.455278	0.166702	-0.010999
H	-3.201054	1.590716	-0.914282	0.179077	0.020621
H	-3.652354	1.470075	0.771307	0.187765	0.043137
H	-5.256510	-1.303697	0.767083	0.181849	0.003931
H	-3.998231	-2.556405	0.569060	0.171084	-0.008848
H	-4.830801	-1.877445	-0.830473	0.196686	0.021131
H	-1.188872	-0.039764	-0.545923	0.317173	0.040578
H	-1.705553	-1.761350	-0.806673	0.149753	-0.018041
H	-1.484414	-1.137717	0.832778	0.250818	0.032399
C	-0.461095	2.518144	0.539660	-0.841369	0.304120
C	0.532709	1.993107	-0.457918	0.180096	-0.731922
C	1.452150	1.020464	-0.138557	-0.406574	0.579581
C	1.481906	0.349524	1.158105	-0.513888	-0.520999
H	0.820854	0.701213	1.944360	0.107106	0.037122
C	2.348465	-0.701719	1.424647	0.131760	0.491670
H	2.324434	-1.154609	2.414372	0.160481	0.018741
C	3.246006	-1.203968	0.461570	-0.483383	-0.774992
H	3.937669	-2.004151	0.695372	0.133693	0.042029
C	3.299661	-0.521013	-0.780795	0.057675	0.384061
H	4.027550	-0.832906	-1.527463	0.151783	0.015879
C	2.456389	0.530531	-1.077636	-0.038100	-0.410663
H	2.538158	1.028496	-2.041362	0.128112	0.012998
Na	0.818630	-1.478551	-0.616488	0.555428	0.762171
H	-1.144866	3.235334	0.075854	0.152553	-0.034892
H	0.012950	3.028172	1.394188	0.159541	-0.104985
H	0.592565	2.469525	-1.433192	0.116666	-0.004811
B	-3.352175	-0.487957	-0.086378	0.665459	0.911062

4M

Electronic energy: -472.39768

Electronic energy + zero-point energy: -472.25399

Electronic energy + thermal energy correction: -472.24022

Electronic energy + thermal enthalpy correction: -472.23904

Electronic energy + thermal free energy correction: -472.29980

BSSE correction: 0.002652

Table S13. Cartesian coordinates, Mulliken and APT charges of all atoms at **4M** in the reaction between phenylsilane and styrene.

Symbol	X	Y	Z	Mulliken	APT
H	-2.860765	1.121872	0.704710	0.136605	-0.086061
C	-3.051231	0.351807	-0.060449	-0.737135	0.309837
C	-1.953068	-0.672711	-0.136089	0.090229	-0.719961
C	-0.637255	-0.335411	-0.358908	-0.384537	0.605862
C	-0.171250	1.046675	-0.441077	-0.478855	-0.520800
H	-0.905206	1.845286	-0.488577	0.115426	0.030690
C	1.179766	1.364643	-0.461574	-0.004794	0.492517
H	1.464345	2.414381	-0.509363	0.154275	0.016827
C	2.188174	0.381865	-0.420578	-0.400494	-0.799729
H	3.237620	0.646421	-0.465623	0.134132	0.042562
C	1.765382	-0.970974	-0.482897	-0.003101	0.401084
H	2.513573	-1.758760	-0.547279	0.149024	0.016177
C	0.432111	-1.324408	-0.467002	-0.001527	-0.406677
H	0.151942	-2.374142	-0.519323	0.122495	0.010928
Na	0.664999	-0.000171	1.794632	0.700450	0.761619
H	-4.007506	-0.116206	0.189567	0.151012	-0.039095
H	-3.198525	0.899191	-1.005721	0.155839	-0.104762
H	-2.226241	-1.725082	-0.127908	0.100957	-0.011018

5M

Electronic energy: -709.63895

Electronic energy + zero-point energy: -709.37631

Electronic energy + thermal energy correction: -709.35026

Electronic energy + thermal enthalpy correction: -709.34907

Electronic energy + thermal free energy correction: -709.43886

BSSE correction: 0.004591

Table S14. Cartesian coordinates, Mulliken and APT charges of all atoms at **5M** in the reaction between phenylsilane and styrene.

Symbol	X	Y	Z	Mulliken	APT
H	0.622403	1.806095	2.480004	0.159632	-0.070463
C	1.097351	2.552062	1.822954	-0.508752	0.291459
C	1.212335	2.084572	0.399517	-0.333527	-0.766276
C	1.746932	0.863149	0.052001	-0.112015	0.543995
C	2.139879	-0.146170	1.027908	-0.341456	-0.493390
H	2.062827	0.088246	2.085226	0.111145	0.040219
C	2.678580	-1.368779	0.648904	-0.035215	0.427289
H	2.979967	-2.066026	1.428592	0.157140	0.020370
C	2.841215	-1.736104	-0.701193	-0.406689	-0.711161
H	3.292035	-2.680655	-0.980596	0.132780	0.041799
C	2.480988	-0.773147	-1.676238	-0.095701	0.371385
H	2.627190	-1.002167	-2.729989	0.152567	0.020349
C	1.946847	0.454305	-1.333186	0.037682	-0.413287
H	1.705313	1.169707	-2.115769	0.106868	0.027653
Na	0.244426	-1.341765	-0.372347	0.309499	0.648094
H	0.495227	3.464300	1.889479	0.148127	-0.034881
H	2.071661	2.775045	2.288444	0.160531	-0.114580
H	1.028206	2.808963	-0.389451	0.107255	0.010750
H	-2.820144	-0.708561	-1.923255	0.172308	0.046993
H	-3.078990	2.157702	-1.936993	-0.037926	-0.321502
H	-2.970165	-2.876706	-0.752592	0.179214	0.051071
C	-2.485359	-0.778678	-0.890743	-0.364351	-0.029902
C	-2.574303	-2.010173	-0.232114	-0.212440	-0.056638
H	-0.705654	1.983060	-2.092601	-0.008361	-0.288005
Si	-1.836117	2.004800	-1.146962	0.148453	1.342348
C	-1.979972	0.360902	-0.239925	0.214583	-0.345031
C	-2.162347	-2.119224	1.098623	-0.172429	-0.060130
H	-2.233203	-3.071852	1.613955	0.184495	0.056545
H	-1.730217	3.110946	-0.182279	-0.017422	-0.298685
C	-1.578260	0.230740	1.099893	-0.132019	-0.051729
C	-1.665770	-0.994824	1.765799	-0.006268	-0.020361
H	-1.172403	1.094101	1.617779	0.106262	0.084448
H	-1.345798	-1.071766	2.800126	0.196027	0.051255

7M

Electronic energy: -709.63897

Electronic energy + zero-point energy: -709.37537

Electronic energy + thermal energy correction: -709.35049

Electronic energy + thermal enthalpy correction: -709.34931

Electronic energy + thermal free energy correction: -709.43625

BSSE correction: 0.004681

Table S15. Cartesian coordinates, Mulliken and APT charges of all atoms at **7M** in the reaction between phenylsilane and styrene.

Symbol	X	Y	Z	Mulliken	APT
H	1.164087	2.828200	1.183199	0.161081	-0.016804
C	1.525551	2.990177	0.157893	-0.562599	0.146625
C	1.432095	1.722703	-0.676627	-0.399712	-0.865426
C	2.330988	0.634231	-0.326166	-0.468615	0.464378
C	2.789606	0.425373	1.000010	-0.081145	-0.241198
H	2.589328	1.179803	1.754405	0.149831	0.056088
C	3.500416	-0.721968	1.359534	-0.089091	0.135016
H	3.841523	-0.836045	2.384824	0.175132	0.037184
C	3.784946	-1.716276	0.417549	-0.313951	-0.296492
H	4.348476	-2.600015	0.696804	0.159759	0.046304
C	3.352914	-1.529299	-0.902347	0.011642	0.123368
H	3.578462	-2.278110	-1.656545	0.178245	0.039171
C	2.641168	-0.386247	-1.263517	0.218992	-0.222089
H	2.316787	-0.259869	-2.292875	0.171889	0.043316
Na	0.898640	-1.499460	0.502930	0.544072	0.783763
H	0.892625	3.771214	-0.273704	0.147630	-0.012264
H	2.547492	3.386467	0.228681	0.162138	-0.076262
H	1.465093	1.932279	-1.751879	0.135860	-0.025030
H	-3.200775	2.004995	0.644720	0.125883	0.022676
H	-1.047918	2.334110	-0.721932	-0.136223	-0.456918
H	-5.434489	1.039816	1.056909	0.144412	0.009413
C	-3.387014	0.963102	0.382206	-0.360030	-0.056782
C	-4.653517	0.425991	0.615696	-0.138675	-0.014142
H	-0.137349	-0.217630	-1.291736	-0.163565	-0.378284
Si	-0.543623	0.955896	-0.395247	0.324440	1.789047
C	-2.349099	0.206579	-0.184245	0.114875	-0.480996
C	-4.921516	-0.901775	0.274721	-0.177113	-0.094467
H	-5.907075	-1.323779	0.448210	0.140219	0.025518
H	-0.141260	0.666280	1.042937	-0.094533	-0.385989
C	-2.653800	-1.117239	-0.526767	-0.177396	-0.097127
C	-3.916207	-1.675482	-0.303469	-0.141811	-0.011469
H	-1.888805	-1.731162	-1.007750	0.104649	0.001704
H	-4.119712	-2.704269	-0.589857	0.133712	0.008165

8M

Electronic energy: -854.17712

Electronic energy + zero-point energy: -853.79844

Electronic energy + thermal energy correction: -853.76144

Electronic energy + thermal enthalpy correction: -853.76026

Electronic energy + thermal free energy correction: -853.87622

BSSE correction: 0.005991

Table S16. Cartesian coordinates, Mulliken and APT charges of all atoms at **8M** in the reaction between phenylsilane and styrene.

Symbol	X	Y	Z	Mulliken	APT
H	1.564003	-2.025838	2.710795	0.160266	-0.018961
C	1.820293	-0.984554	2.953226	-0.639830	0.146576
C	1.612579	-0.065206	1.760682	-0.744404	-0.851552
C	2.511815	-0.239295	0.628836	-0.123790	0.437299
C	3.142019	-1.474795	0.334141	0.137116	-0.234493
H	3.079231	-2.286808	1.051889	0.159193	0.055650
C	3.858132	-1.670201	-0.850611	-0.086072	0.117183
H	4.337494	-2.628771	-1.029350	0.169943	0.036052
C	3.968353	-0.650027	-1.801042	-0.333767	-0.281848
H	4.533046	-0.801404	-2.714694	0.161617	0.044265
C	3.360889	0.584215	-1.530289	-0.077718	0.126310
H	3.446420	1.399208	-2.243936	0.174663	0.042215
C	2.649007	0.781391	-0.348881	0.204675	-0.207135
H	2.183494	1.744008	-0.157532	0.128825	0.049089
Na	1.134511	-1.211764	-1.506060	0.600056	0.783225
H	1.163977	-0.686437	3.776371	0.132882	-0.011155
H	2.852607	-0.980513	3.328738	0.169135	-0.077115
H	1.548681	0.987589	2.055494	0.174299	-0.006143
H	-2.873278	-1.912834	1.933731	0.129674	0.020815
H	-0.871057	-0.283716	2.397141	-0.123153	-0.441091
H	-5.029448	-2.511348	0.893225	0.148770	0.008866
C	-3.075395	-1.596495	0.909875	-0.397371	-0.050180
C	-4.298600	-1.937290	0.329579	-0.119298	-0.009766
H	-0.061913	0.563951	-0.083925	-0.312724	-0.396308
Si	-0.339350	-0.475889	1.004546	0.280830	1.756071
C	-2.104534	-0.855555	0.219187	-0.115176	-0.476444
C	-4.588273	-1.533818	-0.975562	-0.164297	-0.088787
H	-5.540486	-1.790828	-1.430193	0.143932	0.024265
H	0.211713	-1.842102	0.611959	-0.086884	-0.389417
C	-2.431170	-0.455981	-1.083556	0.067484	-0.102282
C	-3.648492	-0.786258	-1.684827	-0.212090	-0.010472
H	-1.722965	0.164502	-1.639418	0.165839	0.003910
H	-3.871700	-0.449408	-2.694161	0.145659	0.011194
C	0.016665	3.338551	1.320090	-0.762930	-0.324303
H	-0.242613	2.750746	2.207855	0.164820	0.015905
H	1.094592	3.266248	1.146576	0.159260	-0.011076
H	-0.190033	4.388872	1.579576	0.157202	0.003776
C	-2.415661	2.696683	0.315741	-0.827422	-0.318697

H	-2.994388	2.477978	-0.586343	0.195690	-0.012384
H	-2.549642	1.859513	1.012172	0.270492	0.030928
H	-2.866252	3.569780	0.810244	0.131598	-0.004200
C	-0.342925	3.202373	-1.402449	-0.668098	-0.302810
H	0.745629	3.144071	-1.502651	0.187930	-0.014350
H	-0.812136	2.523309	-2.122782	0.180106	0.001249
H	-0.638136	4.217729	-1.711697	0.150016	0.004703
B	-0.886753	3.002386	0.067817	0.743052	0.921424

9M

Electronic energy: -854.17409

Electronic energy + zero-point energy: -853.79424

Electronic energy + thermal energy correction: -853.75962

Electronic energy + thermal enthalpy correction: -853.75844

Electronic energy + thermal free energy correction: -853.86458

BSSE correction: 0.006756

Table S17. Cartesian coordinates, Mulliken and APT charges of all atoms at **9M** in the reaction between phenylsilane and styrene.

Symbol	X	Y	Z	Mulliken	APT
C	-1.523608	0.172312	1.966079	-0.425186	-0.804194
C	-2.487811	-0.304827	0.963842	-0.200295	0.365015
C	-3.110970	0.556905	0.034246	-0.437308	-0.215129
H	-3.005111	1.629438	0.151330	0.075281	0.066492
C	-3.867178	0.065342	-1.034518	-0.080751	0.087841
H	-4.329093	0.765351	-1.725263	0.180742	0.043306
C	-4.035919	-1.309473	-1.215252	-0.246295	-0.218312
H	-4.626027	-1.691156	-2.041721	0.173369	0.046643
C	-3.462777	-2.184216	-0.283821	0.038066	0.076878
H	-3.608360	-3.255771	-0.385782	0.181056	0.041609
C	-2.709972	-1.693226	0.781002	0.308503	-0.171113
H	-2.276406	-2.388299	1.493932	0.177789	0.047840
Na	-1.104147	-0.672712	-1.313690	0.506917	0.789303
H	3.238846	0.808286	1.805031	0.136728	0.030176
H	0.922413	0.312427	2.616597	-0.109838	-0.436563
H	5.456097	0.350042	0.817792	0.150672	0.014832
C	3.333627	0.034001	1.043774	0.022177	-0.059816
C	4.591272	-0.222774	0.493906	-0.212318	-0.012654
H	-0.069625	-1.658975	0.960777	-0.182710	-0.374132
Si	0.406494	-0.259409	1.320922	0.458334	1.945477
C	2.191885	-0.674400	0.644924	-0.098788	-0.524080

C	4.739412	-1.222250	-0.469182	-0.122594	-0.070780
H	5.715256	-1.427513	-0.899358	0.159488	0.026214
H	0.121253	0.710902	0.081391	-0.284398	-0.637054
C	2.379225	-1.692298	-0.299806	-0.301505	-0.077613
C	3.627141	-1.968567	-0.860414	-0.222616	-0.017584
H	1.523256	-2.299184	-0.603962	0.068123	0.003716
H	3.736898	-2.764469	-1.592449	0.143171	0.012665
C	1.387556	2.918948	-0.058421	-0.775677	-0.312873
H	0.758635	3.339766	0.733366	0.162707	-0.010450
H	2.260551	2.444572	0.399213	0.184241	0.008272
H	1.764589	3.767582	-0.650019	0.128456	-0.021691
C	-0.820623	2.478691	-1.573471	-0.736304	-0.327582
H	-1.439003	1.774743	-2.146618	0.134811	-0.041133
H	-1.445376	2.925057	-0.794715	0.205950	0.000089
H	-0.577483	3.289605	-2.278181	0.142780	-0.026278
C	1.475193	1.095633	-2.082884	-0.767495	-0.307943
H	2.404748	0.704098	-1.661562	0.232711	0.010066
H	0.959495	0.263216	-2.584836	0.114501	-0.051417
H	1.750287	1.790469	-2.891742	0.140144	-0.018734
B	0.606250	1.963422	-1.061213	0.791705	1.127930
C	-1.607501	1.646297	2.334581	-0.502127	0.109069
H	-1.343273	2.285249	1.481661	0.207255	-0.006160
H	-2.604278	1.950487	2.680572	0.165497	-0.069007
H	-0.891822	1.875690	3.130329	0.138631	-0.004977
H	-1.566731	-0.463748	2.860442	0.176400	-0.036164

10M

Electronic energy: -854.23126

Electronic energy + zero-point energy: -853.84827

Electronic energy + thermal energy correction: -853.81375

Electronic energy + thermal enthalpy correction: -853.81256

Electronic energy + thermal free energy correction: -853.92023

BSSE correction: 0.006746

Table S18. Cartesian coordinates, Mulliken and APT charges of all atoms at **10M** in the reaction between phenylsilane and styrene.

Symbol	X	Y	Z	Mulliken	APT
C	1.691357	-0.559266	1.669450	0.063605	-0.339970
C	1.966669	-0.828236	0.208572	-1.217288	0.094631
C	1.105449	-1.645716	-0.536746	-0.931611	-0.156877
H	0.273128	-2.133732	-0.034314	0.147330	0.092820

C	1.309858	-1.850982	-1.903435	0.025695	-0.022541
H	0.634698	-2.501446	-2.453488	0.164387	0.053815
C	2.389894	-1.248270	-2.549271	0.054446	-0.086010
H	2.555136	-1.410315	-3.609536	0.170559	0.044254
C	3.271169	-0.456596	-1.811961	0.016204	0.018213
H	4.125022	0.003787	-2.299927	0.160205	0.040161
C	3.061611	-0.249901	-0.449207	1.023456	-0.132698
H	3.754797	0.377677	0.106727	0.191104	0.053656
Na	-1.230435	-0.080432	-0.979033	0.216887	0.788967
H	-1.669728	1.844700	1.926965	0.188412	0.063545
H	0.686747	1.478303	3.262092	-0.010580	-0.314172
H	-3.250360	2.661051	0.223527	0.172294	0.061056
C	-1.300897	2.081760	0.932528	-0.006544	-0.033765
C	-2.202248	2.542064	-0.030508	-0.230870	-0.048842
H	2.523782	2.049972	1.794257	-0.043480	-0.319545
Si	1.272222	1.270839	1.922931	0.224365	1.408693
C	0.060340	1.905913	0.631346	0.463321	-0.384617
C	-1.758204	2.828371	-1.322769	-0.125754	-0.037884
H	-2.458205	3.183742	-2.072411	0.193372	0.058902
H	-1.589804	-1.044893	0.839552	-0.437625	-0.438732
C	0.488960	2.204556	-0.676048	-0.510654	-0.060264
C	-0.409011	2.656151	-1.646660	-0.174244	-0.059369
H	1.535585	2.082290	-0.944187	0.139286	0.060575
H	-0.055239	2.882469	-2.647783	0.191739	0.049821
C	-3.152322	-2.564150	1.657719	-0.807622	-0.147566
H	-2.408987	-3.303067	1.989821	0.123837	-0.064247
H	-3.423596	-1.965935	2.539049	0.123108	-0.064126
H	-4.052213	-3.129294	1.369591	0.131520	-0.075699
C	-2.242748	-2.613005	-0.871156	-0.827912	-0.189890
H	-1.891449	-2.134531	-1.806829	0.190405	-0.107764
H	-1.497698	-3.386260	-0.633936	0.178591	-0.053147
H	-3.155804	-3.146857	-1.171396	0.143697	-0.050594
C	-3.769372	-0.545016	-0.011378	-0.702375	-0.188616
H	-4.025069	0.140040	0.809393	0.189638	-0.051631
H	-3.570028	0.100307	-0.888364	0.149525	-0.110299
H	-4.690715	-1.086309	-0.271568	0.143187	-0.057074
B	-2.614175	-1.645784	0.423353	0.847683	0.676215
C	2.855144	-0.970784	2.589247	-0.681811	0.082909
H	3.077489	-2.036359	2.475611	0.183170	-0.031312
H	3.767228	-0.411696	2.357503	0.143124	-0.003167
H	2.609406	-0.785774	3.639638	0.171957	-0.013351
H	0.796529	-1.127318	1.953239	0.182260	-0.004463

11M

Electronic energy: -546.79470

Electronic energy + zero-point energy: -546.53777

Electronic energy + thermal energy correction: -546.51606

Electronic energy + thermal enthalpy correction: -546.51488

Electronic energy + thermal free energy correction: -546.59760

BSSE correction: 0.002705

Table S19. Cartesian coordinates, Mulliken and APT charges of all atoms at **11M** in the reaction between phenylsilane and styrene.

Symbol	X	Y	Z	Mulliken	APT
H	4.614850	-2.327215	0.136544	0.151690	0.030657
H	2.235696	-2.102912	0.758112	0.136931	0.035845
C	4.133582	-1.355576	0.078881	-0.052713	0.012603
C	2.792322	-1.227642	0.430344	-0.200031	-0.123494
H	0.441382	-0.688103	1.437569	0.161487	-0.022498
C	4.857747	-0.239251	-0.340866	-0.067511	-0.107639
C	2.141580	0.013374	0.375523	-0.239724	0.178851
C	0.674960	0.114754	0.725636	-0.194891	-0.396081
H	5.903999	-0.334834	-0.613043	0.144680	0.036458
H	0.298008	2.276236	0.620987	0.197694	0.003143
C	0.256342	1.455524	1.345698	-0.666327	0.053827
H	-2.299871	-2.249713	0.171046	0.151231	0.037328
H	-0.772627	1.401001	1.712479	0.155239	-0.007012
H	-0.020824	0.801812	-1.832547	-0.018766	-0.315440
C	4.223959	0.999992	-0.404112	-0.123014	0.015290
C	2.880074	1.124678	-0.050767	-0.067792	-0.135452
H	-4.684518	-2.144626	0.786028	0.154271	0.030780
C	-2.838950	-1.311893	0.052589	-0.264792	-0.045034
C	-4.188228	-1.259177	0.400611	-0.220348	-0.052233
H	0.908020	1.720164	2.185378	0.177810	-0.026794
H	0.013527	-1.578754	-1.354095	-0.032744	-0.324562
Si	-0.341779	-0.241750	-0.834253	0.233514	1.466204
H	4.776156	1.877133	-0.727930	0.151726	0.029951
H	2.406405	2.100447	-0.105511	0.116106	0.049661
C	-2.173823	-0.183253	-0.451729	0.227276	-0.404879
C	-4.899953	-0.069183	0.248513	-0.117167	-0.028131
H	-5.951236	-0.025896	0.516113	0.153221	0.037597
C	-2.909041	1.003351	-0.598340	-0.231917	-0.050368
C	-4.258917	1.063463	-0.252514	-0.115518	-0.047447
H	-2.423954	1.894030	-0.992164	0.139775	0.038160
H	-4.810023	1.990758	-0.376230	0.160600	0.030711

2aM

Electronic energy: -616.90363

Electronic energy + zero-point energy: -616.64690

Electronic energy + thermal energy correction: -616.62396

Electronic energy + thermal enthalpy correction: -616.62278

Electronic energy + thermal free energy correction: -616.70551

BSSE correction: 0.003512

Table S20. Cartesian coordinates, Mulliken and APT charges of all atoms at **2aM** in the reaction between phenylsilane and styrene.

Symbol	X	Y	Z	Mulliken	APT
Na	-2.437544	1.592583	0.646701	0.746224	0.767055
H	-1.522777	-3.232580	-0.502070	0.133245	-0.052371
H	-3.062814	-0.259683	-1.676956	0.155737	0.004288
C	-1.004907	-2.274694	-0.656084	-0.803711	-0.300685
H	-2.186559	-0.195483	2.188646	0.092942	-0.061716
H	-0.917375	-2.137750	-1.742153	0.155623	-0.018344
C	-3.213871	-0.688133	-0.677067	-0.734578	-0.323304
H	0.007677	-2.387081	-0.250312	0.180140	-0.018227
B	-1.827138	-1.097575	0.051327	1.328246	1.217113
C	-1.785806	-1.080621	1.665910	-0.752447	-0.342103
H	-3.904372	-0.026792	-0.129827	0.086791	-0.075847
H	-3.791511	-1.610022	-0.826776	0.178247	-0.009865
H	-2.414801	-1.911833	2.018091	0.172770	-0.028447
H	-0.778863	-1.256419	2.059354	0.195631	-0.003402
H	-0.990910	0.033131	-0.279414	-0.789103	-0.859846
C	3.312727	-0.468715	-0.782224	-0.223675	0.010127
H	4.060755	-0.867980	-1.460520	0.153131	0.029779
C	3.603128	-0.329147	0.574144	-0.047761	-0.078266
C	2.059249	-0.102623	-1.271944	-0.389094	-0.103557
H	4.576594	-0.618670	0.957332	0.147100	0.033348
H	1.834648	-0.215948	-2.329470	0.143464	0.038046
C	2.631189	0.177879	1.437967	-0.102326	-0.012328
C	1.082335	0.412887	-0.416487	-0.610319	0.051005
C	1.380774	0.542085	0.944311	0.636579	-0.079538
C	-0.256426	0.836036	-0.947313	-0.029288	1.164631
H	2.845878	0.280685	2.497507	0.148765	0.030276
H	-0.463870	0.386481	-1.924875	0.191222	-0.087500
C	-0.630987	2.227272	-0.811073	-0.779983	-0.875137
H	0.618476	0.923460	1.620502	0.140963	0.023311
H	-1.092553	2.690017	-1.680148	0.123169	-0.030235
H	0.066626	2.862580	-0.270102	0.152296	-0.008261

3aM

Electronic energy: -616.92094

Electronic energy + zero-point energy: -616.66092

Electronic energy + thermal energy correction: -616.63606

Electronic energy + thermal enthalpy correction: -616.63488

Electronic energy + thermal free energy correction: -616.72238

BSSE correction: 0.003405

Table S21. Cartesian coordinates, Mulliken and APT charges of all atoms at **3aM** in the reaction between phenylsilane and styrene.

Symbol	X	Y	Z	Mulliken	APT
Na	-1.297123	-1.915682	1.365605	0.921519	0.821996
H	4.086113	-1.142049	-0.469724	0.153185	0.012430
H	1.648264	-2.525559	-1.652352	0.153585	-0.015861
C	3.246471	-0.434075	-0.561137	-0.826595	-0.311108
H	1.169768	-1.606974	2.155068	0.118488	-0.036635
H	3.117693	-0.259409	-1.634881	0.204001	0.015361
C	1.221926	-2.271230	-0.677386	-0.767750	-0.313165
H	3.552306	0.496314	-0.074264	0.193721	0.002843
B	2.004319	-1.138361	0.099583	0.937130	0.859025
C	1.570078	-0.765205	1.574355	-0.828685	-0.296612
H	0.183171	-1.951780	-0.853445	0.098831	0.043015
H	1.159694	-3.192552	-0.081802	0.120538	-0.001779
H	2.371388	-0.308285	2.163358	0.161541	-0.000512
H	0.783974	0.004209	1.491567	0.184558	0.044747
H	-1.367488	-0.913684	-2.052925	0.156210	-0.067131
C	0.927104	2.040545	-0.662569	-0.016718	-0.024536
H	1.882898	2.298001	-1.110067	0.161435	0.035050
C	0.512802	2.669431	0.510737	-0.167954	-0.105060
C	0.119614	1.072233	-1.262058	-0.042607	-0.113656
H	1.138175	3.422372	0.980393	0.163635	0.036308
H	0.451470	0.588154	-2.179286	0.144735	0.038186
C	-0.714659	2.318214	1.075071	-0.091386	0.006316
C	-1.114961	0.706237	-0.710150	-0.880541	0.072856
C	-1.513332	1.344899	0.473127	0.056480	-0.110274
C	-2.002357	-0.327376	-1.374071	0.175563	0.141235
H	-1.051109	2.804607	1.986607	0.164020	0.026251
H	-2.679560	0.237303	-2.044079	0.157292	-0.169509
C	-2.742479	-1.264874	-0.404489	-1.095175	-0.416502
H	-2.467859	1.075448	0.917463	0.131653	0.053560
H	-3.201925	-2.071552	-0.994621	0.077581	-0.107901
H	-3.591454	-0.723047	0.044831	0.081709	-0.118939

4aM

Electronic energy: -472.38130

Electronic energy + zero-point energy: -472.23744

Electronic energy + thermal energy correction: -472.22385

Electronic energy + thermal enthalpy correction: -472.22267

Electronic energy + thermal free energy correction: -472.28828

BSSE correction: 0.002518

Table S22. Cartesian coordinates, Mulliken and APT charges of all atoms at **4aM** in the reaction between phenylsilane and styrene.

Symbol	X	Y	Z	Mulliken	APT
Na	-1.402673	-1.669477	0.868373	0.823938	0.793571
H	-1.836741	0.589696	-1.793855	0.166454	-0.063904
C	1.738265	-0.929658	-0.748042	-0.168076	0.004324
H	2.190946	-1.782974	-1.245605	0.154591	0.028190
C	2.442835	-0.243661	0.242105	-0.100980	-0.114392
C	0.455508	-0.512272	-1.110231	-0.029738	-0.117810
H	3.440337	-0.563478	0.526768	0.151823	0.036700
H	-0.087691	-1.045331	-1.889232	0.127622	0.035441
C	1.857438	0.867723	0.851539	-0.152371	0.017203
C	-0.150759	0.595686	-0.500698	-0.386034	0.104317
C	0.578365	1.281569	0.479919	-0.136702	-0.102434
C	-1.583468	0.966532	-0.794734	-0.149434	0.130587
H	2.401606	1.415687	1.615508	0.150821	0.031451
H	-1.640887	2.068578	-0.854748	0.122830	-0.167690
C	-2.528469	0.335321	0.253335	-0.907699	-0.413570
H	0.127130	2.147197	0.959626	0.156791	0.038636
H	-3.567471	0.435771	-0.090060	0.111796	-0.121087
H	-2.456114	0.931655	1.180338	0.064369	-0.119534

5aM

Electronic energy: -709.60805

Electronic energy + zero-point energy: -709.34612

Electronic energy + thermal energy correction: -709.31963

Electronic energy + thermal enthalpy correction: -709.31844

Electronic energy + thermal free energy correction: -709.41593

BSSE correction: 0.003080

Table S23. Cartesian coordinates, Mulliken and APT charges of all atoms at **5aM** in the reaction between phenylsilane and styrene.

Symbol	X	Y	Z	Mulliken	APT
Na	-1.525012	0.803339	1.464481	0.792077	0.822470
H	-3.491861	2.576997	-0.783691	0.167415	-0.070328
C	-5.058414	-0.546928	1.208364	-0.113103	0.001644
H	-5.610414	-0.443598	2.138524	0.153063	0.026902
C	-4.962195	-1.792846	0.588399	-0.080170	-0.112361
C	-4.458595	0.572236	0.626188	-0.313513	-0.114494
H	-5.429487	-2.665074	1.034750	0.147785	0.036248
H	-4.550261	1.546038	1.105587	0.100890	0.032217
C	-4.271873	-1.903502	-0.620345	-0.160036	0.017770
C	-3.758864	0.477424	-0.585212	-0.339989	0.105033
C	-3.681150	-0.780271	-1.198115	-0.051163	-0.107150
C	-3.024181	1.660414	-1.166203	-0.294743	0.148444
H	-4.199395	-2.867200	-1.116311	0.145176	0.031782
H	-3.196623	1.658460	-2.257648	0.113312	-0.169706
C	-1.531524	1.628828	-0.766155	-0.603922	-0.479203
H	-3.145501	-0.872059	-2.140282	0.146802	0.041447
H	-1.057391	2.575472	-1.064367	0.086206	-0.111398
H	-1.039183	0.843784	-1.366317	0.052645	-0.100255
H	4.181712	1.990909	0.455984	0.125351	0.036203
H	1.547689	1.771018	-0.588958	-0.003211	-0.278482
H	6.579900	1.444956	0.605493	0.159279	0.030043
C	4.506122	0.968224	0.275899	-0.583853	-0.050409
C	5.864757	0.665755	0.359815	-0.018876	-0.052991
H	1.168961	0.274205	1.257369	-0.073686	-0.378290
Si	1.729847	0.391427	-0.111213	0.099703	1.377822
C	3.559666	-0.018107	-0.042466	0.804537	-0.361392
C	6.303777	-0.636594	0.121754	-0.243825	-0.029885
H	7.361337	-0.874455	0.182971	0.155579	0.037913
H	1.052114	-0.589578	-0.977109	0.002252	-0.289970
C	4.023279	-1.320199	-0.283317	-0.619812	-0.053671
C	5.380843	-1.630536	-0.201718	-0.028524	-0.051461
H	3.317633	-2.105573	-0.544915	0.115397	0.035440
H	5.718155	-2.644396	-0.394724	0.160957	0.030069

6aM

Electronic energy: -709.60836

Electronic energy + zero-point energy: -709.34609

Electronic energy + thermal energy correction: -709.32121

Electronic energy + thermal enthalpy correction: -709.32003

Electronic energy + thermal free energy correction: -709.41116

BSSE correction: 0.003765

Table S24. Cartesian coordinates, Mulliken and APT charges of all atoms at **6aM** in the reaction between phenylsilane and styrene.

Symbol	X	Y	Z	Mulliken	APT
Na	1.558122	0.641473	1.566540	0.678555	0.833783
H	1.347484	0.564446	-2.052537	0.141940	-0.055775
C	3.388158	-2.011037	0.285702	-0.054839	0.002895
H	3.033702	-3.008670	0.528805	0.166578	0.035934
C	4.660909	-1.603761	0.689256	-0.146152	-0.113543
C	2.572806	-1.142046	-0.443976	0.126831	-0.120654
H	5.299184	-2.277789	1.251690	0.152728	0.039213
H	1.582701	-1.464144	-0.762284	0.147302	0.041883
C	5.110067	-0.326091	0.350329	-0.163899	0.009681
C	3.008508	0.146552	-0.790655	-0.628774	0.115919
C	4.291940	0.535331	-0.381590	-0.031894	-0.097971
C	2.086670	1.129227	-1.467565	-0.232203	0.118381
H	6.102748	-0.003227	0.650364	0.156666	0.032831
H	2.679031	1.708743	-2.196422	0.133211	-0.157777
C	1.360508	1.985235	-0.405428	-0.778820	-0.578823
H	4.647342	1.528755	-0.645891	0.160197	0.045451
H	0.663678	2.668041	-0.912567	0.123182	-0.079398
H	2.124481	2.651854	0.046381	0.074665	-0.143599
H	-3.828984	1.561414	1.435159	0.136045	0.030610
H	-1.420842	2.174376	0.565020	-0.000681	-0.349117
H	-6.119044	0.647771	1.462248	0.150628	0.020331
C	-4.068212	0.709733	0.800591	-0.480673	-0.057899
C	-5.367242	0.198934	0.819403	-0.024937	-0.040574
H	-0.818572	0.675677	-1.383136	-0.054597	-0.316247
Si	-1.290637	0.819707	0.003445	0.155854	1.718710
C	-3.073279	0.157631	-0.019867	0.572126	-0.428997
C	-5.699706	-0.884870	0.007552	-0.222111	-0.053585
H	-6.709361	-1.284481	0.016587	0.149766	0.031308
H	-0.609289	-0.117597	0.935572	-0.055694	-0.434782
C	-3.435643	-0.928267	-0.832225	-0.600865	-0.058379
C	-4.729820	-1.448634	-0.822186	-0.017737	-0.041296
H	-2.694870	-1.376270	-1.492882	0.113855	0.029433
H	-4.983785	-2.288614	-1.462326	0.153746	0.022051

7aM

Electronic energy: -709.63503

Electronic energy + zero-point energy: -709.37054

Electronic energy + thermal energy correction: -709.34661

Electronic energy + thermal enthalpy correction: -709.34543

Electronic energy + thermal free energy correction: -709.43172

BSSE correction: 0.004511

Table S25. Cartesian coordinates, Mulliken and APT charges of all atoms at **7aM** in the reaction between phenylsilane and styrene.

Symbol	X	Y	Z	Mulliken	APT
Na	-1.402165	1.530879	-0.579591	0.423489	0.773244
H	-1.512932	-2.660983	-0.284841	0.144238	-0.018587
C	-3.922168	0.369706	-1.304775	-0.075380	-0.023113
H	-4.285691	0.506207	-2.318681	0.185470	0.050857
C	-4.310006	1.254893	-0.295943	-0.297033	-0.085602
C	-3.065843	-0.697328	-1.011739	0.174380	-0.094668
H	-4.978862	2.080064	-0.518401	0.167362	0.053525
H	-2.757313	-1.374807	-1.803057	0.183922	0.064310
C	-3.847981	1.052469	1.009102	0.098183	-0.027725
C	-2.582454	-0.903331	0.287683	-0.731493	0.067261
C	-2.994980	-0.014723	1.293316	0.121916	-0.090547
C	-1.625811	-2.030160	0.604961	-0.334636	0.128253
H	-4.153528	1.725844	1.803836	0.193371	0.051967
H	-2.079414	-2.657952	1.383372	0.183356	-0.079238
C	-0.237845	-1.533891	1.057838	-0.586596	-0.305533
H	-2.635145	-0.160333	2.308489	0.165386	0.063490
H	0.364419	-2.407980	1.333730	0.107034	-0.048679
H	-0.337489	-0.903629	1.948950	0.165026	-0.036786
H	2.136163	1.771814	0.920995	0.102331	0.054224
H	0.259389	0.893431	0.406118	-0.170441	-0.672958
H	4.516307	2.417445	1.151937	0.144676	0.011669
C	2.911228	1.131552	0.506656	-0.688328	-0.081301
C	4.251555	1.497355	0.637727	-0.237758	-0.048214
H	1.083194	-1.923642	-1.076079	-0.236176	-0.566410
Si	0.702022	-0.604813	-0.333190	0.312493	1.849651
C	2.528577	-0.049373	-0.146241	0.523552	-0.444668
C	5.252208	0.682005	0.108549	-0.185798	-0.045311
H	6.296844	0.963858	0.205484	0.141308	0.023032
H	-0.148317	-0.155130	-1.520349	-0.050374	-0.468724
C	3.555157	-0.854586	-0.664344	-0.140971	-0.069399
C	4.899610	-0.498851	-0.544540	-0.113056	-0.051016
H	3.289316	-1.779034	-1.171630	0.166551	0.054706
H	5.671078	-1.141895	-0.959205	0.143997	0.012291

8aM

Electronic energy: -854.17488

Electronic energy + zero-point energy: -853.79512

Electronic energy + thermal energy correction: -853.76038

Electronic energy + thermal enthalpy correction: -853.75920

Electronic energy + thermal free energy correction: -853.86973

BSSE correction: 0.006098

Table S26. Cartesian coordinates, Mulliken and APT charges of all atoms at **8aM** in the reaction between phenylsilane and styrene.

Symbol	X	Y	Z	Mulliken	APT
Na	1.384956	-0.476448	-1.612712	0.374197	0.790521
H	1.426149	-0.108649	2.589420	0.123648	-0.017527
C	3.896963	0.360464	-0.530847	-0.031537	-0.034665
H	4.263089	1.332609	-0.846438	0.153257	0.056171
C	4.304488	-0.790387	-1.210032	-0.178303	-0.086567
C	3.016412	0.264145	0.552170	0.239302	-0.097684
H	4.991884	-0.717666	-2.046778	0.175541	0.053632
H	2.690221	1.165817	1.065414	0.144913	0.071879
C	3.832206	-2.038057	-0.789990	0.067062	-0.029118
C	2.528234	-0.978721	0.978295	-0.752646	0.064997
C	2.955139	-2.126443	0.291559	-0.040119	-0.087811
C	1.547992	-1.094378	2.123422	-0.196760	0.123017
H	4.148745	-2.940384	-1.303908	0.188985	0.050203
H	1.986017	-1.752232	2.885518	0.190867	-0.079328
C	0.167856	-1.624264	1.682362	-0.583306	-0.299478
H	2.589202	-3.099447	0.608941	0.166078	0.062061
H	-0.451006	-1.759941	2.577518	0.104183	-0.046809
H	0.277136	-2.602931	1.201380	0.177764	-0.039817
H	-2.222920	-1.924850	-1.615344	0.122732	0.051212
H	-0.316902	-1.314441	-0.828750	-0.082705	-0.673621
H	-4.617180	-2.212792	-2.180369	0.147859	0.011218
C	-2.980775	-1.409844	-1.029627	-0.704015	-0.072808
C	-4.329220	-1.573722	-1.349969	-0.100955	-0.045850
H	-1.084648	0.585283	1.724098	-0.242491	-0.548078
Si	-0.734892	-0.376270	0.543226	0.331233	1.849233
C	-2.569703	-0.598605	0.037662	-0.032364	-0.448098
C	-5.308054	-0.916705	-0.604244	-0.207438	-0.042241
H	-6.358817	-1.039071	-0.851009	0.143789	0.022724
H	0.178852	0.699592	-0.057246	-0.262423	-0.515498
C	-3.574602	0.048371	0.773868	0.174228	-0.074573
C	-4.926333	-0.102416	0.461943	-0.005682	-0.047858
H	-3.285733	0.681894	1.609652	0.141177	0.057528
H	-5.680624	0.413779	1.049393	0.152493	0.014054
C	1.236613	3.064345	-1.289748	-0.816107	-0.308387

H	2.252211	2.825705	-0.957430	0.209684	-0.014281
H	0.952642	2.425003	-2.134763	0.158706	-0.020450
H	1.276724	4.086264	-1.698037	0.154472	0.003487
C	0.632593	3.305898	1.373739	-0.863372	-0.312231
H	-0.006446	4.018110	1.908789	0.142115	-0.005885
H	0.493071	2.345863	1.894451	0.267692	0.055695
H	1.679012	3.607341	1.489031	0.137540	-0.027650
C	-1.374085	3.059103	-0.442363	-0.844841	-0.335314
H	-1.631762	2.599135	-1.401651	0.147503	-0.008945
H	-1.946267	2.565386	0.352195	0.194525	0.035021
H	-1.729547	4.100524	-0.470971	0.146834	0.001661
B	0.169308	3.087220	-0.119530	1.066680	0.946255

10aM

Electronic energy: -854.22291

Electronic energy + zero-point energy: -853.83994

Electronic energy + thermal energy correction: -853.80444

Electronic energy + thermal enthalpy correction: -853.80326

Electronic energy + thermal free energy correction: -853.91690

BSSE correction: 0.006126

Table S27. Cartesian coordinates, Mulliken and APT charges of all atoms at **10aM** in the reaction between phenylsilane and styrene.

Symbol	X	Y	Z	Mulliken	APT
Na	2.120088	-0.058178	-1.484450	0.398392	0.817737
H	1.171151	0.463629	2.064244	0.215552	0.010690
C	3.826291	-1.802575	0.122414	-0.046471	-0.025006
H	4.895216	-1.613347	0.133453	0.188554	0.056763
C	3.285044	-2.722808	-0.781963	-0.157437	-0.095223
C	2.992956	-1.112355	1.000966	0.297270	-0.100905
H	3.929793	-3.260647	-1.469423	0.175974	0.053861
H	3.415893	-0.374401	1.677596	0.126381	0.078351
C	1.907935	-2.948326	-0.782693	-0.004163	-0.012609
C	1.604636	-1.322519	1.008018	-0.727349	0.072741
C	1.077998	-2.256107	0.106440	-0.178838	-0.103641
C	0.751106	-0.545688	1.987610	-0.213952	0.141526
H	1.474818	-3.666310	-1.472422	0.183390	0.049253
H	0.877516	-1.010712	2.974590	0.198114	-0.080560
C	-0.744353	-0.461955	1.658116	-0.499319	-0.337282
H	0.009535	-2.446197	0.083639	0.115289	0.057008
H	-1.253463	0.041717	2.489447	0.159673	-0.004092

H	-1.193459	-1.462840	1.618328	0.178864	-0.009592
H	-2.890620	-1.875606	-0.745110	0.133952	0.024116
H	-0.589658	-0.041592	-1.098292	-0.045623	-0.389816
H	-5.306029	-2.301910	-0.971349	0.159341	0.029092
C	-3.594244	-1.074659	-0.521824	-0.280425	-0.046086
C	-4.959208	-1.323372	-0.652985	-0.132607	-0.053649
H	-1.045196	1.929912	0.241205	0.032133	-0.290132
Si	-1.276202	0.481758	0.110893	0.200085	1.505190
C	-3.116130	0.181584	-0.115289	0.197369	-0.390520
C	-5.879338	-0.311270	-0.375842	-0.174643	-0.035372
H	-6.943558	-0.500607	-0.477314	0.150821	0.036158
H	1.446912	1.319084	-0.140261	-0.656493	-0.480258
C	-4.058354	1.184335	0.155576	-0.222356	-0.051140
C	-5.427412	0.943639	0.028471	-0.097091	-0.043190
H	-3.721419	2.170165	0.467674	0.166292	0.040785
H	-6.138997	1.735202	0.242976	0.163090	0.029090
C	3.611086	1.933664	-1.049850	-0.831605	-0.211476
H	4.191589	1.091785	-0.634503	0.136293	-0.075270
H	3.498582	1.757410	-2.137378	0.088487	-0.090933
H	4.280970	2.801436	-0.989852	0.169735	-0.038727
C	2.587331	2.737717	1.310746	-0.909084	-0.171958
H	3.209904	3.645769	1.324749	0.126057	-0.072785
H	1.692312	2.963497	1.909819	0.154793	-0.060924
H	3.153048	1.969303	1.860963	0.180449	-0.075489
C	1.410604	3.497810	-1.006513	-0.828172	-0.163224
H	1.089564	3.219947	-2.023278	0.118115	-0.079968
H	0.506230	3.815274	-0.468481	0.157572	-0.060220
H	2.041001	4.394013	-1.116284	0.137406	-0.077356
B	2.217709	2.309737	-0.223335	1.296184	0.725040

11aM

Electronic energy: -546.79585

Electronic energy + zero-point energy: -546.53847

Electronic energy + thermal energy correction: -546.51720

Electronic energy + thermal enthalpy correction: -546.51602

Electronic energy + thermal free energy correction: -546.59703

BSSE correction: 0.003147

Table S28. Cartesian coordinates, Mulliken and APT charges of all atoms at **11aM** in the reaction between phenylsilane and styrene.

Symbol	X	Y	Z	Mulliken	APT

H	-3.858350	-2.665370	0.734291	0.151700	0.037179
C	-3.284115	-1.846385	0.312629	-0.032974	-0.064309
C	-3.827458	-0.561361	0.262027	-0.173731	-0.017675
C	-2.002664	-2.071247	-0.186593	-0.231747	-0.013188
H	-4.828044	-0.378880	0.642230	0.150134	0.033130
H	-1.572732	-3.067991	-0.155796	0.158489	0.038033
C	-3.087585	0.488584	-0.276676	0.089009	-0.075186
C	-1.266720	-1.016423	-0.728552	-0.255785	-0.086593
C	-1.796470	0.276460	-0.774910	-0.197477	0.024941
H	-3.515196	1.488437	-0.311673	0.141289	0.037685
H	-0.264096	-1.195508	-1.110319	0.130725	0.041045
C	-0.975105	1.436382	-1.288107	-0.202296	0.141910
C	-0.519305	2.376452	-0.152419	-0.602673	-0.312742
H	-1.557027	2.005970	-2.022538	0.170611	-0.068046
H	-1.387886	2.889774	0.279730	0.183546	-0.012746
H	0.124134	3.164759	-0.562652	0.173982	-0.024810
H	-0.095559	1.045822	-1.811775	0.190227	-0.021547
H	-0.525644	0.705411	2.087410	-0.025377	-0.308908
H	4.135276	0.273767	-1.840212	0.161373	0.032390
H	2.445073	1.790704	-0.887120	0.149135	0.033196
C	3.500902	-0.069476	-1.028565	-0.070906	-0.047816
C	2.543246	0.784642	-0.482568	-0.204762	-0.040161
C	3.640059	-1.365713	-0.531920	-0.158020	-0.025619
Si	0.390995	1.513017	1.255783	0.227728	1.422098
C	1.707177	0.367370	0.564720	0.169411	-0.391631
H	4.382974	-2.034290	-0.955974	0.158311	0.038686
C	2.820143	-1.800308	0.509147	-0.189099	-0.041482
C	1.863045	-0.940072	1.048028	-0.327129	-0.055362
H	2.922624	-2.809226	0.897367	0.163170	0.034197
H	1.217837	-1.298300	1.847093	0.162777	0.040423
H	1.011794	2.549260	2.111522	-0.059641	-0.347091

6L

Electronic energy: -709.61232

Electronic energy + zero-point energy: -709.35251

Electronic energy + thermal energy correction: -709.32726

Electronic energy + thermal enthalpy correction: -709.32608

Electronic energy + thermal free energy correction: -709.41413

BSSE correction: 0.003459

Table S29. Cartesian coordinates, Mulliken and APT charges of all atoms at **6L** in the reaction between phenylsilane and styrene.

Symbol	X	Y	Z	Mulliken	APT
H	2.050749	2.416710	1.496357	0.133700	-0.021201
C	2.887985	2.371907	0.779416	-0.605186	0.268520
C	2.551056	1.482011	-0.391349	0.041446	-1.242304
C	2.414294	0.084208	-0.205131	-0.098452	0.441432
C	2.182867	-0.494522	1.083976	-0.235579	-0.270874
H	2.262405	0.131699	1.967065	0.145148	0.043554
C	1.930977	-1.858954	1.242552	-0.226273	0.258513
H	1.802010	-2.257436	2.245949	0.169826	0.034706
C	1.843091	-2.718642	0.140144	-0.150085	-0.464272
H	1.667012	-3.780431	0.270371	0.158913	0.043410
C	2.022565	-2.165181	-1.144231	-0.216713	0.226891
H	1.963373	-2.807822	-2.018976	0.161514	0.032143
C	2.283101	-0.812682	-1.314576	-0.150804	-0.252968
H	2.428193	-0.417438	-2.317264	0.158513	0.029581
Na	-0.234071	-0.989158	-0.099466	0.450891	0.625727
H	3.067963	3.397380	0.444434	0.167813	-0.023181
H	3.773449	2.042535	1.340826	0.166187	-0.070076
H	2.915449	1.796015	-1.368774	0.168368	0.034802
H	-2.347223	0.655378	-2.201216	0.170095	0.031673
H	-0.992415	2.981042	-1.645969	-0.041472	-0.312763
H	-3.899746	-1.222661	-1.843034	0.175889	0.031261
C	-2.562686	0.332655	-1.184494	0.105242	-0.173516
C	-3.444182	-0.733376	-0.986927	-0.037679	0.066328
H	1.068545	1.791616	-0.487373	-0.019804	0.837835
Si	-0.601817	2.314045	-0.375991	0.034228	0.496946
C	-1.952623	1.003681	-0.104214	-0.837811	-0.208180
C	-3.745165	-1.165327	0.306248	-0.223719	-0.150387
H	-4.429346	-1.992887	0.463514	0.168790	0.044856
H	-0.830813	3.316452	0.696608	-0.047587	-0.321405
C	-2.286165	0.552864	1.190735	0.048916	-0.181978
C	-3.166997	-0.509518	1.396531	-0.071877	0.071724
H	-1.843055	1.044329	2.055155	0.160674	0.040347
H	-3.405033	-0.825117	2.408231	0.176887	0.032856

7L

Electronic energy: -709.65527

Electronic energy + zero-point energy: -709.38857

Electronic energy + thermal energy correction: -709.36262

Electronic energy + thermal enthalpy correction: -709.36144

Electronic energy + thermal free energy correction: -709.45370

BSSE correction: 0.001859

Table S30. Cartesian coordinates, Mulliken and APT charges of all atoms at **7L** in the reaction between phenylsilane and styrene.

Symbol	X	Y	Z	Mulliken	APT
H	-0.301990	1.601488	0.411215	0.160090	0.004863
C	0.356833	2.473476	0.331368	-0.705773	0.039988
C	1.616698	2.135989	-0.458318	-0.254434	0.087872
C	2.426430	0.976938	0.081048	-0.515432	0.058379
C	2.190663	0.409699	1.339262	-0.284608	-0.146547
H	1.400258	0.803173	1.969862	0.153044	0.078222
C	2.948892	-0.675505	1.793055	-0.011173	-0.008811
H	2.746289	-1.099046	2.771930	0.192726	0.052032
C	3.958381	-1.213469	0.994421	-0.260191	-0.087641
H	4.548360	-2.053127	1.347266	0.171268	0.054229
C	4.212608	-0.649046	-0.260637	-0.060001	-0.018671
H	4.999899	-1.052859	-0.889685	0.179561	0.051560
C	3.453136	0.431426	-0.707024	0.448772	-0.117062
H	3.646687	0.857878	-1.688291	0.185004	0.061958
Na	1.377481	-1.635580	-0.538065	0.526582	0.717377
H	-0.201419	3.263791	-0.176508	0.170517	-0.003392
H	0.589141	2.825836	1.341228	0.156805	-0.023214
H	2.270794	3.015630	-0.512740	0.179895	-0.043988
H	-2.612655	-2.426208	-0.124217	0.104373	0.016897
H	-1.588793	-1.283726	-2.929789	-0.067455	-0.375375
H	-4.504177	-2.177903	1.428129	0.131041	0.011880
C	-3.018533	-1.431457	0.058789	-0.505721	-0.107845
C	-4.087924	-1.298612	0.943509	-0.252071	0.013982
H	1.335995	1.894809	-1.490092	0.167717	0.002232
Si	-0.956323	-0.556259	-1.776717	-0.096500	0.433153
C	-2.454320	-0.326767	-0.605246	-0.273112	-0.205043
C	-4.621021	-0.036270	1.211280	-0.126578	-0.120828
H	-5.449756	0.074646	1.904218	0.146286	0.024669
H	-0.848174	0.826263	-2.361536	-0.055862	-0.354819
C	-3.017507	0.929446	-0.321811	0.147332	-0.145640
C	-4.078344	1.078976	0.574419	-0.046820	0.013852
H	-2.622906	1.812164	-0.820775	0.145211	0.025249
H	-4.487272	2.067257	0.767867	0.149506	0.010481

8L

Electronic energy: -398.89777

Electronic energy + zero-point energy: -398.79052

Electronic energy + thermal energy correction: -398.77785

Electronic energy + thermal enthalpy correction: -398.77667

Electronic energy + thermal free energy correction: -398.83706

BSSE correction: 0.000426

Table S31. Cartesian coordinates, Mulliken and APT charges of all atoms at **8L** in the reaction between phenylsilane and styrene.

Symbol	X	Y	Z	Mulliken	APT
H	1.732789	-0.209471	2.195505	-0.094549	-0.361912
H	1.699705	1.883198	1.202897	-0.083585	-0.360675
C	-0.168388	0.181896	0.373780	0.379428	-0.166206
C	-0.798157	-1.065669	0.531722	-0.654949	-0.132567
C	-0.932596	1.203374	-0.216280	-0.551955	-0.139357
C	-2.115553	-1.284622	0.129771	0.061208	0.022193
H	-0.247094	-1.886840	0.988472	0.076298	0.014097
C	-2.250412	0.995555	-0.626890	0.032531	0.024349
H	-0.491099	2.189390	-0.350166	0.091492	0.014825
C	-2.849956	-0.252328	-0.456216	-0.209289	-0.132624
H	-2.571884	-2.260076	0.276377	0.141893	0.011527
H	-2.812725	1.811269	-1.073680	0.143077	0.010931
H	-3.876345	-0.417065	-0.770045	0.144537	0.025375
Si	1.666862	0.428765	0.839478	-0.143865	0.404840
Na	3.447359	-0.525668	-1.148852	0.667726	0.765204

9L

Electronic energy: -708.43074

Electronic energy + zero-point energy: -708.18807

Electronic energy + thermal energy correction: -708.16252

Electronic energy + thermal enthalpy correction: -708.16134

Electronic energy + thermal free energy correction: -708.25378

BSSE correction: 0.002467

Table S32. Cartesian coordinates, Mulliken and APT charges of all atoms at **9L** in the reaction between phenylsilane and styrene.

Symbol	X	Y	Z	Mulliken	APT
H	-2.102839	3.152517	1.267580	-0.085026	-0.356705
H	-2.130874	3.261152	-1.047283	-0.083089	-0.355369
C	-2.432813	0.835199	0.002625	-0.160835	-0.144183
C	-2.701275	0.094345	1.168120	-0.240675	-0.163276
C	-2.758684	0.220853	-1.220324	-0.292448	-0.165046
C	-3.254952	-1.185666	1.121229	-0.151712	0.031370

H	-2.469383	0.529563	2.139437	0.130309	0.022870
C	-3.313703	-1.058246	-1.281769	-0.127427	0.031537
H	-2.573145	0.756363	-2.150325	0.126182	0.021409
C	-3.560794	-1.773547	-0.108177	-0.143306	-0.147385
H	-3.451725	-1.725367	2.044054	0.153517	0.017451
H	-3.556777	-1.497625	-2.245783	0.154163	0.016649
H	-3.992213	-2.769013	-0.150184	0.156433	0.030097
Si	-1.487364	2.493538	0.068905	-0.074356	0.376495
Na	1.227368	1.662862	0.016681	0.479462	0.706890
C	0.785141	-1.094880	1.194871	0.034669	-0.049551
C	2.133162	-0.757081	1.329327	-0.028264	-0.078456
C	0.229401	-1.273125	-0.072098	-0.253661	-0.078254
C	2.951421	-0.581383	0.200928	-0.027037	0.036861
C	2.381299	-0.774648	-1.070013	-0.195358	-0.087182
C	1.034815	-1.111631	-1.202856	-0.166088	-0.056668
H	0.162839	-1.210838	2.076747	0.203607	0.065649
H	-0.821427	-1.524131	-0.177540	0.144672	0.100402
H	0.609789	-1.253637	-2.191582	0.207138	0.060128
H	2.998451	-0.679945	-1.958237	0.122894	0.056651
H	2.561085	-0.623815	2.319677	0.180666	0.057816
C	4.367450	-0.204245	0.388959	-0.397387	0.097383
C	5.183647	0.285532	-0.549033	-0.121954	-0.185817
H	4.748331	-0.332482	1.400885	0.138147	0.024224
H	4.862145	0.455964	-1.572791	0.152200	0.059509
H	6.213115	0.531432	-0.313557	0.164566	0.054502

10L

Electronic energy: -708.40424

Electronic energy + zero-point energy: -708.16181

Electronic energy + thermal energy correction: -708.13917

Electronic energy + thermal enthalpy correction: -708.13799

Electronic energy + thermal free energy correction: -708.22043

BSSE correction: 0.002524

Table S33. Cartesian coordinates, Mulliken and APT charges of all atoms at **10L** in the reaction between phenylsilane and styrene.

Symbol	X	Y	Z	Mulliken	APT
H	1.219492	-2.661326	-0.980447	-0.096617	-0.436668
H	0.034796	-0.681942	-1.162796	-0.081769	-0.413619
C	2.472239	-0.477251	-0.247859	-0.069366	-0.059346
C	2.512844	0.902237	-0.518311	0.074500	-0.165498

C	3.696990	-1.096042	0.062829	-0.480241	-0.158643
C	3.705359	1.626512	-0.478159	-0.184770	0.006172
H	1.592120	1.421310	-0.776984	0.099574	0.014412
C	4.894804	-0.383629	0.099990	-0.165341	0.051373
H	3.715753	-2.163304	0.278259	0.142788	0.028799
C	4.904936	0.986332	-0.168293	-0.138804	-0.128737
H	3.698844	2.691272	-0.696223	0.145689	0.012152
H	5.822329	-0.897231	0.338274	0.139318	0.007348
H	5.835404	1.545286	-0.140183	0.141016	0.022997
Na	-2.025487	-0.883872	-1.531804	0.598673	0.730199
C	-4.008327	1.259918	-0.688178	-0.003593	0.183792
C	-2.767684	1.568329	-0.145363	-0.356193	-0.361304
C	-4.635086	0.038678	-0.388929	-0.368347	-0.272099
C	-2.088684	0.673322	0.720671	-0.190196	0.705031
C	-2.735786	-0.556759	1.008489	-0.445808	-0.149141
C	-3.993233	-0.853219	0.472264	0.269446	0.062461
H	-4.496932	1.971453	-1.347229	0.173738	0.038665
H	-5.609866	-0.196738	-0.802299	0.164346	0.045017
H	-4.468513	-1.796377	0.726832	0.192169	0.041460
H	-2.260691	-1.275416	1.666427	0.065777	0.053907
H	-2.292532	2.515126	-0.389499	0.158056	0.047468
C	-0.752963	0.967215	1.181635	0.421903	-1.024731
C	0.012560	0.062493	1.866363	-0.741996	0.726242
H	-0.294171	1.876485	0.801167	0.130394	0.023340
H	-0.423764	-0.765796	2.408235	0.175336	-0.046533
H	1.030305	0.317053	2.145685	0.155407	0.023953
Si	0.847855	-1.463291	-0.134448	0.074909	0.391531

11L

Electronic energy: -708.44930

Electronic energy + zero-point energy: -708.20549

Electronic energy + thermal energy correction: -708.18169

Electronic energy + thermal enthalpy correction: -708.18051

Electronic energy + thermal free energy correction: -708.26639

BSSE correction: 0.003846

Table S34. Cartesian coordinates, Mulliken and APT charges of all atoms at **11L** in the reaction between phenylsilane and styrene.

Symbol	X	Y	Z	Mulliken	APT
H	-1.418785	2.943181	-0.409197	-0.065553	-0.399556
H	-0.026030	1.220401	-1.246696	-0.064409	-0.355923

C	-2.389191	0.424818	-0.116303	-0.093179	-0.361172
C	-2.588370	-0.549660	0.872849	0.350992	-0.084268
C	-3.352981	0.531523	-1.132110	-0.671683	-0.037968
C	-3.704484	-1.387218	0.849334	-0.131636	-0.026246
H	-1.861924	-0.659641	1.673729	0.138053	0.062971
C	-4.468897	-0.304100	-1.165352	-0.115829	-0.067751
H	-3.237367	1.285732	-1.908534	0.170961	0.034998
C	-4.645965	-1.267713	-0.172022	-0.144892	-0.052446
H	-3.839050	-2.131172	1.628910	0.165474	0.029716
H	-5.202035	-0.199568	-1.959652	0.148609	0.026367
H	-5.515651	-1.917471	-0.191646	0.149592	0.036033
Na	1.771245	-0.819960	-1.527379	0.649205	0.748868
C	3.860083	-1.510681	0.073717	-0.104971	0.384715
C	2.756219	-1.289405	0.870928	0.177658	-0.437146
C	4.385053	-0.506546	-0.778347	-0.350947	-0.756848
C	2.032010	-0.024464	0.868210	-0.827762	0.705611
C	2.676902	1.022060	0.085927	-0.411926	-0.543135
C	3.794733	0.767980	-0.697931	0.204559	0.509596
H	4.340515	-2.486438	0.105657	0.144299	0.015603
H	5.268101	-0.683623	-1.380218	0.132357	0.037967
H	4.220015	1.587873	-1.273623	0.159679	0.019634
H	2.266702	2.026781	0.104289	0.075237	0.032561
H	2.385075	-2.087432	1.510033	0.134426	0.012383
C	0.820368	0.136585	1.509828	0.132789	-0.794772
C	0.051118	1.435307	1.508608	-0.649416	-0.127782
H	0.438941	-0.688222	2.106185	0.078424	-0.001211
H	0.696747	2.313173	1.653500	0.186691	-0.070149
H	-0.672772	1.459540	2.332018	0.167592	-0.005271
Si	-0.906126	1.583252	-0.100544	0.265605	1.464622

12L

Electronic energy: -945.69596

Electronic energy + zero-point energy: -945.33348

Electronic energy + thermal energy correction: -945.29722

Electronic energy + thermal enthalpy correction: -945.29604

Electronic energy + thermal free energy correction: -945.40916

BSSE correction: 0.006321

Table S35. Cartesian coordinates, Mulliken and APT charges of all atoms at **12L** in the reaction between phenylsilane and styrene.

Symbol	X	Y	Z	Mulliken	APT

H	1.228840	-2.840381	-2.484437	-0.061146	-0.386805
H	-0.059769	-0.997939	-1.735592	-0.005712	-0.346799
C	2.149055	-1.575198	-0.260486	-0.183408	-0.353409
C	2.235700	-1.745209	1.129250	0.403105	-0.090673
C	3.173085	-0.856128	-0.897475	-0.748399	-0.064842
C	3.293558	-1.201956	1.859725	-0.129364	-0.016404
H	1.457401	-2.293358	1.653696	0.228099	0.067204
C	4.232100	-0.305445	-0.174416	-0.116835	-0.071698
H	3.143174	-0.715223	-1.976580	0.146817	0.047935
C	4.290114	-0.472619	1.209677	-0.083587	-0.057178
H	3.337958	-1.343147	2.935641	0.160325	0.035403
H	5.007854	0.254353	-0.688499	0.160431	0.037695
H	5.109317	-0.041941	1.777179	0.175351	0.041443
Si	0.683199	-2.198791	-1.260390	0.266766	1.412058
Na	-1.572890	0.645562	-0.525704	0.148680	0.662587
C	-3.931639	0.188230	0.852344	0.078840	0.340026
C	-2.986996	-0.720800	1.279356	0.164219	-0.460316
C	-4.325188	0.279850	-0.504687	-0.404421	-0.701682
C	-2.299582	-1.616201	0.362025	-0.739467	0.631539
C	-2.833939	-1.599035	-0.992416	-0.148368	-0.503602
C	-3.792664	-0.676050	-1.388751	0.153882	0.467408
H	-4.380033	0.859198	1.582810	0.156544	0.019779
H	-5.083080	0.984720	-0.824728	0.130693	0.039623
H	-4.135298	-0.695313	-2.421534	0.162099	0.019709
H	-2.458677	-2.311413	-1.720454	0.108604	0.031585
H	-2.701128	-0.749269	2.328840	0.148514	0.022501
C	-1.197759	-2.359722	0.740068	-0.230759	-0.767126
C	-0.449248	-3.264570	-0.208798	-0.554130	-0.116946
H	-0.892393	-2.336691	1.783035	0.062578	0.006516
H	-1.114105	-3.870093	-0.840898	0.179419	-0.074025
H	0.172674	-3.980665	0.341271	0.156609	-0.003029
H	1.860419	0.908962	0.696974	0.004273	0.078931
H	1.726548	1.578892	-2.662774	-0.006688	-0.295995
H	0.274830	0.559911	2.542770	0.223918	0.064021
C	0.959844	1.515629	0.741086	-0.921977	-0.021353
C	0.068691	1.323953	1.798941	-0.195043	-0.078463
H	3.290365	2.669834	-1.200265	-0.049477	-0.278640
Si	1.902388	2.681422	-1.694951	0.106667	1.254010
C	0.709594	2.473269	-0.258588	0.693142	-0.363208
C	-1.085938	2.105507	1.889334	-0.094252	0.012081
H	-1.782740	1.956351	2.707484	0.193790	0.059034
H	1.603328	3.961705	-2.364045	-0.004472	-0.282544
C	-0.458313	3.249492	-0.150090	0.038040	-0.029856
C	-1.347446	3.072719	0.914910	-0.140380	-0.091998
H	-0.676937	4.006751	-0.899104	0.179128	0.048662
H	-2.243151	3.682447	0.980662	0.187353	0.056839

13L

Electronic energy: -945.66437

Electronic energy + zero-point energy: -945.30497

Electronic energy + thermal energy correction: -945.26950

Electronic energy + thermal enthalpy correction: -945.26832

Electronic energy + thermal free energy correction: -945.38156

BSSE correction: 0.005889

Table S36. Cartesian coordinates, Mulliken and APT charges of all atoms at **13L** in the reaction between phenylsilane and styrene.

Symbol	X	Y	Z	Mulliken	APT
H	-3.530141	-2.161462	-2.216127	-0.080165	-0.369703
H	-2.341790	-2.682600	-0.208693	-0.067522	-0.342255
C	-4.114980	-0.593824	-0.045484	0.011851	-0.398820
C	-5.243774	-1.228978	0.496300	-0.830635	-0.014957
C	-3.976647	0.786493	0.162946	0.435102	-0.051598
C	-6.201841	-0.515661	1.214931	-0.164361	-0.065449
H	-5.381534	-2.299328	0.354352	0.159940	0.031053
C	-4.931966	1.507982	0.881179	0.011206	-0.047218
H	-3.107386	1.307172	-0.233293	0.104051	0.051927
C	-6.046346	0.857718	1.408298	-0.156448	-0.038846
H	-7.067706	-1.028273	1.623304	0.151108	0.024772
H	-4.804250	2.576249	1.029229	0.168125	0.031047
H	-6.790898	1.416970	1.966884	0.147344	0.031278
Si	-2.850605	-1.567799	-1.041671	0.212729	1.525952
Na	2.959925	0.848822	-0.379624	0.384052	0.616137
C	1.518538	2.932340	0.613283	0.022815	0.245708
C	0.666119	1.842219	0.700873	0.223255	-0.308327
C	1.987346	3.390346	-0.636763	-0.228724	-0.441099
C	0.201825	1.144421	-0.458945	-0.359073	0.627746
C	0.712083	1.609756	-1.709706	-0.014446	-0.328977
C	1.566779	2.714311	-1.786079	-0.057541	0.231776
H	1.822183	3.444294	1.522595	0.175562	0.036041
H	2.635239	4.257057	-0.703896	0.161948	0.044969
H	1.908052	3.049997	-2.762121	0.168100	0.032184
H	0.394923	1.118688	-2.624506	0.171120	0.052889
H	0.313829	1.512664	1.675785	0.170678	0.036264
C	-0.610111	-0.024636	-0.365119	-0.650096	-1.303420
C	-1.439010	-0.456070	-1.557591	-0.665404	-0.134629
H	-1.039188	-0.193732	0.625343	0.118419	0.023881
H	-0.818552	-1.020641	-2.281577	0.180924	-0.018186
H	-1.849257	0.398046	-2.119428	0.188217	-0.046685
H	1.781610	-1.275926	2.001210	0.161244	0.044739

H	0.412232	-1.120153	-0.543672	0.083347	0.744783
H	3.528634	-0.068703	3.248726	0.184519	0.043863
C	2.770093	-1.166421	1.558236	-0.213419	-0.136763
C	3.752947	-0.472923	2.265955	-0.039848	0.030991
H	1.059783	-3.561500	0.053786	-0.072874	-0.293730
Si	1.562947	-2.403588	-0.731655	0.031856	0.512706
C	3.015108	-1.707151	0.277272	-0.295265	-0.171698
C	5.021523	-0.287580	1.707252	-0.248740	-0.109980
H	5.786728	0.255704	2.252262	0.174809	0.047025
H	2.213212	-2.990288	-1.936313	-0.043855	-0.414117
C	4.308081	-1.520757	-0.253914	-0.143207	-0.138461
C	5.296745	-0.819145	0.444544	-0.011190	0.037635
H	4.543925	-1.930695	-1.233436	0.157998	0.035102
H	6.283310	-0.695810	0.007198	0.182496	0.034449

14L

Electronic energy: -945.70857

Electronic energy + zero-point energy: -945.34262

Electronic energy + thermal energy correction: -945.30661

Electronic energy + thermal enthalpy correction: -945.30543

Electronic energy + thermal free energy correction: -945.41983

BSSE correction: 0.006491

Table S37. Cartesian coordinates, Mulliken and APT charges of all atoms at **14L** in the reaction between phenylsilane and styrene.

Symbol	X	Y	Z	Mulliken	APT
H	2.666589	3.373762	-1.469182	-0.051771	-0.330846
H	3.026928	3.609368	0.909229	-0.058158	-0.340276
C	3.072081	1.045577	-0.106558	0.179071	-0.401816
C	3.399003	0.366605	-1.291658	-0.181960	-0.048596
C	3.207696	0.354810	1.108260	-0.337334	-0.057905
C	3.852370	-0.952825	-1.264480	-0.160348	-0.053305
H	3.301775	0.873896	-2.249280	0.161043	0.038141
C	3.659258	-0.964351	1.142448	-0.048115	-0.071224
H	2.944492	0.841847	2.045113	0.173163	0.050135
C	3.984697	-1.618582	-0.045697	-0.084192	-0.023468
H	4.099215	-1.461187	-2.191926	0.169385	0.037547
H	3.734706	-1.483977	2.092178	0.173064	0.059706
H	4.328646	-2.647908	-0.022198	0.176830	0.045502
Si	2.387219	2.787396	-0.138871	0.193820	1.469870
Na	-2.407686	-0.172371	1.406606	0.322871	0.735224

C	-3.628122	0.258465	-1.116761	0.065453	-0.029243
C	-2.271266	0.529285	-1.294877	0.056154	-0.129563
C	-4.404533	1.074591	-0.287000	-0.207539	-0.084122
C	-1.658505	1.619743	-0.655347	-0.521991	0.076318
C	-2.446112	2.427011	0.176323	0.187196	-0.121678
C	-3.807269	2.159398	0.358526	-0.086690	-0.008668
H	-4.073574	-0.596121	-1.616852	0.202075	0.056334
H	-5.460711	0.868167	-0.147495	0.180782	0.055179
H	-4.399037	2.800548	1.004430	0.182748	0.050242
H	-1.996291	3.268738	0.693151	0.179206	0.079153
H	-1.670531	-0.127755	-1.919078	0.117356	0.087608
C	-0.187431	1.885859	-0.899933	-0.402307	0.086144
C	0.527548	2.741798	0.149714	-0.739971	-0.360397
H	-0.090797	2.358336	-1.887546	0.179794	-0.033241
H	0.354293	2.324778	1.151081	0.166799	0.025795
H	0.144889	3.769606	0.154761	0.116724	-0.019917
H	1.255995	-1.093212	-0.133072	-0.291255	0.048307
H	0.309927	0.911347	-0.983753	0.466559	0.011037
H	0.845070	-1.941974	-2.394148	0.177415	0.030534
C	0.361005	-1.684486	-0.316980	-0.930530	-0.150961
C	0.133879	-2.168632	-1.602929	0.090590	0.029172
H	-1.491297	-1.416278	3.092556	-0.075326	-0.385572
Si	-0.057953	-1.331179	2.539589	0.000210	0.346266
C	-0.518920	-1.947232	0.754584	0.200954	-0.148231
C	-0.999226	-2.940974	-1.876207	-0.128393	-0.136393
H	-1.179974	-3.321073	-2.877160	0.156541	0.032272
H	-0.174659	0.166294	2.204424	-0.014968	-0.386747
C	-1.640299	-2.744036	0.449397	-0.221598	-0.179573
C	-1.885450	-3.228774	-0.839706	-0.030343	0.018649
H	-2.338769	-3.008149	1.244514	0.140212	0.014874
H	-2.764500	-3.839513	-1.029172	0.156777	0.017732

8S

Electronic energy: -1019.1770

Electronic energy + zero-point energy: -1018.7777

Electronic energy + thermal energy correction: -1018.7401

Electronic energy + thermal enthalpy correction: -1018.7389

Electronic energy + thermal free energy correction: -1018.8551

BSSE correction: 0.007222

Table S38. Cartesian coordinates, Mulliken and APT charges of all atoms at **8S** in the reaction between phenylsilane and styrene.

Symbol	X	Y	Z	Mulliken	APT
H	-2.577552	2.776434	-1.733918	0.172883	-0.018159
C	-3.063190	3.112111	-0.806183	-0.504485	0.157466
C	-2.597831	2.301602	0.392000	-0.726450	-0.836866
C	-3.011667	0.909522	0.452843	-0.179986	0.444662
C	-3.251984	0.137683	-0.713720	-0.073988	-0.244709
H	-3.277454	0.632244	-1.679815	0.157348	0.059166
C	-3.460541	-1.241341	-0.652106	-0.047015	0.116304
H	-3.641148	-1.792467	-1.571420	0.184018	0.042353
C	-3.434713	-1.919572	0.570457	-0.276006	-0.301743
H	-3.601804	-2.990587	0.615206	0.173044	0.050000
C	-3.213934	-1.179241	1.739681	0.016507	0.117333
H	-3.208710	-1.679335	2.704250	0.178659	0.039783
C	-3.002936	0.197349	1.681719	0.231742	-0.218443
H	-2.831994	0.752253	2.600323	0.190213	0.044342
Na	-0.820325	-0.733440	0.297518	0.036749	0.698931
H	-2.791601	4.164313	-0.677355	0.133016	-0.015873
H	-4.148462	3.062716	-0.970141	0.166621	-0.079538
H	-2.778250	2.815840	1.342348	0.114138	-0.027817
H	1.630028	2.543550	-1.926632	0.114415	0.022009
H	-0.441156	3.713973	0.184618	-0.119168	-0.448274
H	4.060909	2.175086	-2.122944	0.153797	0.014940
C	2.189638	2.216722	-1.048401	-0.509573	-0.068797
C	3.563970	2.009695	-1.170376	-0.073687	-0.018483
H	-0.490104	1.407816	1.563691	-0.148327	-0.364021
Si	-0.456758	2.218964	0.272997	0.366923	1.698846
C	1.503157	2.001339	0.158530	0.104576	-0.458834
C	4.306097	1.591018	-0.061211	-0.119462	-0.099038
H	5.377466	1.433650	-0.146916	0.161933	0.031151
H	-0.674512	1.407577	-0.993783	-0.142313	-0.356354
C	2.274868	1.578227	1.249736	-0.180978	-0.109487
C	3.657310	1.384970	1.155483	-0.190558	-0.016053
H	1.784587	1.389672	2.205677	0.137088	0.026740
H	4.224230	1.065284	2.026586	0.151145	0.019567
C	-0.346710	-2.975671	-1.424749	-0.084606	-0.038604
C	0.464714	-3.254092	-0.323040	0.213581	-0.099555
C	-0.085305	-1.856824	-2.218564	-0.210975	-0.088801
C	1.554368	-2.428700	0.003911	-0.098145	0.098161
C	1.800468	-1.298663	-0.797475	-0.489439	-0.100849
C	0.989631	-1.020849	-1.897060	0.092967	-0.044135
H	-1.184606	-3.625760	-1.656125	0.194145	0.058094
H	-0.720080	-1.627226	-3.068302	0.200048	0.066549
H	1.186264	-0.130886	-2.486526	0.224258	0.077521
H	2.611111	-0.616150	-0.555036	0.078558	0.084139
H	0.257812	-4.126495	0.291238	0.191854	0.057898
C	2.387753	-2.777450	1.171213	-0.248339	0.025616
C	3.540635	-2.195177	1.512735	-0.165601	-0.143754
H	2.009477	-3.597340	1.780111	0.148129	0.024496
H	3.974111	-1.382098	0.937978	0.135925	0.072973

H	4.086839	-2.525670	2.389694	0.164825	0.049146

9S

Electronic energy: -1019.1435

Electronic energy + zero-point energy: -1018.7448

Electronic energy + thermal energy correction: -1018.7089

Electronic energy + thermal enthalpy correction: -1018.7078

Electronic energy + thermal free energy correction: -1018.8183

BSSE correction: 0.008543

Table S39. Cartesian coordinates, Mulliken and APT charges of all atoms at **9S** in the reaction between phenylsilane and styrene.

Symbol	X	Y	Z	Mulliken	APT
H	0.977834	-4.088015	-0.552654	0.167517	0.334869
C	1.249542	-3.832840	0.478888	-0.543225	-2.079465
C	1.143005	-2.330394	0.754620	-0.354294	0.010204
C	2.195921	-1.536792	0.096879	-0.834510	-0.433087
C	2.554039	-1.757822	-1.255057	0.381318	-0.317154
H	2.075824	-2.561321	-1.806279	0.165754	0.475794
C	3.513576	-0.971940	-1.895710	0.026547	-0.425002
H	3.764556	-1.176220	-2.932592	0.180030	0.778650
C	4.154953	0.067523	-1.214887	-0.145556	-0.506045
H	4.906869	0.672443	-1.710371	0.174675	0.898991
C	3.821359	0.300245	0.124260	-0.041894	-0.430310
H	4.312610	1.097255	0.675195	0.191973	0.658461
C	2.858323	-0.482066	0.761633	-0.060315	-0.990170
H	2.599890	-0.280124	1.798029	0.146400	0.302128
Na	1.330576	0.760374	-1.083176	0.287578	0.522393
H	0.565252	-4.389086	1.125526	0.143636	0.512946
H	2.267009	-4.206524	0.655206	0.163507	0.610721
H	1.142099	-2.132958	1.831834	0.131393	0.388978
H	-2.041007	-0.127243	-2.283937	0.142362	0.195297
H	-1.326669	-3.298318	-0.028098	-0.073974	0.378344
H	-4.196941	0.987855	-2.762477	0.152841	0.668427
C	-2.853296	-0.198601	-1.558961	-0.006649	-0.702067
C	-4.066601	0.436693	-1.834596	-0.115998	-0.456857
H	-1.019577	-1.117187	1.633202	-0.108619	0.075778
C	-2.651887	-0.919340	-0.376394	-0.350959	-0.409455
C	-5.114095	0.362240	-0.915913	-0.222216	-0.554248
H	-6.058670	0.856857	-1.121613	0.149764	1.052003
H	-0.214701	-1.267436	-1.322000	-0.185642	-0.121604

C	-3.718450	-0.980019	0.530533	-0.181883	-0.648048
C	-4.938545	-0.352474	0.270175	-0.122879	-0.570095
H	-3.594762	-1.526908	1.466527	0.151760	0.370885
H	-5.749377	-0.415405	0.990914	0.152114	0.908839
C	1.614526	3.339227	0.225512	-0.133697	-0.424432
C	1.412087	2.500961	1.314506	0.064982	-0.555747
C	0.647636	3.450107	-0.786885	-0.096693	-0.698761
C	0.228490	1.729265	1.456183	-0.223570	-1.208731
C	-0.723524	1.835079	0.406289	-0.577552	-0.690473
C	-0.523684	2.692336	-0.677607	-0.108175	-0.457016
H	2.533779	3.914375	0.158674	0.179023	0.832692
H	0.801407	4.117701	-1.627928	0.172628	0.789084
H	-1.292745	2.757376	-1.443086	0.166271	0.518329
H	-1.643010	1.261431	0.447571	0.108186	0.342260
H	2.174698	2.431798	2.086633	0.157140	0.612842
C	0.050399	0.832087	2.562714	0.213383	0.266234
C	-1.055961	0.008613	2.683561	-0.440331	-1.225421
H	0.898936	0.684770	3.225759	0.152981	0.612698
H	-2.018240	0.317814	2.277390	0.213209	0.340058
H	-1.128289	-0.636234	3.555704	0.156483	0.678858
Si	-0.868571	-1.813810	0.048526	0.435177	-0.232574

10S

Electronic energy: -1019.2106

Electronic energy + zero-point energy: -1018.8081

Electronic energy + thermal energy correction: -1018.7704

Electronic energy + thermal enthalpy correction: -1018.7692

Electronic energy + thermal free energy correction: -1018.8866

BSSE correction: 0.008225

Table S40. Cartesian coordinates, Mulliken and APT charges of all atoms at **10S** in the reaction between phenylsilane and styrene.

Symbol	X	Y	Z	Mulliken	APT
H	-5.180950	-1.130479	-0.295716	0.144016	0.003426
C	-4.911221	-0.869334	0.732226	-0.703909	0.092457
C	-3.497971	-0.265953	0.812884	0.069219	-0.347703
C	-2.407888	-1.220173	0.387053	-1.150505	0.097110
C	-2.449289	-1.859049	-0.859884	0.349209	-0.106148
H	-3.291166	-1.687461	-1.526118	0.160388	0.054852
C	-1.422344	-2.711798	-1.264909	0.127601	0.011156
H	-1.476852	-3.196659	-2.234731	0.176970	0.044945

C	-0.328093	-2.941097	-0.430743	0.000667	-0.083664
H	0.474138	-3.599803	-0.746023	0.196299	0.059828
C	-0.268951	-2.308676	0.813240	-0.512358	-0.052289
H	0.584785	-2.459122	1.468208	0.258017	0.078567
C	-1.299458	-1.456261	1.213733	0.199987	-0.121590
H	-1.242223	-0.969598	2.184692	0.175118	0.058350
Na	0.886207	-0.037679	-0.450155	-0.162718	0.663138
H	-5.659164	-0.159742	1.098914	0.174618	-0.016926
H	-4.979268	-1.779496	1.336150	0.188899	-0.031071
H	-3.304238	0.023005	1.854240	0.148138	-0.022066
H	-1.419593	1.936768	-2.401087	0.166844	0.053275
H	-4.274525	2.341725	0.349007	-0.031103	-0.338276
H	0.902155	2.780458	-2.413352	0.218210	0.055593
C	-0.923004	2.142043	-1.455858	-0.158436	-0.038141
C	0.390112	2.623499	-1.469022	-0.182253	-0.076088
H	2.708579	1.289832	2.717471	0.160436	-0.069437
C	-1.608499	1.932410	-0.248100	0.157914	-0.413552
C	1.043836	2.894349	-0.265344	-0.238153	0.014067
H	2.063472	3.263713	-0.270999	0.201205	0.059498
H	-3.784923	1.020989	-1.613929	-0.009915	-0.306519
C	-0.924282	2.196635	0.952142	-0.291986	-0.014011
C	0.387663	2.670956	0.947926	0.143169	-0.077338
H	-1.419874	2.035950	1.907631	0.195799	0.053119
H	0.898230	2.865973	1.885554	0.160514	0.062535
C	2.832396	-1.641078	-1.580501	0.167491	0.353529
C	2.893689	-1.800558	-0.211870	0.181937	-0.416799
C	3.026115	-0.381501	-2.198498	-0.352403	-0.715469
C	3.109487	-0.681246	0.693822	-0.866220	0.512284
C	3.468269	0.557322	0.018037	-0.228376	-0.499575
C	3.406089	0.683614	-1.360558	-0.049558	0.402125
H	2.627745	-2.511883	-2.200957	0.177692	0.022028
H	2.998724	-0.272141	-3.276067	0.131928	0.044843
H	3.651745	1.646463	-1.806799	0.146977	0.017921
H	3.766342	1.412504	0.617586	0.150513	0.041283
H	2.739248	-2.786435	0.222494	0.114729	0.022611
C	2.937466	-0.772795	2.060298	0.176258	-0.679402
C	3.241956	0.367174	2.993447	-0.677827	0.291301
H	2.738309	-1.750578	2.493822	0.073921	-0.004984
H	4.311939	0.633984	3.019574	0.153450	-0.118439
H	2.948710	0.123871	4.018881	0.151596	-0.038518
Si	-3.379007	1.313696	-0.222419	0.215993	1.418163

Phenylgermane + styrene

5M

Electronic energy: -709.50492

Electronic energy + zero-point energy: -709.24496

Electronic energy + thermal energy correction: -709.21829

Electronic energy + thermal enthalpy correction: -709.21710

Electronic energy + thermal free energy correction: -709.30978

BSSE correction: 0.004709

Table S41. Cartesian coordinates, Mulliken and APT charges of all atoms at **5M** in the reaction between phenylgermane and styrene.

Symbol	X	Y	Z	Mulliken	APT
H	-0.560586	-1.404965	2.778963	0.159380	-0.067225
C	-0.644438	-2.351647	2.222038	-0.486197	0.288092
C	-0.745251	-2.144950	0.737057	-0.342036	-0.770227
C	-1.635433	-1.265751	0.159442	-0.045095	0.547934
C	-2.481472	-0.360305	0.927709	-0.312902	-0.492885
H	-2.458176	-0.413979	2.011856	0.112234	0.040818
C	-3.367408	0.518397	0.317871	-0.026542	0.429978
H	-3.991537	1.146907	0.950539	0.157495	0.020921
C	-3.478986	0.627001	-1.082424	-0.422695	-0.706628
H	-4.197737	1.293695	-1.543208	0.132380	0.042900
C	-2.684053	-0.251839	-1.859290	-0.105800	0.368817
H	-2.770410	-0.229244	-2.943857	0.153540	0.020379
C	-1.795548	-1.140559	-1.284415	-0.065607	-0.413096
H	-1.220292	-1.808750	-1.920975	0.110173	0.028592
Na	-0.991846	1.265018	-0.516700	0.281608	0.640200
H	0.236959	-2.949777	2.476490	0.157167	-0.036496
H	-1.518770	-2.868684	2.650832	0.159458	-0.114873
H	-0.222669	-2.845284	0.090677	0.123189	0.010693
H	2.247893	1.639985	-1.736266	0.181660	0.048889
H	3.653267	-0.940160	-1.253763	-0.132880	-0.363488
H	1.424341	3.830916	-0.951530	0.177177	0.047925
C	1.783128	1.711900	-0.755403	-0.103797	-0.048173
C	1.319136	2.957357	-0.315515	-0.209335	-0.054622
H	1.326910	-1.740850	-1.653842	-0.068188	-0.316295
Ge	2.281519	-1.186944	-0.584571	0.189630	1.474856
C	1.660778	0.566937	0.049552	0.367277	-0.339772
C	0.728831	3.076147	0.945197	-0.164532	-0.065258
H	0.370384	4.040898	1.290007	0.184587	0.056761
H	2.449147	-2.139681	0.605774	-0.076313	-0.325309
C	1.071395	0.707613	1.316011	-0.340479	-0.068152
C	0.607779	1.948109	1.763213	-0.075417	-0.019193
H	0.951656	-0.167147	1.947906	0.135307	0.084347
H	0.150575	2.032670	2.744079	0.195553	0.049587

7M

Electronic energy: -709.50230

Electronic energy + zero-point energy: -709.24170

Electronic energy + thermal energy correction: -709.21598

Electronic energy + thermal enthalpy correction: -709.21480

Electronic energy + thermal free energy correction: -709.30469

BSSE correction: 0.004475

Table S42. Cartesian coordinates, Mulliken and APT charges of all atoms at **7M** in the reaction between phenylgermane and styrene.

Symbol	X	Y	Z	Mulliken	APT
H	1.328183	2.662478	1.344072	0.171601	-0.017499
C	1.704812	2.887552	0.335778	-0.566181	0.159542
C	1.627421	1.677891	-0.575005	-0.125575	-0.931162
C	2.460400	0.539898	-0.269393	-0.418485	0.517527
C	2.917007	0.256915	1.047579	0.014954	-0.272234
H	2.757325	0.989758	1.832149	0.149255	0.054125
C	3.584256	-0.930541	1.355235	-0.126156	0.163616
H	3.928299	-1.096569	2.372537	0.171910	0.035429
C	3.824063	-1.899634	0.374153	-0.340200	-0.339144
H	4.356894	-2.813403	0.613678	0.157504	0.045778
C	3.389968	-1.642989	-0.934656	0.016642	0.156989
H	3.580035	-2.369942	-1.719579	0.177202	0.038117
C	2.721738	-0.461367	-1.247160	-0.092676	-0.251729
H	2.398945	-0.282661	-2.269121	0.165520	0.042625
Na	0.997846	-1.624668	0.524094	0.598674	0.771494
H	1.080421	3.696394	-0.055950	0.160013	-0.011259
H	2.725297	3.279090	0.450374	0.159499	-0.081540
H	1.642010	1.932301	-1.638965	0.181978	-0.011860
H	-3.247375	1.838467	0.770185	0.129179	0.022816
H	-0.979304	2.348479	-0.609020	-0.177561	-0.501949
H	-5.459563	0.808856	1.140003	0.147553	0.008805
C	-3.408745	0.802768	0.469835	-0.168334	-0.057568
C	-4.663709	0.228707	0.680390	-0.154183	-0.017065
H	-0.052070	-0.287338	-1.312834	-0.214600	-0.394324
Ge	-0.488318	0.890258	-0.321782	0.377109	1.938350
C	-2.357808	0.085424	-0.119275	0.097088	-0.489140
C	-4.899496	-1.092709	0.295158	-0.184294	-0.091018
H	-5.875386	-1.542573	0.452288	0.140822	0.025977
H	-0.028581	0.529775	1.156554	-0.202991	-0.411456
C	-2.625566	-1.233430	-0.505048	-0.322489	-0.106740
C	-3.875624	-1.826083	-0.303464	-0.178876	-0.009916
H	-1.842351	-1.814329	-0.998099	0.119304	0.006859

H	-4.055230	-2.850089	-0.621047	0.136793	0.007555

8M

Electronic energy: -854.04038

Electronic energy + zero-point energy: -853.66470

Electronic energy + thermal energy correction: -853.62689

Electronic energy + thermal enthalpy correction: -853.62571

Electronic energy + thermal free energy correction: -853.74470

BSSE correction: 0.005742

Table S43. Cartesian coordinates, Mulliken and APT charges of all atoms at **8M** in the reaction between phenylgermane and styrene.

Symbol	X	Y	Z	Mulliken	APT
H	1.519444	-2.547083	2.212780	0.178348	-0.018143
C	1.815115	-1.589160	2.664237	-0.481250	0.149293
C	1.679154	-0.440734	1.683318	-0.551988	-0.892640
C	2.538669	-0.433946	0.520536	-0.159368	0.480673
C	3.117219	-1.614586	-0.016995	0.200173	-0.260767
H	3.036537	-2.544779	0.536717	0.156842	0.053751
C	3.808858	-1.605709	-1.231183	-0.111544	0.138389
H	4.250410	-2.529183	-1.595888	0.166855	0.034096
C	3.946147	-0.428971	-1.975754	-0.329545	-0.319905
H	4.493771	-0.424787	-2.911957	0.161507	0.044566
C	3.387023	0.751890	-1.465311	0.007186	0.149768
H	3.491296	1.684134	-2.014350	0.170657	0.042640
C	2.699898	0.748349	-0.254228	-0.184137	-0.232079
H	2.274437	1.674524	0.121942	0.116600	0.052093
Na	1.148704	-0.935449	-1.769115	0.587724	0.771039
H	1.155662	-1.432136	3.523381	0.142421	-0.008449
H	2.837907	-1.711762	3.046941	0.166102	-0.080009
H	1.634395	0.537667	2.169614	0.199625	0.000837
H	-3.165879	-1.808391	1.631290	0.124039	0.025749
H	-0.920187	-0.666147	2.318556	-0.145872	-0.488889
H	-5.374000	-2.050421	0.551698	0.151423	0.007966
C	-3.320094	-1.392747	0.635073	0.023376	-0.060835
C	-4.572566	-1.531655	0.032300	-0.153236	-0.010485
H	-0.004123	0.595819	-0.131813	-0.299430	-0.415010
Ge	-0.401794	-0.622168	0.837977	0.404999	1.918357
C	-2.264099	-0.728861	-0.002733	-0.041575	-0.492587
C	-4.797881	-0.997485	-1.237340	-0.158512	-0.084631
H	-5.770979	-1.097900	-1.708916	0.144002	0.024486

H	0.115925	-1.974454	0.172236	-0.210760	-0.415494
C	-2.522070	-0.193123	-1.270049	-0.358297	-0.098859
C	-3.766523	-0.322092	-1.890971	-0.213107	-0.013783
H	-1.739392	0.375224	-1.780224	0.132211	0.001974
H	-3.938827	0.113302	-2.872081	0.147682	0.009720
C	0.439399	3.611771	-0.873792	-0.766782	-0.292629
H	1.473720	3.891561	-0.649374	0.180042	-0.019009
H	0.460646	2.794960	-1.609080	0.243278	0.006112
H	-0.049175	4.452297	-1.383451	0.143512	-0.004507
C	0.215585	3.059403	1.815685	-0.744126	-0.324991
H	-0.257276	2.312952	2.463309	0.191581	0.015910
H	1.300688	2.917861	1.833609	0.170821	-0.004003
H	0.025002	4.038069	2.285618	0.151679	0.007350
C	-1.972849	2.950033	0.203596	-0.815266	-0.327324
H	-2.303114	2.818105	-0.831566	0.186157	-0.002248
H	-2.375703	2.126964	0.803956	0.243505	0.020890
H	-2.450288	3.868807	0.579483	0.149238	0.000701
B	-0.417032	3.145966	0.372849	0.683211	0.910917

9M

Electronic energy: -854.03868

Electronic energy + zero-point energy: -853.66130

Electronic energy + thermal energy correction: -853.62607

Electronic energy + thermal enthalpy correction: -853.62489

Electronic energy + thermal free energy correction: -853.73293

BSSE correction: 0.006369

Table S44. Cartesian coordinates, Mulliken and APT charges of all atoms at **9M** in the reaction between phenylgermane and styrene.

Symbol	X	Y	Z	Mulliken	APT
C	-1.608877	0.073891	1.877787	-0.153077	0.488121
C	-2.566364	-0.352638	0.859218	-0.317573	-0.663366
C	-3.209787	0.558053	-0.011399	-0.273021	-0.575329
H	-3.105574	1.622777	0.163625	0.079206	0.397573
C	-3.985472	0.122555	-1.088451	-0.067418	-0.649042
H	-4.465659	0.857680	-1.728384	0.181397	0.734628
C	-4.155832	-1.241855	-1.342340	-0.280512	-0.393099
H	-4.765931	-1.578992	-2.173476	0.171210	0.954049
C	-3.555089	-2.164580	-0.476795	0.042490	-0.620111
H	-3.696551	-3.229535	-0.637058	0.183640	0.750332
C	-2.780323	-1.731137	0.597881	0.030002	-0.949431

H	-2.329617	-2.462947	1.261722	0.164820	0.413765
Na	-1.316928	-0.622505	-1.518565	0.571888	0.644893
H	3.277552	0.813884	1.634191	0.136211	0.356780
H	0.950038	0.349807	2.471887	-0.147016	0.117900
H	5.518319	0.419255	0.668189	0.153549	0.884589
C	3.397699	0.064814	0.851436	0.041992	-0.551135
C	4.667533	-0.156422	0.313913	-0.197772	-0.556491
H	-0.085380	-1.720704	0.641311	-0.239377	-0.059138
Ge	0.414899	-0.278234	1.126743	0.558626	0.008774
C	2.279144	-0.652155	0.410091	-0.135143	-0.269989
C	4.844596	-1.123014	-0.677304	-0.159104	-0.429690
H	5.829854	-1.299342	-1.098731	0.156992	1.063763
H	0.037596	0.766532	-0.134444	-0.291176	-0.322531
C	2.489581	-1.636499	-0.561881	-0.213926	-0.900169
C	3.751152	-1.874053	-1.110405	-0.302408	-0.570043
H	1.648075	-2.247266	-0.894227	0.093918	0.203510
H	3.885586	-2.643942	-1.865612	0.146160	0.707915
C	1.285470	2.930112	-0.017128	-0.801906	-1.430674
H	0.692965	3.209152	0.861390	0.170933	0.364856
H	2.218557	2.470116	0.322653	0.190386	0.352821
H	1.561354	3.868548	-0.522153	0.121599	0.714043
C	-0.948049	2.604097	-1.523932	-0.736380	-1.320904
H	-1.582865	1.933824	-2.118772	0.130083	0.352186
H	-1.552072	3.001561	-0.702500	0.211940	0.415099
H	-0.723504	3.455351	-2.185598	0.141175	0.730953
C	1.352114	1.298604	-2.200629	-0.791893	-1.315244
H	2.241393	0.790585	-1.817834	0.225711	0.341683
H	0.805677	0.592850	-2.843518	0.101874	0.326142
H	1.705179	2.092037	-2.877586	0.141394	0.720462
B	0.486768	2.039544	-1.075152	0.753212	-0.485376
C	-1.691031	1.517105	2.345583	-0.513822	-1.845100
H	-1.454298	2.216310	1.532980	0.208033	0.196726
H	-2.681179	1.787482	2.736526	0.161463	0.662673
H	-0.958196	1.698533	3.138056	0.161182	0.426524
H	-1.594517	-0.631501	2.717686	0.190438	0.576105

10M

Electronic energy: -854.09558

Electronic energy + zero-point energy: -853.71473

Electronic energy + thermal energy correction: -853.67845

Electronic energy + thermal enthalpy correction: -853.67727

Electronic energy + thermal free energy correction: -853.79265

BSSE correction: 0.007057

Table S45. Cartesian coordinates, Mulliken and APT charges of all atoms at **10M** in the reaction between phenylgermane and styrene.

Symbol	X	Y	Z	Mulliken	APT
C	1.667000	0.548244	-1.472750	0.149715	-0.320035
C	1.785141	1.096335	-0.073180	-1.206031	0.096923
C	0.823924	1.990139	0.419943	-0.869245	-0.158557
H	0.027488	2.325252	-0.240068	0.135467	0.093362
C	0.882743	2.459756	1.734094	0.041832	-0.018832
H	0.131784	3.163048	2.084902	0.166770	0.051265
C	1.914245	2.050030	2.579758	0.041336	-0.091629
H	1.966377	2.416640	3.599887	0.170282	0.043728
C	2.893895	1.184128	2.091710	-0.029974	0.017384
H	3.710700	0.871259	2.735224	0.161343	0.040289
C	2.829932	0.714015	0.780855	0.795539	-0.135788
H	3.597681	0.031782	0.421887	0.195469	0.051584
Na	-1.467259	0.361067	0.989563	0.212429	0.785360
H	-1.646092	-2.230217	-1.316613	0.184379	0.064217
H	0.710966	-1.899011	-2.730959	-0.066882	-0.348846
H	-3.262690	-2.760071	0.463918	0.176875	0.057403
C	-1.321825	-2.196022	-0.279654	0.259685	-0.058486
C	-2.244279	-2.492965	0.727043	-0.185390	-0.041274
H	2.611997	-2.115648	-1.069698	-0.118275	-0.352527
Ge	1.283521	-1.395725	-1.393172	0.277977	1.514999
C	-0.000565	-1.834295	0.029603	0.462580	-0.378752
C	-1.862235	-2.423952	2.068262	-0.128954	-0.040938
H	-2.579224	-2.651511	2.850731	0.195251	0.055794
H	-1.611854	0.855484	-1.042270	-0.625190	-0.439458
C	0.367936	-1.775327	1.386150	-0.799212	-0.080932
C	-0.553168	-2.061403	2.398569	-0.198467	-0.045658
H	1.382581	-1.499427	1.662774	0.136091	0.062787
H	-0.246902	-2.010684	3.438920	0.191237	0.047561
C	-3.126103	2.012548	-2.382272	-0.797528	-0.148415
H	-2.377962	2.703197	-2.797208	0.122954	-0.063651
H	-3.258358	1.205668	-3.116754	0.122828	-0.061865
H	-4.077976	2.564625	-2.343774	0.136171	-0.076903
C	-2.561867	2.725634	0.145223	-0.813500	-0.187297
H	-2.257746	2.519693	1.190592	0.186503	-0.111236
H	-1.868070	3.498897	-0.215035	0.176322	-0.052988
H	-3.543080	3.212510	0.240186	0.145089	-0.051774
C	-3.860909	0.397318	-0.360077	-0.712670	-0.187094
H	-3.961120	-0.486046	-1.006911	0.184374	-0.053344
H	-3.763170	0.003431	0.669679	0.152219	-0.109631
H	-4.835508	0.906946	-0.366991	0.145329	-0.057485
B	-2.711454	1.454059	-0.908088	0.972239	0.676140
C	2.913350	0.801486	-2.335384	-0.497432	0.073229
H	3.121364	1.874251	-2.404908	0.179463	-0.033553
H	3.800957	0.315584	-1.917810	0.157636	-0.001604
H	2.772498	0.418359	-3.350996	0.172673	-0.013066

H	0.796521	1.013139	-1.949324	0.240693	-0.010405

11M

Electronic energy: -546.65853

Electronic energy + zero-point energy: -546.40401

Electronic energy + thermal energy correction: -546.38165

Electronic energy + thermal enthalpy correction: -546.38046

Electronic energy + thermal free energy correction: -546.46642

BSSE correction: 0.002839

Table S46. Cartesian coordinates, Mulliken and APT charges of all atoms at **11M** in the reaction between phenylgermane and styrene.

Symbol	X	Y	Z	Mulliken	APT
H	4.675482	-2.288029	0.439743	0.151510	0.031141
H	2.304484	-1.973316	1.051184	0.128612	0.035899
C	4.209351	-1.317026	0.302087	-0.073328	0.018257
C	2.872859	-1.138028	0.647640	-0.457386	-0.130642
H	0.542734	-0.456398	1.638311	0.237192	-0.027583
C	4.948997	-0.252098	-0.214249	-0.067798	-0.114324
C	2.240317	0.104637	0.490664	-0.198963	0.188850
C	0.780979	0.255380	0.838181	0.070820	-0.382137
H	5.991865	-0.387527	-0.482392	0.144813	0.036564
H	0.406459	2.385387	0.460092	0.206489	0.004334
C	0.361521	1.661539	1.281614	-0.674671	0.044603
H	-2.360829	-2.201656	0.446549	0.158731	0.036330
H	-0.668616	1.654193	1.649612	0.167133	-0.005800
H	0.030920	0.661731	-1.887032	-0.088535	-0.345785
C	4.334588	0.987426	-0.378311	-0.180880	0.019641
C	2.994876	1.163988	-0.030355	0.043021	-0.142437
H	-4.736393	-2.009892	1.075301	0.153993	0.027893
C	-2.882291	-1.262393	0.273697	-0.134185	-0.066519
C	-4.227283	-1.160424	0.630029	-0.239783	-0.045309
H	1.009691	2.031067	2.084232	0.169835	-0.029645
H	0.053008	-1.758195	-1.107474	-0.091766	-0.354293
Ge	-0.298285	-0.305245	-0.729376	0.253199	1.558053
H	4.898928	1.825240	-0.776819	0.151314	0.029434
H	2.537661	2.139913	-0.163852	0.119572	0.050138
C	-2.203756	-0.180966	-0.306690	0.214207	-0.390240
C	-4.917281	0.031494	0.410347	-0.117433	-0.035763
H	-5.964577	0.112618	0.684643	0.152768	0.036827
C	-2.914339	1.009184	-0.520741	-0.347278	-0.071039

C	-4.259355	1.117600	-0.166456	-0.158552	-0.042313
H	-2.417341	1.864343	-0.974365	0.146782	0.037776
H	-4.793456	2.046467	-0.342447	0.160567	0.028090

5aM

Electronic energy: -709.47387

Electronic energy + zero-point energy: -709.21433

Electronic energy + thermal energy correction: -709.18735

Electronic energy + thermal enthalpy correction: -709.18617

Electronic energy + thermal free energy correction: -709.28557

BSSE correction: 0.003003

Table S47. Cartesian coordinates, Mulliken and APT charges of all atoms at **5aM** in the reaction between phenylgermane and styrene.

Symbol	X	Y	Z	Mulliken	APT
Na	1.771177	-0.749288	1.487645	0.833625	0.824132
H	3.725332	-2.551746	-0.730716	0.164733	-0.070794
C	5.309559	0.591959	1.214028	-0.125652	0.000292
H	5.861761	0.498827	2.145137	0.151710	0.027023
C	5.219174	1.829451	0.576763	-0.074749	-0.112299
C	4.703360	-0.532202	0.648198	-0.292527	-0.113208
H	5.691349	2.705418	1.010444	0.147120	0.036305
H	4.791344	-1.499753	1.140834	0.102088	0.032172
C	4.528173	1.926742	-0.632803	-0.157983	0.017519
C	4.003636	-0.450925	-0.564145	-0.355398	0.104644
C	3.931332	0.798630	-1.194290	-0.058265	-0.107399
C	3.264762	-1.638674	-1.129939	-0.269427	0.149952
H	4.460006	2.883810	-1.142032	0.145310	0.032059
H	3.442695	-1.655071	-2.220352	0.114738	-0.169875
C	1.769885	-1.592704	-0.738590	-0.624802	-0.484020
H	3.395499	0.879913	-2.137313	0.146322	0.041670
H	1.292992	-2.540961	-1.027529	0.098660	-0.110216
H	1.287160	-0.814038	-1.354933	0.051725	-0.099305
H	-4.042501	-1.910635	0.503733	0.150686	0.034860
H	-1.334626	-1.797418	-0.597072	-0.076001	-0.304097
H	-6.435088	-1.344224	0.661663	0.162429	0.026903
C	-4.359431	-0.887394	0.313251	-0.545594	-0.068547
C	-5.715710	-0.573323	0.402127	0.023963	-0.047499
H	-0.913504	-0.217397	1.315440	-0.204900	-0.413826
Ge	-1.502824	-0.353074	-0.111345	0.126850	1.501187
C	-3.410430	0.088883	-0.022479	0.855297	-0.352252

C	-6.146675	0.729464	0.152526	-0.304075	-0.037231
H	-7.201961	0.976049	0.218195	0.154266	0.036806
H	-0.807860	0.666125	-1.026990	-0.065968	-0.317822
C	-3.863088	1.391508	-0.274234	-0.566427	-0.073134
C	-5.218274	1.712754	-0.187508	-0.009014	-0.045491
H	-3.153634	2.169397	-0.548269	0.137811	0.034693
H	-5.549171	2.727225	-0.388740	0.163450	0.026797

6aM

Electronic energy: -709.47466

Electronic energy + zero-point energy: -709.21504

Electronic energy + thermal energy correction: -709.18955

Electronic energy + thermal enthalpy correction: -709.18837

Electronic energy + thermal free energy correction: -709.28225

BSSE correction: 0.003706

Table S48. Cartesian coordinates, Mulliken and APT charges of all atoms at **6aM** in the reaction between phenylgermane and styrene.

Symbol	X	Y	Z	Mulliken	APT
Na	-1.713131	-0.559292	1.565924	0.744543	0.820368
H	-1.503548	-0.478168	-2.053125	0.163874	0.157658
C	-3.573312	2.072809	0.286409	-0.038678	-0.462338
H	-3.230229	3.074299	0.529968	0.166621	0.469971
C	-4.841324	1.650876	0.689822	-0.158669	-0.449245
C	-2.748150	1.213503	-0.443711	0.112320	-0.620648
H	-5.487208	2.317327	1.252599	0.151936	0.996053
H	-1.761792	1.547004	-0.761907	0.140204	0.068109
C	-5.275919	0.368333	0.350311	-0.148506	-0.388497
C	-3.169166	-0.079810	-0.790980	-0.626313	-0.911747
C	-4.448069	-0.483372	-0.382047	-0.049941	-0.528829
C	-2.236228	-1.051605	-1.468389	-0.179059	-0.567111
H	-6.264845	0.034045	0.650233	0.156678	1.081481
H	-2.821984	-1.637486	-2.197496	0.131160	0.606323
C	-1.500317	-1.899788	-0.406685	-0.819625	-1.605313
H	-4.792147	-1.480654	-0.646802	0.160030	0.639276
H	-0.795780	-2.574376	-0.914173	0.131256	0.303137
H	-2.256629	-2.575277	0.044840	0.071461	0.518717
H	3.684096	-1.417765	1.433894	0.164504	0.313440
H	1.283050	-2.057701	0.563563	-0.081557	0.188977
H	5.963604	-0.478116	1.461322	0.153357	0.949910
C	3.913581	-0.563117	0.799718	-0.180134	-0.814831

C	5.206711	-0.037567	0.818719	-0.063411	-0.582965
H	0.663665	-0.565041	-1.383863	-0.169106	0.000438
C	2.912388	-0.021994	-0.020440	0.535560	-0.403666
C	5.526774	1.050335	0.007365	-0.245771	-0.182501
H	6.531814	1.461413	0.016548	0.149618	1.180361
H	0.445467	0.224707	0.935227	-0.218003	-0.092648
C	3.262326	1.068342	-0.832301	-0.566167	-0.776427
C	4.550494	1.603408	-0.822068	-0.063859	-0.564647
H	2.516469	1.508191	-1.492717	0.141293	0.119800
H	4.794848	2.446527	-1.461822	0.156258	0.740037
Ge	1.137402	-0.704338	0.002631	0.178124	-0.202642

7aM

Electronic energy: -709.49755

Electronic energy + zero-point energy: -709.23618

Electronic energy + thermal energy correction: -709.21144

Electronic energy + thermal enthalpy correction: -709.21025

Electronic energy + thermal free energy correction: -709.29912

BSSE correction: 0.004391

Table S49. Cartesian coordinates, Mulliken and APT charges of all atoms at **7aM** in the reaction between phenylgermane and styrene.

Symbol	X	Y	Z	Mulliken	APT
Na	-1.517815	1.626710	-0.560902	0.487530	0.765695
H	-1.672668	-2.619398	-0.171326	0.146699	-0.017124
C	-4.013222	0.425736	-1.304582	-0.081553	-0.024112
H	-4.355959	0.545060	-2.327828	0.185396	0.051388
C	-4.415988	1.331354	-0.320079	-0.311153	-0.082542
C	-3.170449	-0.641309	-0.974422	0.167477	-0.092273
H	-5.076079	2.155486	-0.570780	0.167221	0.053511
H	-2.852611	-1.336438	-1.746510	0.179044	0.063530
C	-3.980315	1.151530	0.997417	0.090856	-0.029863
C	-2.716422	-0.826528	0.338343	-0.682005	0.061228
C	-3.140696	0.084519	1.318474	0.068684	-0.087758
C	-1.785464	-1.962221	0.699363	-0.346884	0.116271
H	-4.296348	1.842214	1.772908	0.194088	0.052592
H	-2.264562	-2.561218	1.485420	0.180088	-0.079877
C	-0.397825	-1.486200	1.167370	-0.569121	-0.305202
H	-2.801936	-0.044006	2.343169	0.165518	0.064187
H	0.186253	-2.360508	1.476337	0.152646	-0.052182
H	-0.491615	-0.817767	2.029227	0.199692	-0.034429

H	2.074742	1.884097	0.919211	0.125506	0.062727
H	0.135217	1.060972	0.493406	-0.292161	-0.707096
H	4.447545	2.577547	1.134669	0.147109	0.010451
C	2.864369	1.246163	0.529309	-0.680369	-0.106726
C	4.198844	1.637068	0.650284	-0.258532	-0.040976
H	1.046602	-1.973374	-1.031612	-0.278375	-0.599474
C	2.511202	0.039455	-0.087374	0.828414	-0.424576
C	5.213931	0.821276	0.149748	-0.196270	-0.049703
H	6.253357	1.123648	0.239859	0.141931	0.023301
H	-0.253287	-0.099765	-1.523591	-0.162518	-0.496639
C	3.546145	-0.768576	-0.578500	-0.246154	-0.087237
C	4.884245	-0.386018	-0.465853	-0.188278	-0.046859
H	3.296726	-1.712774	-1.057935	0.161331	0.054626
H	5.667974	-1.028644	-0.857409	0.148406	0.011307
Ge	0.626953	-0.578951	-0.286071	0.355736	1.973834

8aM

Electronic energy: -854.03747

Electronic energy + zero-point energy: -853.66082

Electronic energy + thermal energy correction: -853.62637

Electronic energy + thermal enthalpy correction: -853.62519

Electronic energy + thermal free energy correction: -853.73604

BSSE correction: 0.006027

Table S50. Cartesian coordinates, Mulliken and APT charges of all atoms at **8aM** in the reaction between phenylgermane and styrene.

Symbol	X	Y	Z	Mulliken	APT
Na	-1.566595	0.347907	1.521906	0.378367	0.766287
H	-1.657968	-1.580520	-2.441014	0.126693	-0.012723
C	-3.887701	0.825565	-0.152956	0.018487	-0.033654
H	-4.116267	1.848842	-0.435126	0.171774	0.058783
C	-4.422514	0.282558	1.018918	-0.270133	-0.085005
C	-3.057366	0.049675	-0.966499	0.337375	-0.093230
H	-5.076504	0.877290	1.648662	0.178941	0.055473
H	-2.632545	0.476289	-1.871313	0.164113	0.066771
C	-4.125203	-1.040613	1.362940	0.112554	-0.032572
C	-2.742027	-1.273954	-0.629471	-0.675325	0.058206
C	-3.291558	-1.806885	0.546045	-0.103838	-0.080520
C	-1.806205	-2.095926	-1.484842	-0.396060	0.109046
H	-4.545851	-1.474896	2.264589	0.192992	0.050971
H	-2.289601	-3.054934	-1.712027	0.184972	-0.078665

C	-0.440491	-2.334613	-0.814106	-0.589345	-0.301954
H	-3.060711	-2.832835	0.821805	0.163471	0.061485
H	0.174422	-2.951413	-1.479816	0.140175	-0.050702
H	-0.568137	-2.876569	0.128856	0.188648	-0.037241
H	2.135044	-0.874552	2.167104	0.126625	0.060250
H	0.138250	-0.782605	1.317916	-0.229272	-0.692872
H	4.539939	-0.806488	2.775775	0.146848	0.011422
C	2.886990	-0.738503	1.393343	-0.555641	-0.102943
C	4.239675	-0.698918	1.736974	-0.239575	-0.036753
H	0.884444	-0.373990	-2.071012	-0.213118	-0.590611
C	2.469992	-0.604082	0.063542	0.496617	-0.420055
C	5.206485	-0.519645	0.747614	-0.129273	-0.041515
H	6.259590	-0.485458	1.011666	0.149568	0.022936
H	-0.331942	0.681468	-0.420610	-0.416535	-0.563025
C	3.457168	-0.427792	-0.916096	-0.111425	-0.086985
C	4.811818	-0.385211	-0.583745	-0.215032	-0.042651
H	3.154967	-0.313629	-1.955053	0.158569	0.059866
H	5.558164	-0.244581	-1.360684	0.156342	0.012548
C	-0.156653	2.841769	1.318139	-0.833415	-0.308790
H	-1.222511	2.818685	1.586522	0.124192	-0.048287
H	0.389800	2.013385	1.790664	0.178300	0.013310
H	0.245078	3.751877	1.786586	0.156384	0.023269
C	-1.001505	3.359092	-1.258053	-0.770464	-0.302752
H	-0.647288	4.114001	-1.968972	0.160083	-0.011483
H	-1.264100	2.479470	-1.861393	0.242512	0.025220
H	-1.921732	3.722021	-0.787830	0.168440	-0.028026
C	1.616843	2.805443	-0.752840	-0.878515	-0.333288
H	2.302509	2.320663	-0.051029	0.198710	0.000176
H	1.672764	2.274582	-1.711584	0.222260	0.033479
H	1.994546	3.821198	-0.944418	0.154027	-0.001803
B	0.132147	2.933859	-0.238461	1.019729	0.963725
Ge	0.559718	-0.639729	-0.485949	0.409202	1.964884

10aM

Electronic energy: -854.08717

Electronic energy + zero-point energy: -853.70637

Electronic energy + thermal energy correction: -853.67033

Electronic energy + thermal enthalpy correction: -853.66915

Electronic energy + thermal free energy correction: -853.78495

BSSE correction: 0.006153

Table S51. Cartesian coordinates, Mulliken and APT charges of all atoms at **10aM** in the reaction between phenylgermane and styrene.

Symbol	X	Y	Z	Mulliken	APT
Na	2.283096	-0.091914	-1.477713	0.464948	0.812490
H	1.350954	0.410918	2.066960	0.145445	0.011685
C	3.980220	-1.863752	0.097998	-0.033353	-0.024832
H	5.050710	-1.683363	0.104617	0.189955	0.056647
C	3.426745	-2.773926	-0.809394	-0.172814	-0.093241
C	3.157062	-1.172764	0.985569	0.412155	-0.100868
H	4.063618	-3.312337	-1.503694	0.175620	0.053643
H	3.589570	-0.444180	1.666363	0.128757	0.078087
C	2.048071	-2.989186	-0.803863	-0.105283	-0.012703
C	1.766983	-1.371726	0.998011	-0.314593	0.071570
C	1.228258	-2.295584	0.093614	-0.500023	-0.104231
C	0.924077	-0.595073	1.986413	-0.605684	0.129239
H	1.605673	-3.699378	-1.495724	0.184932	0.049601
H	1.054651	-1.066650	2.970252	0.193313	-0.083151
C	-0.571276	-0.501900	1.670350	-0.157368	-0.319084
H	0.158273	-2.477414	0.075788	0.095158	0.056851
H	-1.071119	0.014607	2.498024	0.238431	-0.009773
H	-1.031159	-1.497061	1.632288	0.214311	-0.017608
H	-2.799311	-1.979380	-0.631020	0.109874	0.023850
H	-0.440874	-0.059421	-1.222804	-0.177088	-0.421837
H	-5.207012	-2.463378	-0.809288	0.161867	0.025813
C	-3.515236	-1.176635	-0.459033	-0.749913	-0.064025
C	-4.876732	-1.458702	-0.562555	-0.224007	-0.047247
H	-0.947886	1.995037	0.183048	-0.035587	-0.315610
Ge	-1.142794	0.478539	0.054445	0.232156	1.612671
C	-3.060764	0.112856	-0.144196	0.461999	-0.382702
C	-5.814101	-0.447430	-0.348233	-0.170012	-0.042749
H	-6.875205	-0.663102	-0.427287	0.150829	0.034912
H	1.592704	1.287225	-0.137563	-0.608438	-0.487747
C	-4.017910	1.114748	0.065781	0.154573	-0.070302
C	-5.383249	0.840366	-0.033952	-0.124914	-0.037904
H	-3.698645	2.125706	0.309299	0.177020	0.039680
H	-6.108429	1.631205	0.132867	0.163148	0.025867
C	3.760004	1.899727	-1.044037	-0.832884	-0.212979
H	4.337410	1.049727	-0.640596	0.134542	-0.075818
H	3.643890	1.738720	-2.133390	0.088199	-0.088993
H	4.434762	2.762792	-0.973586	0.169470	-0.038167
C	2.747355	2.680875	1.328147	-0.888056	-0.174602
H	3.371156	3.587792	1.352236	0.126461	-0.072002
H	1.855318	2.898934	1.934365	0.165106	-0.059032
H	3.314506	1.903662	1.864234	0.182118	-0.075406
C	1.571902	3.478123	-0.977732	-0.823806	-0.166602
H	1.234081	3.209268	-1.991421	0.116542	-0.077967
H	0.679537	3.807675	-0.427205	0.164753	-0.058809
H	2.215063	4.364690	-1.091401	0.135690	-0.076931

B	2.370935	2.275079	-0.210020	1.186452	0.730314

11aM

Electronic energy: -546.65744

Electronic energy + zero-point energy: -546.40251

Electronic energy + thermal energy correction: -546.38049

Electronic energy + thermal enthalpy correction: -546.37931

Electronic energy + thermal free energy correction: -546.46396

BSSE correction: 0.002758

Table S52. Cartesian coordinates, Mulliken and APT charges of all atoms at **11aM** in the reaction between phenylgermane and styrene.

Symbol	X	Y	Z	Mulliken	APT
H	5.150534	2.240296	-0.352403	0.153239	0.039954
C	4.479059	1.406292	-0.174381	-0.229076	-0.066968
C	4.096926	1.078163	1.127570	0.090238	-0.012252
C	3.996772	0.653347	-1.242994	0.010551	-0.007501
H	4.473073	1.656042	1.966347	0.158894	0.035101
H	4.291445	0.898302	-2.258858	0.160075	0.037112
C	3.234031	0.008310	1.353622	-0.379333	-0.085069
C	3.134060	-0.418832	-1.010591	-0.459109	-0.107616
C	2.738771	-0.752670	0.288099	0.041051	0.036350
H	2.938560	-0.242997	2.370079	0.123623	0.040901
H	2.759798	-1.002444	-1.848627	0.131383	0.045457
C	1.740636	-1.858533	0.540412	-0.256265	0.147607
C	0.343653	-1.305519	0.879071	-0.439865	-0.314719
H	2.094589	-2.493135	1.361968	0.176427	-0.080508
H	0.374523	-0.754675	1.826625	0.234267	-0.011710
H	-0.365375	-2.130196	1.017731	0.193793	-0.035107
H	1.676407	-2.495732	-0.348876	0.177716	-0.029475
H	-0.179571	-0.743653	-1.880228	-0.152140	-0.367121
H	-4.559418	2.561876	0.734860	0.161301	0.026803
H	-2.151350	2.265031	0.291412	0.167903	0.036667
C	-4.181122	1.584849	0.449425	-0.041585	-0.039765
C	-2.818813	1.411331	0.198295	-0.054552	-0.073224
C	-5.054008	0.504480	0.332848	-0.238404	-0.039080
Ge	-0.389665	-0.095717	-0.491366	0.232894	1.541689
C	-2.304896	0.161396	-0.172587	0.564251	-0.361904
H	-6.114053	0.636872	0.526593	0.156088	0.036409
C	-4.561364	-0.747738	-0.036361	-0.068407	-0.047997
C	-3.199584	-0.913517	-0.285424	-0.835940	-0.063282

H	-5.237424	-1.592201	-0.131149	0.159967	0.027175
H	-2.834803	-1.897210	-0.575541	0.129311	0.030843
H	0.287629	1.288596	-0.458256	-0.068295	-0.338772

6L

Electronic energy: -709.48593

Electronic energy + zero-point energy: -709.22839

Electronic energy + thermal energy correction: -709.20266

Electronic energy + thermal enthalpy correction: -709.20147

Electronic energy + thermal free energy correction: -709.29155

BSSE correction: 0.003459

Table S53. Cartesian coordinates, Mulliken and APT charges of all atoms at **6L** in the reaction between phenylgermane and styrene.

Symbol	X	Y	Z	Mulliken	APT
H	-2.106886	-2.286012	1.426276	0.165282	-0.027175
C	-2.952655	-2.191761	0.723482	-0.615187	0.287685
C	-2.615887	-1.284392	-0.432999	0.171229	-1.245723
C	-2.459443	0.101245	-0.228503	-0.313927	0.529728
C	-2.158975	0.650456	1.064055	-0.328775	-0.316315
H	-2.162786	-0.004655	1.929779	0.127444	0.048832
C	-1.935573	2.014841	1.249347	-0.123234	0.283572
H	-1.747506	2.384507	2.254665	0.173133	0.035094
C	-1.946971	2.914162	0.174216	-0.209006	-0.506496
H	-1.799434	3.976789	0.329623	0.154107	0.044945
C	-2.198344	2.394575	-1.113956	-0.202246	0.243055
H	-2.223312	3.066931	-1.968057	0.154350	0.029896
C	-2.422582	1.040397	-1.314387	-0.078556	-0.304704
H	-2.627967	0.675304	-2.318042	0.151039	0.026941
Na	0.127669	1.318573	-0.340594	0.395139	0.641986
H	-3.177746	-3.201657	0.368821	0.157635	-0.025352
H	-3.814297	-1.843896	1.311083	0.166380	-0.073094
H	-2.961618	-1.589545	-1.419250	0.170324	0.022038
H	2.493588	-0.602912	-2.040696	0.192001	0.031262
H	1.209250	-2.957738	-1.273336	-0.123601	-0.394362
H	3.901525	1.414149	-1.885890	0.177764	0.031180
C	2.580644	-0.089569	-1.085205	0.181917	-0.129582
C	3.381922	1.053541	-1.002864	-0.081207	0.034592
H	-1.045404	-1.637668	-0.451707	-0.014086	0.756267
Ge	0.608337	-2.110345	-0.115333	0.026802	0.813292
C	1.895440	-0.593208	0.036765	-0.257219	-0.328813

C	3.522802	1.725205	0.212624	-0.242548	-0.117444
H	4.146613	2.610670	0.280381	0.173062	0.045916
H	0.867695	-2.934953	1.176178	-0.125385	-0.414613
C	2.058747	0.101123	1.252329	-0.317701	-0.147357
C	2.860724	1.240769	1.344271	-0.081296	0.044577
H	1.545945	-0.255278	2.144347	0.192733	0.045146
H	2.972107	1.748401	2.297958	0.183634	0.035025

7L

Electronic energy: -709.53755

Electronic energy + zero-point energy: -709.27301

Electronic energy + thermal energy correction: -709.2465

Electronic energy + thermal enthalpy correction: -709.24532

Electronic energy + thermal free energy correction: -709.33945

BSSE correction: 0.001859

Table S54. Cartesian coordinates, Mulliken and APT charges of all atoms at **7L** in the reaction between phenylgermane and styrene.

Symbol	X	Y	Z	Mulliken	APT
H	-1.498833	-1.978720	1.708134	0.174184	0.000233
C	-2.295357	-1.519375	2.303667	-0.560519	0.046780
C	-3.256207	-0.723265	1.423677	-0.266573	0.117083
C	-2.608292	0.343224	0.564189	-0.058074	0.058184
C	-1.296068	0.779153	0.777067	-0.220732	-0.145550
H	-0.693251	0.335435	1.561846	0.131259	0.095734
C	-0.720092	1.767314	-0.027733	-0.312955	-0.022795
H	0.309635	2.065556	0.154424	0.128712	0.077699
C	-1.455230	2.339947	-1.065521	-0.328482	-0.087386
H	-1.012331	3.107925	-1.691506	0.183273	0.055865
C	-2.770142	1.915300	-1.293445	-0.111911	-0.019363
H	-3.353824	2.357137	-2.095376	0.174067	0.044392
C	-3.336008	0.926906	-0.486677	0.294126	-0.101800
H	-4.358556	0.603407	-0.667823	0.163132	0.048116
Na	-1.212436	-0.544402	-1.822327	0.494223	0.712835
H	-2.833669	-2.315845	2.822634	0.165068	-0.019248
H	-1.827929	-0.887172	3.064138	0.176808	-0.005132
H	-4.017239	-0.241985	2.050819	0.191853	-0.035738
H	2.656238	0.359716	-1.889701	0.128827	0.018533
H	2.208400	-2.697155	-1.451150	-0.193475	-0.440431
H	3.630513	2.457463	-1.050566	0.148150	0.013145
C	2.617274	0.568832	-0.820461	-0.558490	-0.140860

C	3.166193	1.763953	-0.354106	-0.180904	0.024442
H	-3.803331	-1.409271	0.765994	0.162316	-0.030370
Ge	1.034831	-1.953863	-0.702989	-0.089615	0.595735
C	2.017145	-0.364709	0.042792	0.185266	-0.235876
C	3.116106	2.071711	1.007376	-0.147709	-0.124507
H	3.534681	3.003224	1.376393	0.158384	0.027844
H	0.954301	-2.841910	0.601993	-0.151808	-0.415626
C	2.000779	-0.038731	1.408683	-0.012798	-0.161375
C	2.531455	1.161565	1.888919	-0.180154	0.009529
H	1.561714	-0.739578	2.117838	0.161638	0.026595
H	2.496345	1.382850	2.952581	0.152912	0.013313

8L

Electronic energy: -398.77724

Electronic energy + zero-point energy: -398.67207

Electronic energy + thermal energy correction: -398.65882

Electronic energy + thermal enthalpy correction: -398.65764

Electronic energy + thermal free energy correction: -398.72114

BSSE correction: 0.000426

Table S55. Cartesian coordinates, Mulliken and APT charges of all atoms at **8L** in the reaction between phenylgermane and styrene.

Symbol	X	Y	Z	Mulliken	APT
H	1.510655	-0.540713	-1.985076	-0.182128	-0.437673
H	1.479580	-2.062057	-0.115980	-0.160570	-0.429703
C	-0.549584	-0.196197	-0.169632	0.489225	-0.232461
C	-1.198097	0.860262	-0.830540	-0.766104	-0.128833
C	-1.319666	-0.948867	0.731166	-0.381351	-0.142173
C	-2.544861	1.151899	-0.610255	0.070113	0.012935
H	-0.641710	1.468389	-1.543175	0.099509	0.013148
C	-2.666909	-0.664240	0.964575	0.034265	0.014535
H	-0.861458	-1.783881	1.258452	0.126521	0.016988
C	-3.286641	0.390038	0.293828	-0.248657	-0.120331
H	-3.017410	1.971440	-1.145474	0.143089	0.007723
H	-3.235044	-1.270251	1.665508	0.143922	0.007353
H	-4.334965	0.612598	0.469245	0.143786	0.024178
Ge	1.415731	-0.513838	-0.410716	-0.182561	0.616414
Na	3.017411	1.317267	1.114959	0.670942	0.777901

9L

Electronic energy: -708.30941

Electronic energy + zero-point energy: -708.06842

Electronic energy + thermal energy correction: -708.04259

Electronic energy + thermal enthalpy correction: -708.0414

Electronic energy + thermal free energy correction: -708.13508

BSSE correction: 0.002467

Table S56. Cartesian coordinates, Mulliken and APT charges of all atoms at **9L** in the reaction between phenylgermane and styrene.

Symbol	X	Y	Z	Mulliken	APT
H	1.791586	-3.157597	0.565398	-0.194912	-0.441344
H	1.762727	-2.462004	-1.735338	-0.156495	-0.420562
C	2.059184	-0.442997	0.108533	0.262647	-0.230268
C	2.057480	0.041631	1.427469	-0.644849	-0.140763
C	2.685880	0.358961	-0.858523	-0.019746	-0.155464
C	2.648701	1.258251	1.770214	-0.258321	0.007918
H	1.580669	-0.546069	2.212243	0.148688	0.021004
C	3.274842	1.583501	-0.531984	-0.140169	0.011902
H	2.716520	0.021184	-1.892688	0.155448	0.026517
C	3.258221	2.040580	0.786313	-0.108570	-0.122410
H	2.635396	1.598093	2.802707	0.147499	0.013976
H	3.753221	2.178474	-1.305807	0.154690	0.012386
H	3.718148	2.989474	1.045806	0.158372	0.028393
Ge	1.055886	-2.114742	-0.366953	-0.119124	0.605454
Na	-1.798297	-1.690979	-0.160220	0.615078	0.748474
C	-0.404828	1.843667	-0.222216	-0.141804	-0.028309
C	-1.247213	1.283426	0.736575	0.383428	-0.091080
C	-0.853404	1.998811	-1.531493	-0.270814	-0.041733
C	-2.545264	0.870437	0.403572	-0.659603	-0.042273
C	-2.993538	1.052648	-0.916506	-0.275208	-0.096386
C	-2.149960	1.606341	-1.875343	-0.065390	-0.038517
H	0.605399	2.132518	0.051974	0.145243	0.083764
H	-0.195175	2.422647	-2.282997	0.174094	0.059160
H	-2.508076	1.743672	-2.890774	0.169562	0.044408
H	-4.010198	0.782092	-1.187306	0.120180	0.054322
H	-0.884246	1.145351	1.752307	0.181887	0.068194
C	-3.370644	0.208253	1.435640	-0.049677	0.128034
C	-4.441643	-0.562856	1.211377	-0.197504	-0.222631
H	-3.030738	0.345900	2.460987	0.147763	0.039477
H	-4.829574	-0.746004	0.212052	0.161178	0.058505
H	-4.979621	-1.019142	2.034589	0.176426	0.059852

10L

Electronic energy: -708.28684

Electronic energy + zero-point energy: -708.04624

Electronic energy + thermal energy correction: -708.02215

Electronic energy + thermal enthalpy correction: -708.02097

Electronic energy + thermal free energy correction: -708.10852

BSSE correction: 0.002524

Table S57. Cartesian coordinates, Mulliken and APT charges of all atoms at **10L** in the reaction between phenylgermane and styrene.

Symbol	X	Y	Z	Mulliken	APT
H	1.179567	-2.594485	-0.529432	-0.188518	-0.540726
H	-0.096289	-0.588631	-1.029338	-0.268579	-0.478597
C	2.464604	-0.228011	-0.134479	0.564312	-0.168138
C	2.512237	1.176645	-0.132765	-0.992578	-0.159177
C	3.687326	-0.905439	-0.268057	0.301349	-0.162856
C	3.714070	1.872235	-0.268463	-0.356493	-0.011965
H	1.589070	1.744846	-0.032909	0.048434	0.022194
C	4.897328	-0.220184	-0.396229	-0.055115	0.019154
H	3.696104	-1.993588	-0.280505	0.146186	0.033430
C	4.915363	1.174269	-0.399957	-0.208296	-0.108437
H	3.714003	2.959048	-0.272274	0.154489	0.010727
H	5.825579	-0.775687	-0.499819	0.142333	0.003327
H	5.853248	1.711337	-0.505688	0.140444	0.023681
Ge	0.757822	-1.227323	0.178933	0.107704	0.693584
Na	-2.111982	-0.585592	-1.654967	0.665219	0.713409
C	-4.233352	1.264357	-0.811862	0.004834	0.205029
C	-3.045921	1.672613	-0.220271	-0.314856	-0.401616
C	-4.757617	-0.016206	-0.557895	-0.357566	-0.311436
C	-2.317212	0.826007	0.659731	-0.151439	0.785595
C	-2.869462	-0.459908	0.912857	-0.468181	-0.208427
C	-4.070639	-0.858869	0.319237	0.199269	0.128159
H	-4.760551	1.941798	-1.477321	0.171198	0.036995
H	-5.690685	-0.331414	-1.012006	0.163775	0.043906
H	-4.467632	-1.845517	0.541617	0.188511	0.040929
H	-2.356772	-1.145244	1.578381	0.045689	0.050793
H	-2.649480	2.662107	-0.433807	0.154039	0.043329
C	-1.033619	1.222689	1.169072	0.301562	-1.142645
C	-0.245017	0.393534	1.937256	-0.661052	0.883651
H	-0.613728	2.142692	0.769614	0.142986	0.014145
H	-0.677627	-0.394654	2.540155	0.203980	-0.068586
H	0.728174	0.740863	2.273080	0.176360	0.010569

11L

Electronic energy: -708.31385

Electronic energy + zero-point energy: -708.07259

Electronic energy + thermal energy correction: -708.04921

Electronic energy + thermal enthalpy correction: -708.04803

Electronic energy + thermal free energy correction: -708.13241

BSSE correction: 0.003846

Table S58. Cartesian coordinates, Mulliken and APT charges of all atoms at **11L** in the reaction between phenylgermane and styrene.

Symbol	X	Y	Z	Mulliken	APT
H	-1.374497	2.822298	-0.336968	-0.134905	-0.447938
H	0.106896	1.067022	-1.266362	-0.147760	-0.396831
C	-2.329884	0.162147	-0.103396	0.408335	-0.346671
C	-2.480213	-0.857468	0.846828	-0.685979	-0.099220
C	-3.313734	0.287928	-1.095601	0.041757	-0.056370
C	-3.572281	-1.726105	0.805536	-0.333583	-0.024839
H	-1.733629	-0.984013	1.626902	0.102139	0.060522
C	-4.407392	-0.576594	-1.143427	-0.045152	-0.060903
H	-3.234777	1.077725	-1.840488	0.140476	0.034537
C	-4.536980	-1.588169	-0.191422	-0.172348	-0.055838
H	-3.669449	-2.509201	1.551673	0.169098	0.027600
H	-5.159203	-0.458361	-1.918170	0.152305	0.023522
H	-5.388180	-2.261413	-0.224072	0.148468	0.035392
Ge	-0.809068	1.405485	-0.050696	0.252027	1.530965
Na	1.894051	-0.922964	-1.543611	0.661326	0.747496
C	4.023819	-1.634162	-0.014382	-0.149879	0.379370
C	2.933599	-1.469770	0.815133	0.294523	-0.441359
C	4.513165	-0.582997	-0.830585	-0.332715	-0.749929
C	2.189239	-0.219257	0.885587	-0.388751	0.710641
C	2.801147	0.874031	0.142387	-0.541151	-0.531155
C	3.904589	0.675974	-0.677361	0.041349	0.508479
H	4.521107	-2.601652	-0.038396	0.143762	0.015640
H	5.384993	-0.716820	-1.459428	0.133007	0.037688
H	4.302261	1.530304	-1.221798	0.160399	0.020067
H	2.378334	1.870615	0.220636	0.051426	0.031040
H	2.589463	-2.303154	1.423516	0.137356	0.010671
C	0.986440	-0.108865	1.556036	-0.721635	-0.815242
C	0.194385	1.168532	1.625398	0.072095	-0.045171
H	0.622170	-0.970804	2.109203	0.070121	-0.006646
H	0.816774	2.052596	1.815792	0.249666	-0.082534
H	-0.542048	1.130570	2.435577	0.224222	-0.012982

12L

Electronic energy: -945.42633

Electronic energy + zero-point energy: -945.06895

Electronic energy + thermal energy correction: -945.03137

Electronic energy + thermal enthalpy correction: -945.03019

Electronic energy + thermal free energy correction: -945.14881

BSSE correction: 0.006321

Table S59. Cartesian coordinates, Mulliken and APT charges of all atoms at **12L** in the reaction between phenylgermane and styrene.

Symbol	X	Y	Z	Mulliken	APT
H	0.715172	-2.914838	-2.425739	-0.129458	-0.434088
H	-0.311403	-0.809935	-1.611736	-0.090456	-0.384885
C	1.648594	-1.934121	0.078959	0.421478	-0.345355
C	1.524787	-2.170323	1.455356	-0.552742	-0.106509
C	2.859759	-1.406727	-0.393056	-0.222889	-0.083689
C	2.567421	-1.872561	2.334515	-0.279806	-0.016261
H	0.596440	-2.573420	1.852242	0.205597	0.065737
C	3.905686	-1.102321	0.480256	0.010087	-0.066832
H	2.992991	-1.222365	-1.457676	0.125116	0.048066
C	3.757714	-1.329420	1.848915	-0.123338	-0.057055
H	2.449650	-2.059874	3.397864	0.162253	0.033909
H	4.832021	-0.687090	0.094211	0.169087	0.034464
H	4.566743	-1.089766	2.532014	0.174926	0.040379
Ge	0.148947	-2.227930	-1.154865	0.265349	1.479377
Na	-1.594031	0.894132	-0.290595	0.063775	0.637508
C	-4.123087	0.898495	0.839037	0.101056	0.334879
C	-3.434959	-0.217836	1.265636	0.219184	-0.458806
C	-4.357439	1.156372	-0.533139	-0.429155	-0.687553
C	-2.864210	-1.179417	0.335577	-0.264090	0.646140
C	-3.261057	-0.970426	-1.049004	-0.393201	-0.501254
C	-3.959878	0.162040	-1.445432	0.081198	0.464494
H	-4.487164	1.604632	1.583054	0.156401	0.021596
H	-4.914972	2.027643	-0.855153	0.130535	0.039066
H	-4.200711	0.280129	-2.500133	0.164595	0.021245
H	-2.976550	-1.701775	-1.799185	0.086789	0.031130
H	-3.258531	-0.369640	2.328532	0.151440	0.021159
C	-1.964666	-2.151147	0.734353	-0.863461	-0.787846
C	-1.327749	-3.127753	-0.216017	-0.101508	-0.034818
H	-1.747406	-2.248668	1.795090	0.052559	0.003237
H	-2.030358	-3.551188	-0.945798	0.232103	-0.082699
H	-0.896240	-3.978872	0.321985	0.197936	-0.011483
H	1.701705	0.532480	1.142979	0.059301	0.075862

H	1.933874	1.175612	-2.304768	-0.056917	-0.320498
H	-0.038165	0.469472	2.878129	0.224606	0.061642
C	0.924623	1.292507	1.138141	-1.175414	-0.042661
C	-0.055197	1.260155	2.133694	-0.184024	-0.072152
H	3.651739	1.998352	-0.666557	-0.113861	-0.306112
Ge	2.269522	2.274061	-1.277602	0.162069	1.376335
C	0.913657	2.283458	0.141080	0.847264	-0.355973
C	-1.056674	2.234055	2.160207	-0.100078	-0.002568
H	-1.823607	2.206745	2.927236	0.195687	0.057962
H	2.239000	3.648774	-1.967901	-0.090247	-0.317301
C	-0.099420	3.257094	0.184446	0.253583	-0.044022
C	-1.075825	3.236813	1.186555	-0.116322	-0.078983
H	-0.130772	4.043414	-0.566027	0.185673	0.050388
H	-1.852602	3.994920	1.202335	0.187325	0.054827

13L

Electronic energy: -945.40150

Electronic energy + zero-point energy: -945.04690

Electronic energy + thermal energy correction: -945.01006

Electronic energy + thermal enthalpy correction: -945.00887

Electronic energy + thermal free energy correction: -945.12808

BSSE correction: 0.005889

Table S60. Cartesian coordinates, Mulliken and APT charges of all atoms at **13L** in the reaction between phenylgermane and styrene.

Symbol	X	Y	Z	Mulliken	APT
H	-3.517429	-1.770574	-2.172763	-0.141162	-0.404892
H	-2.202128	-2.334300	-0.121707	-0.101100	-0.369701
C	-4.077917	-0.202484	0.163816	0.344844	-0.382475
C	-5.055167	-0.890596	0.897525	-0.237561	-0.037910
C	-4.057247	1.197041	0.241888	-0.381039	-0.072466
C	-5.986623	-0.206568	1.678327	-0.121493	-0.057194
H	-5.093768	-1.977687	0.863768	0.147833	0.030610
C	-4.985896	1.888316	1.022261	-0.159025	-0.040542
H	-3.300986	1.758386	-0.303222	0.111359	0.046017
C	-5.952821	1.186900	1.741087	-0.191304	-0.040167
H	-6.735770	-0.758736	2.238120	0.152609	0.022870
H	-4.951858	2.972737	1.070620	0.168338	0.028295
H	-6.675610	1.722443	2.349219	0.146917	0.030973
Ge	-2.783185	-1.167095	-0.953207	0.237817	1.623264
Na	3.185700	1.066817	-0.397785	0.381143	0.650422

C	1.883935	3.286526	0.500990	-0.002378	0.268931
C	0.908833	2.314095	0.644206	0.206521	-0.347413
C	2.423556	3.600895	-0.766669	-0.224996	-0.511204
C	0.370397	1.597052	-0.476611	-0.330817	0.701245
C	0.962879	1.905962	-1.744346	-0.023706	-0.381823
C	1.938905	2.898185	-1.875557	-0.188118	0.285737
H	2.235069	3.818971	1.381305	0.168024	0.033098
H	3.164030	4.384692	-0.879048	0.155823	0.043350
H	2.326864	3.125151	-2.865793	0.162002	0.029799
H	0.598806	1.402412	-2.634334	0.160168	0.052488
H	0.506195	2.100213	1.631840	0.166846	0.034461
C	-0.592958	0.571666	-0.316725	-0.796385	-1.362691
C	-1.362733	0.055853	-1.508385	-0.361631	-0.089734
H	-1.085405	0.545634	0.656845	0.171876	0.041125
H	-0.704040	-0.521395	-2.184368	0.243464	-0.039414
H	-1.799627	0.855805	-2.127136	0.204593	-0.067108
H	2.058167	-0.560918	2.271210	0.169186	0.045853
H	0.350012	-0.715804	-0.259575	0.056028	0.722574
H	4.053745	0.552998	3.188474	0.188782	0.042607
C	3.009146	-0.666858	1.751756	-0.708774	-0.132918
C	4.135067	-0.025069	2.272624	-0.091772	0.009749
H	0.868973	-3.178710	0.755717	-0.154864	-0.380228
Ge	1.385288	-2.114304	-0.252554	0.027055	0.824959
C	3.070344	-1.425688	0.565585	0.225084	-0.307080
C	5.363635	-0.119818	1.611740	-0.255020	-0.088322
H	6.239972	0.380692	2.011001	0.177656	0.046701
H	1.904928	-2.927680	-1.475698	-0.108648	-0.468984
C	4.321477	-1.515975	-0.071981	0.146707	-0.118633
C	5.454622	-0.873069	0.439483	-0.099683	0.017218
H	4.414294	-2.098779	-0.985731	0.177899	0.035991
H	6.406972	-0.963971	-0.074835	0.180901	0.032562

14L

Electronic energy: -945.45976

Electronic energy + zero-point energy: -945.09789

Electronic energy + thermal energy correction: -945.06101

Electronic energy + thermal enthalpy correction: -945.05983

Electronic energy + thermal free energy correction: -945.17688

BSSE correction: 0.006491

Table S61. Cartesian coordinates, Mulliken and APT charges of all atoms at **14L** in the reaction between phenylgermane and styrene.

Symbol	X	Y	Z	Mulliken	APT
H	-3.280643	-2.826086	-1.253603	-0.108417	-0.364518
H	-3.637324	-2.643834	1.242511	-0.135171	-0.374164
C	-3.040485	-0.208613	-0.177979	0.251356	-0.382086
C	-3.247211	0.350961	-1.447934	0.108543	-0.069544
C	-2.950305	0.657378	0.921840	-0.556123	-0.078501
C	-3.369913	1.731563	-1.613654	-0.149508	-0.044247
H	-3.317406	-0.295145	-2.320616	0.190823	0.038038
C	-3.073278	2.038228	0.762576	-0.107991	-0.069764
H	-2.769458	0.259753	1.918568	0.179289	0.050625
C	-3.286549	2.576168	-0.506631	-0.102298	-0.032084
H	-3.529009	2.146926	-2.604507	0.169579	0.034922
H	-2.983683	2.690371	1.625588	0.176774	0.055305
H	-3.375183	3.650589	-0.633621	0.175842	0.044926
Ge	-2.808033	-2.137004	0.046109	0.227816	1.571096
Na	2.634287	-0.175789	1.207796	0.357988	0.735761
C	3.678002	-1.230167	-1.229698	0.169448	-0.033747
C	2.290190	-1.172434	-1.358020	0.070432	-0.133631
C	4.263947	-2.117866	-0.320737	-0.190725	-0.080661
C	1.455814	-1.999316	-0.586982	-0.679622	0.072432
C	2.054977	-2.883900	0.318916	0.185110	-0.125340
C	3.446340	-2.944759	0.451340	-0.117440	-0.007313
H	4.298689	-0.573040	-1.831319	0.203174	0.055216
H	5.343275	-2.165160	-0.218700	0.179685	0.052261
H	3.888821	-3.638693	1.159241	0.180746	0.047664
H	1.433911	-3.526431	0.934824	0.181848	0.082090
H	1.843438	-0.458040	-2.045958	0.105486	0.084630
C	-0.045355	-1.903823	-0.769612	-0.382905	0.072412
C	-0.901135	-2.521673	0.336667	-0.636685	-0.345980
H	-0.295942	-2.364375	-1.735863	0.207597	-0.032570
H	-0.619030	-2.099904	1.309462	0.214081	0.015040
H	-0.767213	-3.607827	0.393638	0.118302	-0.027308
H	-0.759164	1.438239	-0.566029	-0.311362	0.045912
H	-0.291905	-0.839399	-0.873228	0.282637	0.012333
H	-0.226064	1.807597	-2.929164	0.178962	0.027247
C	0.252450	1.739553	-0.833529	-1.167345	-0.125737
C	0.548221	1.951976	-2.179068	0.143052	0.002570
H	2.157908	1.504800	2.663443	-0.209014	-0.463274
Ge	0.616611	1.708328	2.140849	0.042650	0.619990
C	1.211230	1.914769	0.184105	0.290346	-0.257554
C	1.833137	2.347034	-2.562157	-0.105927	-0.105758
H	2.069526	2.512705	-3.609018	0.158775	0.031267
H	0.435588	0.084841	1.986537	-0.119347	-0.463813
C	2.487897	2.334811	-0.232053	0.072361	-0.165885
C	2.802918	2.541395	-1.580047	-0.038469	-0.002293
H	3.260983	2.522178	0.514760	0.140093	0.019675
H	3.802886	2.863542	-1.859430	0.155554	0.014361

8S

Electronic energy: -1019.0403

Electronic energy + zero-point energy: -1018.6441

Electronic energy + thermal energy correction: -1018.6056

Electronic energy + thermal enthalpy correction: -1018.6044

Electronic energy + thermal free energy correction: -1018.7249

BSSE correction: 0.006996

Table S62. Cartesian coordinates, Mulliken and APT charges of all atoms at **8S** in the reaction between phenylgermane and styrene.

Symbol	X	Y	Z	Mulliken	APT
H	-2.663707	-2.516009	1.766655	0.175796	-0.018402
C	-3.179630	-2.837645	0.849808	-0.487311	0.172860
C	-2.718271	-2.047575	-0.358565	-0.714663	-0.904938
C	-3.034703	-0.642883	-0.418369	-0.073945	0.504947
C	-3.234947	0.144846	0.749931	-0.075515	-0.281463
H	-3.286999	-0.346176	1.716652	0.162854	0.058157
C	-3.382200	1.530847	0.685201	-0.073371	0.147096
H	-3.537493	2.089973	1.604474	0.182231	0.040133
C	-3.330475	2.207875	-0.538146	-0.272438	-0.352628
H	-3.454613	3.284530	-0.584299	0.170593	0.050021
C	-3.139784	1.455631	-1.706625	0.017515	0.150429
H	-3.112765	1.953957	-2.671921	0.176255	0.038645
C	-2.987625	0.072260	-1.649285	0.112804	-0.249730
H	-2.844184	-0.489425	-2.568479	0.185808	0.042278
Na	-0.793094	0.973902	-0.289685	0.073479	0.688113
H	-2.949522	-3.899632	0.718879	0.147867	-0.015536
H	-4.258888	-2.750793	1.040311	0.164661	-0.087181
H	-2.886987	-2.559501	-1.310171	0.128001	-0.017526
H	1.705403	-2.297011	2.030024	0.126478	0.023893
H	-0.500764	-3.612533	-0.182700	-0.178162	-0.483121
H	4.139073	-1.941779	2.223944	0.156224	0.014265
C	2.273846	-2.021780	1.140063	-0.468644	-0.074561
C	3.650090	-1.821358	1.260674	-0.107098	-0.019628
H	-0.463711	-1.183793	-1.552423	-0.208313	-0.387745
C	1.603189	-1.861037	-0.082219	0.192498	-0.471206
C	4.402757	-1.467236	0.137104	-0.161146	-0.093001
H	5.474710	-1.314591	0.222576	0.163237	0.031478
H	-0.686464	-1.240019	1.119346	-0.176678	-0.371968
C	2.382378	-1.503050	-1.190321	-0.223193	-0.115339
C	3.765522	-1.318510	-1.094571	-0.152464	-0.018254
H	1.899819	-1.355889	-2.157459	0.150344	0.030307
H	4.342994	-1.050806	-1.976219	0.156926	0.018795

C	-0.237986	3.211362	1.430498	-0.070934	-0.037407
C	0.555128	3.469290	0.310536	0.211958	-0.100308
C	0.012845	2.086555	2.218873	-0.186027	-0.086285
C	1.614985	2.616179	-0.041381	-0.047656	0.097148
C	1.854499	1.483478	0.758732	-0.519240	-0.102661
C	1.061148	1.225479	1.875548	0.035760	-0.049012
H	-1.054207	3.882043	1.679776	0.194917	0.060447
H	-0.608167	1.872645	3.082681	0.206421	0.067364
H	1.252210	0.333912	2.464261	0.214286	0.078725
H	2.649786	0.786439	0.506164	0.067162	0.083691
H	0.355152	4.345536	-0.300504	0.192304	0.058677
C	2.425307	2.941833	-1.231568	-0.301708	0.028803
C	3.512373	2.285380	-1.646767	-0.125740	-0.145054
H	2.085202	3.808742	-1.796126	0.142891	0.023881
H	3.904607	1.417848	-1.124312	0.128852	0.075658
H	4.043530	2.607375	-2.536053	0.166518	0.047888
Ge	-0.438458	-2.056175	-0.218232	0.419605	1.849256

9S

Electronic energy: -1019.0112

Electronic energy + zero-point energy: -1018.6155

Electronic energy + thermal energy correction: -1018.5787

Electronic energy + thermal enthalpy correction: -1018.5775

Electronic energy + thermal free energy correction: -1018.6913

BSSE correction: 0.008434

Table S63. Cartesian coordinates, Mulliken and APT charges of all atoms at **9S** in the reaction between phenylgermane and styrene.

Symbol	X	Y	Z	Mulliken	APT
H	1.055266	-3.984867	-0.259445	0.174618	-0.009491
C	1.128416	-3.587364	0.758699	-0.330066	0.137998
C	1.097749	-2.056034	0.784845	-0.276041	-0.542598
C	2.223249	-1.422185	0.064708	-0.926721	0.219104
C	2.501380	-1.712111	-1.290747	0.365842	-0.160546
H	1.915082	-2.470313	-1.802286	0.146205	0.054994
C	3.501326	-1.035137	-1.989938	0.083321	0.052539
H	3.686349	-1.282581	-3.031172	0.181237	0.041026
C	4.262810	-0.042357	-1.363742	-0.184145	-0.179682
H	5.041055	0.481522	-1.908585	0.175651	0.050228
C	4.014437	0.250172	-0.019698	-0.062508	0.084659
H	4.599927	1.010784	0.489002	0.192374	0.046282

C	3.012070	-0.427367	0.676685	-0.182111	-0.162950
H	2.818472	-0.183211	1.717755	0.134241	0.052811
Na	1.430693	0.880750	-1.088133	0.299781	0.634880
H	0.283256	-3.998442	1.320280	0.141306	-0.016628
H	2.052654	-3.976222	1.204623	0.155675	-0.082145
H	1.090519	-1.701560	1.820643	0.179499	-0.038938
H	-1.975054	0.260599	-2.285138	0.141858	0.020357
H	-1.216521	-2.980319	-0.443085	-0.171837	-0.403743
H	-4.133271	1.374787	-2.754278	0.151925	0.010835
C	-2.795939	0.159198	-1.574002	0.204469	-0.123847
C	-4.010246	0.794649	-1.843315	-0.109342	0.012111
H	-1.114761	-1.097164	1.648593	-0.038984	-0.735933
C	-2.603991	-0.596074	-0.411626	-0.342967	-0.451463
C	-5.066996	0.685847	-0.938489	-0.207387	-0.074617
H	-6.011913	1.182136	-1.138623	0.149662	0.025591
H	-0.142645	-0.777769	-1.292485	-0.238048	-0.394262
C	-3.677917	-0.690416	0.481980	-0.381887	-0.080221
C	-4.899308	-0.062678	0.227220	-0.156492	-0.007799
H	-3.557350	-1.261877	1.403348	0.141664	0.031275
H	-5.716402	-0.150519	0.938148	0.153543	0.010361
C	1.889965	3.334955	0.371484	-0.107476	0.123414
C	1.620588	2.445559	1.404808	0.166624	-0.287858
C	0.937846	3.585545	-0.628794	-0.127865	-0.293296
C	0.381872	1.756779	1.500114	-0.305680	0.505616
C	-0.562113	2.018960	0.471250	-0.513146	-0.208822
C	-0.292562	2.921204	-0.558117	-0.092217	0.125102
H	2.851107	3.840575	0.340971	0.176262	0.039858
H	1.145244	4.289862	-1.427214	0.170223	0.048221
H	-1.054560	3.098552	-1.312666	0.171137	0.053985
H	-1.525878	1.521487	0.482292	0.104676	0.071417
H	2.374203	2.271321	2.169018	0.156889	0.041107
C	0.135687	0.811444	2.555377	0.068296	-0.831403
C	-1.035881	0.081496	2.672079	-0.415863	0.865637
H	0.971640	0.576854	3.209991	0.131377	0.021267
H	-1.968570	0.473139	2.269100	0.211664	-0.044510
H	-1.159593	-0.556336	3.543431	0.159522	-0.013535
Ge	-0.831891	-1.529163	-0.032420	0.481243	1.763615

10S

Electronic energy: -1019.0719

Electronic energy + zero-point energy: -1018.6719

Electronic energy + thermal energy correction: -1018.6336

Electronic energy + thermal enthalpy correction: -1018.6324

Electronic energy + thermal free energy correction: -1018.7525

BSSE correction: 0.008139

Table S64. Cartesian coordinates, Mulliken and APT charges of all atoms at **10S** in the reaction between phenylgermane and styrene.

Symbol	X	Y	Z	Mulliken	APT
H	-4.321508	-2.162104	-0.237478	0.160223	0.004556
C	-4.053601	-1.877768	0.785338	-0.562003	0.074281
C	-2.777959	-1.017236	0.820253	0.232095	-0.344608
C	-1.565549	-1.765756	0.327115	-1.312871	0.123577
C	-1.533935	-2.317619	-0.964869	0.099839	-0.123202
H	-2.382666	-2.179338	-1.630039	0.188652	0.059354
C	-0.436464	-3.057457	-1.406625	0.099991	0.000505
H	-0.439069	-3.478892	-2.407208	0.186574	0.049840
C	0.658741	-3.264308	-0.562896	-0.264459	-0.089562
H	1.513782	-3.839476	-0.902478	0.198304	0.060419
C	0.649612	-2.709727	0.718748	-0.204499	-0.022655
H	1.505496	-2.824045	1.375961	0.227573	0.085756
C	-0.448543	-1.962619	1.153450	0.423346	-0.122549
H	-0.436855	-1.536853	2.153867	0.178684	0.068690
Na	1.121590	-0.521353	-0.883785	0.169267	0.687971
H	-4.902516	-1.335092	1.211715	0.160912	-0.014240
H	-3.914827	-2.799592	1.359698	0.180373	-0.031388
H	-2.591726	-0.712840	1.857531	0.175410	-0.024263
H	-1.444775	2.172838	-2.289786	0.169991	0.043331
H	-4.292648	1.375461	0.362167	-0.112089	-0.374653
H	0.428595	3.774922	-2.186252	0.181244	0.042169
C	-0.996775	2.407111	-1.326341	0.160853	-0.072011
C	0.057876	3.320707	-1.272199	-0.164211	-0.046253
H	1.637604	0.926549	2.842009	0.176757	-0.093314
C	-1.493664	1.808041	-0.158690	0.275685	-0.382263
C	0.630856	3.650214	-0.045590	-0.173518	-0.038213
H	1.452572	4.358706	-0.000860	0.182332	0.054001
H	-3.333804	0.272369	-1.691507	-0.062899	-0.344379
C	-0.888334	2.136283	1.065269	-0.665435	-0.081763
C	0.161812	3.051478	1.123474	-0.202009	-0.048646
H	-1.242435	1.683388	1.989729	0.159133	0.047781
H	0.619489	3.291444	2.078615	0.168305	0.049048
C	3.708058	-1.078840	-1.532582	0.057532	0.359930
C	3.626423	-1.328393	-0.178126	0.169382	-0.415142
C	3.401550	0.189301	-2.087297	-0.351276	-0.724893
C	3.222381	-0.311781	0.784649	-0.382970	0.506771
C	2.962333	0.993126	0.185299	-0.531592	-0.490612
C	3.066954	1.215433	-1.181009	-0.002514	0.416146
H	4.012786	-1.887993	-2.194028	0.152880	0.018648
H	3.501681	0.380520	-3.148955	0.129752	0.041027
H	2.864103	2.215650	-1.560167	0.152996	0.026401

H	2.690677	1.819297	0.834113	0.147041	0.046246
H	3.872825	-2.319566	0.198574	0.122969	0.019441
C	3.054394	-0.565659	2.126239	-0.037895	-0.690439
C	2.617882	0.491496	3.102115	-0.701225	0.316652
H	3.306614	-1.551929	2.508950	0.087975	-0.000865
H	3.316619	1.342259	3.163885	0.154589	-0.101530
H	2.526850	0.080440	4.111913	0.136371	-0.042939
Ge	-3.063396	0.644768	-0.216647	0.264435	1.517844

Diphenylgermane + styrene

5M

Electronic energy: -940.47873

Electronic energy + zero-point energy: -940.13476

Electronic energy + thermal energy correction: -940.10074

Electronic energy + thermal enthalpy correction: -940.09956

Electronic energy + thermal free energy correction: -940.21068

BSSE correction: 0.004945

Table S65. Cartesian coordinates, Mulliken and APT charges of all atoms at **5M** in the reaction between diphenylgermane and styrene.

Symbol	X	Y	Z	Mulliken	APT
H	2.438807	-0.909440	-2.899335	0.155675	-0.066290
C	2.309445	-1.942759	-2.541735	-0.509775	0.287522
C	1.991171	-2.022773	-1.074647	-0.368966	-0.798555
C	2.728693	-1.375029	-0.106297	-0.007892	0.565720
C	3.794005	-0.427894	-0.408768	-0.290148	-0.501058
H	4.056474	-0.248588	-1.447113	0.106741	0.040042
C	4.528568	0.201937	0.586658	-0.056463	0.420557
H	5.330141	0.876430	0.291116	0.159140	0.020503
C	4.268739	0.001441	1.957148	-0.371967	-0.701863
H	4.872877	0.472464	2.723068	0.132649	0.042298
C	3.245543	-0.920719	2.287299	-0.144261	0.371371
H	3.037845	-1.133087	3.334238	0.148208	0.022248
C	2.496480	-1.564488	1.319998	-0.040558	-0.421347
H	1.735973	-2.280674	1.622205	0.127213	0.029341
Na	2.057907	1.033607	0.990631	0.311040	0.649268
H	1.508276	-2.387136	-3.141366	0.152179	-0.032495
H	3.242173	-2.464935	-2.812287	0.161833	-0.117495
H	1.278813	-2.778894	-0.754737	0.103844	0.013069
H	-1.374256	1.649743	1.183708	0.186885	0.055377

H	-0.219285	3.834698	1.196808	0.185949	0.046037
C	-0.594998	1.845781	0.449957	-0.031328	-0.061607
C	0.051980	3.086516	0.458304	-0.027083	-0.042320
H	-0.587638	-1.790809	0.663071	-0.062427	-0.342249
Ge	-1.149100	-0.896703	-0.455897	0.183707	1.750293
C	-0.260425	0.859688	-0.494252	0.324504	-0.396769
C	1.040839	3.363848	-0.489110	-0.192513	-0.061800
H	1.543501	4.325857	-0.486323	0.187847	0.053603
H	-1.055539	-1.537139	-1.849379	-0.101069	-0.372947
C	0.726368	1.161220	-1.445877	-0.504821	-0.055978
C	1.373637	2.400255	-1.446335	-0.105377	-0.029681
H	1.010764	0.407259	-2.173703	0.120575	0.084460
H	2.138987	2.609662	-2.187153	0.201741	0.047401
C	-3.016073	-0.522738	0.024522	0.210171	-0.407006
C	-3.641637	-1.201735	1.078408	-0.053069	-0.063496
C	-3.756079	0.447986	-0.667938	-0.576812	-0.068049
C	-4.965582	-0.927605	1.428521	-0.149305	-0.041736
H	-3.092474	-1.955832	1.638296	0.168353	0.039609
C	-5.077906	0.727343	-0.324379	-0.117840	-0.047620
H	-3.295936	1.000581	-1.485345	0.135047	0.039152
C	-5.685153	0.037400	0.726114	-0.225902	-0.034500
H	-5.432470	-1.465820	2.247967	0.160390	0.024758
H	-5.634044	1.481327	-0.873425	0.163550	0.026965
H	-6.714450	0.253102	0.995909	0.150333	0.035264

6M

Electronic energy: -940.47541

Electronic energy + zero-point energy: -940.13092

Electronic energy + thermal energy correction: -940.09876

Electronic energy + thermal enthalpy correction: -940.09758

Electronic energy + thermal free energy correction: -940.20120

BSSE correction: 0.005688

Table S66. Cartesian coordinates, Mulliken and APT charges of all atoms at **6M** in the reaction between diphenylgermane and styrene.

Symbol	X	Y	Z	Mulliken	APT
H	-1.692512	-0.904086	2.933324	0.166871	-0.019635
C	-1.529076	-1.906379	2.521505	-0.448747	0.154827
C	-1.286786	-1.903791	1.022930	-0.476877	-0.947973
C	-2.330064	-1.388892	0.160523	-0.226239	0.568844
C	-3.290562	-0.427653	0.582750	-0.214694	-0.301965

H	-3.313538	-0.124042	1.624596	0.132668	0.051617
C	-4.221158	0.122283	-0.296274	-0.092054	0.158049
H	-4.943573	0.842334	0.078360	0.180295	0.039113
C	-4.245450	-0.249212	-1.648370	-0.251433	-0.332896
H	-4.983334	0.166270	-2.325977	0.162409	0.047028
C	-3.325150	-1.209027	-2.088697	-0.118357	0.154270
H	-3.342529	-1.539745	-3.123612	0.170324	0.038376
C	-2.390996	-1.761872	-1.212594	0.146078	-0.258511
H	-1.706656	-2.523296	-1.573088	0.180159	0.048454
Na	-1.771758	0.892768	-1.287224	0.508588	0.719751
H	-0.653971	-2.309315	3.040710	0.137065	-0.008489
H	-2.398072	-2.515170	2.808456	0.162363	-0.091427
H	-0.959396	-2.891254	0.678676	0.163343	-0.000762
H	2.338972	-1.034155	-2.159393	0.152271	0.029779
H	1.105713	-1.342171	1.950956	-0.144331	-0.568647
H	4.688891	-0.611434	-2.822157	0.144456	0.004695
C	3.067371	-0.744772	-1.400163	-0.022623	-0.099749
C	4.391573	-0.508762	-1.781570	-0.068478	-0.016444
H	0.321662	-1.374567	-0.990618	-0.198541	-0.449907
Ge	0.705196	-0.886258	0.490408	0.477987	2.163189
C	2.651840	-0.628976	-0.068817	-0.201057	-0.509333
C	5.335321	-0.146795	-0.820461	-0.251340	-0.076795
H	6.366602	0.036306	-1.108132	0.137111	0.020669
C	3.622340	-0.276115	0.878771	-0.349661	-0.076449
C	4.947642	-0.030941	0.516319	-0.114448	-0.018466
H	3.335329	-0.193394	1.927843	0.119045	0.034278
H	5.679555	0.244983	1.271038	0.149978	0.004678
C	0.150764	1.036708	0.512040	-0.177027	-0.421341
C	0.643124	1.903851	-0.483122	-0.487623	-0.087718
C	-0.751948	1.578781	1.440676	0.210388	-0.051787
C	0.232389	3.238198	-0.564704	-0.137222	-0.029220
H	1.375237	1.530220	-1.197372	0.165207	0.066203
C	-1.156553	2.916090	1.380447	0.019616	-0.031544
H	-1.144311	0.948425	2.232614	0.074686	0.050139
C	-0.672582	3.747235	0.369584	-0.315371	-0.066133
H	0.631968	3.882419	-1.342651	0.178892	0.035200
H	-1.848769	3.306544	2.120692	0.186674	0.035559
H	-0.986434	4.785199	0.317485	0.169647	0.040470

7M

Electronic energy: -940.48215

Electronic energy + zero-point energy: -940.13694

Electronic energy + thermal energy correction: -940.10429

Electronic energy + thermal enthalpy correction: -940.10311

Electronic energy + thermal free energy correction: -940.21024

BSSE correction: 0.005518

Table S67. Cartesian coordinates, Mulliken and APT charges of all atoms at **7M** in the reaction between diphenylgermane and styrene.

Symbol	X	Y	Z	Mulliken	APT
H	-0.985370	-0.875102	3.050559	0.184969	-0.005499
C	-0.565923	-1.803268	2.647590	-0.559039	0.082240
C	-0.439608	-1.762145	1.124436	-0.255135	-0.539125
C	-1.741860	-1.751612	0.402769	-0.982794	0.255901
C	-2.816537	-0.940400	0.819160	0.350160	-0.171551
H	-2.722558	-0.356987	1.730171	0.174807	0.064155
C	-3.996083	-0.854333	0.077512	-0.041836	0.043052
H	-4.802290	-0.216495	0.427387	0.182376	0.044391
C	-4.145343	-1.583831	-1.106165	-0.238765	-0.165448
H	-5.065921	-1.524451	-1.677427	0.169085	0.047590
C	-3.098727	-2.407698	-1.528842	-0.050149	0.029421
H	-3.201490	-2.995287	-2.436411	0.179708	0.041714
C	-1.916921	-2.484730	-0.787704	0.124840	-0.131187
H	-1.106905	-3.121739	-1.131076	0.183443	0.050341
Na	-1.704238	0.115735	-1.604354	0.373189	0.763961
H	0.420701	-1.913890	3.104442	0.136243	-0.004650
H	-1.198899	-2.635761	2.978139	0.154332	-0.057088
H	0.139993	-2.626547	0.777138	0.145660	-0.029527
H	2.253430	-0.935097	-2.055429	0.128097	0.049060
H	1.081911	0.240140	2.049655	-0.193535	-0.609313
H	4.649403	-1.084232	-2.683793	0.144390	0.008951
C	3.021730	-0.687862	-1.325311	-0.468604	-0.095706
C	4.369078	-0.771610	-1.681473	-0.175796	-0.037306
H	0.273038	-0.589052	-1.158181	-0.043833	-0.647189
Ge	0.716035	-0.152130	0.510509	0.469650	2.128855
C	2.630331	-0.291580	-0.040653	0.407974	-0.462195
C	5.357025	-0.452992	-0.749304	-0.177473	-0.052862
H	6.406529	-0.515147	-1.022389	0.143950	0.021040
C	3.638443	0.019862	0.881755	-0.322121	-0.093366
C	4.988854	-0.055216	0.536330	-0.182662	-0.036791
H	3.356586	0.327453	1.886982	0.129086	0.055598
H	5.752680	0.194643	1.267578	0.153011	0.008737
C	-0.269120	1.583331	0.217405	-0.210601	-0.456269
C	-0.203352	2.278598	-1.000611	-0.112850	-0.100311
C	-1.042955	2.149648	1.241214	-0.265377	-0.064014
C	-0.889172	3.481478	-1.198305	-0.125649	-0.027347
H	0.412199	1.875256	-1.806974	0.148976	0.042937
C	-1.758976	3.332345	1.047267	-0.186160	-0.009211
H	-1.075610	1.659757	2.213562	0.157637	0.043134
C	-1.681679	4.002635	-0.175038	-0.119680	-0.065991
H	-0.797994	4.013687	-2.141266	0.156553	0.022893

H	-2.366390	3.739258	1.850824	0.156099	0.024140
H	-2.224776	4.930943	-0.324079	0.157820	0.033835

8M

Electronic energy: -1085.0198

Electronic energy + zero-point energy: -1084.5582

Electronic energy + thermal energy correction: -1084.5143

Electronic energy + thermal enthalpy correction: -1084.5131

Electronic energy + thermal free energy correction: -1084.6441

BSSE correction: 0.006686

Table S68. Cartesian coordinates, Mulliken and APT charges of all atoms at **8M** in the reaction between diphenylgermane and styrene.

Symbol	X	Y	Z	Mulliken	APT
H	-0.870291	-2.452418	-2.910005	0.167675	-0.004198
C	-0.388075	-1.547669	-3.293502	-0.352808	0.091890
C	-0.396213	-0.418139	-2.262558	-0.498291	-0.519955
C	-1.760904	0.067386	-1.904694	-0.758858	0.228588
C	-2.782487	-0.823289	-1.518604	0.583795	-0.160189
H	-2.591101	-1.892468	-1.539177	0.189657	0.062624
C	-4.027262	-0.363044	-1.091354	-0.111942	0.039549
H	-4.789905	-1.077198	-0.795535	0.182096	0.044739
C	-4.295975	1.008654	-1.040284	-0.089958	-0.149411
H	-5.266634	1.367676	-0.714282	0.184334	0.047341
C	-3.302696	1.908461	-1.430035	-0.137220	0.020656
H	-3.498675	2.976635	-1.409083	0.156043	0.046890
C	-2.054550	1.442440	-1.853849	-0.008480	-0.147527
H	-1.286461	2.150990	-2.153032	0.155510	0.053856
Na	-1.744876	0.762963	0.763641	0.264482	0.776921
H	0.640676	-1.827300	-3.539264	0.139683	-0.008525
H	-0.898349	-1.252060	-4.218059	0.158799	-0.059025
H	0.183983	0.432877	-2.640141	0.107189	-0.038505
H	2.345233	1.371571	0.504337	-0.196126	0.058341
H	0.833847	-2.482176	-1.061647	-0.218034	-0.599618
H	4.780130	1.822383	0.651593	0.153716	0.014417
C	3.055185	0.636752	0.135127	-0.779012	-0.088193
C	4.424739	0.893417	0.213169	-0.135005	-0.044311
H	0.272048	0.758482	0.024762	-0.799251	-0.694505
Ge	0.624579	-0.948997	-0.556188	0.463436	2.159204
C	2.566019	-0.551765	-0.419509	0.359494	-0.455788
C	5.336987	-0.042120	-0.275926	-0.035075	-0.047092

H	6.403885	0.154077	-0.221288	0.148920	0.020261
C	3.498338	-1.481497	-0.900134	0.146081	-0.083150
C	4.870449	-1.231898	-0.835688	-0.186411	-0.041203
H	3.142031	-2.416608	-1.327623	0.144819	0.050066
H	5.574945	-1.964880	-1.218872	0.156213	0.010158
C	-0.372142	-1.559798	1.088486	0.605159	-0.476609
C	-0.264148	-0.873484	2.308460	-0.811303	-0.105550
C	-1.167040	-2.714793	1.066052	0.143250	-0.062109
C	-0.932140	-1.307671	3.457556	-0.344555	-0.031772
H	0.367894	0.013811	2.358035	0.183395	0.057406
C	-1.864596	-3.142129	2.197756	-0.099229	-0.016207
H	-1.229286	-3.297596	0.148278	0.164867	0.044157
C	-1.747416	-2.438542	3.397944	-0.146778	-0.059961
H	-0.809238	-0.772096	4.395146	0.162190	0.026899
H	-2.488956	-4.029841	2.149324	0.158339	0.023294
H	-2.277364	-2.777131	4.283113	0.166820	0.033013
C	0.653278	2.827752	2.540282	-0.793150	-0.329250
H	-0.173939	2.302673	3.032065	0.174122	-0.021389
H	1.542324	2.189123	2.551003	0.216334	0.020929
H	0.895468	3.694023	3.177537	0.153674	0.001775
C	-1.159991	3.827471	0.744036	-0.806583	-0.336851
H	-1.351150	3.863264	-0.332250	0.210743	0.017366
H	-1.966898	3.272927	1.240049	0.128377	-0.038929
H	-1.267334	4.862978	1.105320	0.171677	0.008315
C	1.469604	3.873765	0.130464	-0.825121	-0.312961
H	2.481221	3.813084	0.543606	0.166946	-0.010558
H	1.435595	3.224312	-0.755429	0.263604	0.027918
H	1.297548	4.893878	-0.235053	0.128042	-0.013063
B	0.324415	3.422152	1.117074	1.073711	0.969830

9M

Electronic energy: -1085.0217

Electronic energy + zero-point energy: -1084.561

Electronic energy + thermal energy correction: -1084.5179

Electronic energy + thermal enthalpy correction: -1084.5167

Electronic energy + thermal free energy correction: -1084.6463

BSSE correction: 0.007269

Table S69. Cartesian coordinates, Mulliken and APT charges of all atoms at **9M** in the reaction between diphenylgermane and styrene.

Symbol	X	Y	Z	Mulliken	APT

H	-1.025878	-1.517879	-3.401228	0.174190	-0.003548
C	-0.492648	-0.578441	-3.578977	-0.385111	0.084508
C	-0.391128	0.271511	-2.311029	-0.371187	-0.517811
C	-1.698516	0.786368	-1.811293	-0.855168	0.219297
C	-2.836363	-0.037124	-1.714131	0.213020	-0.159940
H	-2.791234	-1.057368	-2.084049	0.167685	0.064217
C	-4.019421	0.424184	-1.131998	0.011197	0.028690
H	-4.878367	-0.237013	-1.068316	0.193170	0.047126
C	-4.101497	1.726452	-0.630490	-0.245221	-0.148389
H	-5.021044	2.084834	-0.179654	0.184047	0.050408
C	-2.989334	2.566601	-0.736885	-0.051323	0.018487
H	-3.038631	3.585994	-0.364821	0.179367	0.049783
C	-1.809447	2.100438	-1.319063	0.361787	-0.131439
H	-0.945530	2.754346	-1.389120	0.168510	0.058290
Na	-1.861298	0.470127	0.868567	0.289958	0.735848
H	0.505537	-0.853874	-3.929458	0.147388	-0.004740
H	-1.007532	-0.038186	-4.382348	0.161525	-0.058494
H	0.265312	1.131102	-2.496134	0.135163	-0.027803
H	2.293503	1.760118	-0.404542	0.088777	0.054989
H	0.809161	-2.071145	-1.721086	-0.192817	-0.603100
H	4.727336	2.225433	-0.236974	0.159139	0.017974
C	3.008195	0.940495	-0.443921	-1.051646	-0.084754
C	4.374370	1.202394	-0.335835	-0.328004	-0.042588
H	0.251419	0.759773	0.267238	-0.895081	-0.770334
Ge	0.598138	-0.737483	-0.820701	0.525502	2.170870
C	2.527209	-0.365658	-0.584952	0.341317	-0.450920
C	5.285972	0.145607	-0.342816	-0.186995	-0.051229
H	6.349791	0.342089	-0.246490	0.152704	0.023635
C	3.458017	-1.411600	-0.615997	0.463276	-0.062638
C	4.825346	-1.164389	-0.478855	-0.103326	-0.039997
H	3.109227	-2.433339	-0.754947	0.137169	0.041583
H	5.531099	-1.990242	-0.487706	0.153590	0.013294
C	-0.450981	-1.762607	0.555864	-0.096436	-0.475824
C	-0.337909	-1.493175	1.929113	-0.393426	-0.103660
C	-1.323517	-2.788740	0.164712	0.212725	-0.057317
C	-1.072291	-2.210796	2.877659	-0.088514	-0.031698
H	0.339805	-0.704535	2.254465	0.118846	0.066974
C	-2.087883	-3.490144	1.100322	-0.109609	-0.021173
H	-1.396676	-3.050956	-0.889872	0.180099	0.042584
C	-1.960713	-3.203568	2.460520	-0.158940	-0.056849
H	-0.948406	-1.999507	3.936369	0.180276	0.028921
H	-2.771872	-4.267485	0.771876	0.161604	0.025119
H	-2.542705	-3.756869	3.191310	0.166992	0.034173
C	1.685138	1.556550	2.832245	-0.746313	-0.331325
H	1.378563	0.820104	3.583102	0.138268	-0.028130
H	2.335752	1.059272	2.104135	0.262025	0.039148
H	2.316695	2.301131	3.338371	0.124807	-0.015531
C	-0.981038	2.163660	2.708270	-0.779797	-0.350031
H	-1.785243	2.555835	2.070075	0.122350	-0.017890

H	-1.230977	1.163991	3.090023	0.177377	-0.013239
H	-0.993109	2.806042	3.602175	0.161207	0.004711
C	0.794912	3.574752	1.215911	-0.664269	-0.323281
H	1.778183	3.559788	0.736824	0.172353	-0.000071
H	0.030007	3.763525	0.456044	0.193416	-0.002350
H	0.786671	4.448798	1.886757	0.151506	-0.022976
B	0.492836	2.313535	2.121185	0.770850	1.088439

10M

Electronic energy: -1085.0743

Electronic energy + zero-point energy: -1084.6093

Electronic energy + thermal energy correction: -1084.5657

Electronic energy + thermal enthalpy correction: -1084.5645

Electronic energy + thermal free energy correction: -1084.6944

BSSE correction: 0.007384

Table S70. Cartesian coordinates, Mulliken and APT charges of all atoms at **10M** in the reaction between diphenylgermane and styrene.

Symbol	X	Y	Z	Mulliken	APT
C	0.239782	-1.583703	-1.287597	-0.410948	-0.389479
C	1.729460	-1.514618	-1.083234	-0.111001	0.146320
C	2.443892	-0.367620	-1.460103	-0.406756	-0.175725
H	1.919382	0.427575	-1.986194	0.193541	0.087105
C	3.810033	-0.249855	-1.196748	0.124512	-0.005773
H	4.343948	0.641891	-1.515635	0.180816	0.043055
C	4.494209	-1.284848	-0.558169	-0.211367	-0.107942
H	5.557059	-1.198676	-0.356697	0.164116	0.041403
C	3.801923	-2.444448	-0.207666	-0.048974	0.034568
H	4.326399	-3.264987	0.272776	0.174864	0.037433
C	2.436745	-2.557750	-0.468103	-0.019849	-0.156996
H	1.913006	-3.464844	-0.175183	0.142399	0.055418
Na	1.652324	1.913901	0.234010	0.183118	0.803663
H	-1.466461	1.291558	1.611344	0.152352	0.073557
H	-0.367401	2.987576	3.021189	0.182032	0.053268
C	-0.457784	1.107795	1.973720	0.018658	-0.069089
C	0.163071	2.074599	2.769226	-0.173930	-0.043990
H	-0.600011	-2.783411	1.178745	-0.085748	-0.388740
Ge	-0.677660	-1.412079	0.465170	0.281343	1.771354
C	0.206404	-0.076812	1.617257	0.366226	-0.423637
C	1.467809	1.872569	3.223908	-0.144208	-0.053631
H	1.952120	2.622374	3.841727	0.195473	0.050057

H	0.027087	1.551321	-1.049130	-0.830731	-0.443543
C	1.517403	-0.266793	2.091156	-0.411657	-0.062530
C	2.146201	0.698369	2.883553	-0.157936	-0.061201
H	2.065109	-1.170593	1.834771	0.116614	0.064862
H	3.159037	0.530815	3.237266	0.187741	0.043254
C	-1.184907	2.792999	-2.617385	-0.771187	-0.158178
H	-1.148245	1.986361	-3.364263	0.135343	-0.052391
H	-2.179416	2.751953	-2.149035	0.168717	-0.066841
H	-1.146672	3.741233	-3.174957	0.120921	-0.079665
C	1.471084	2.992360	-2.305361	-0.710747	-0.187696
H	2.413006	2.926268	-1.725472	0.173395	-0.112941
H	1.615179	2.330895	-3.171627	0.160650	-0.048871
H	1.464718	4.019130	-2.698117	0.149686	-0.058444
C	-0.219795	3.816423	-0.329734	-0.703840	-0.188187
H	-1.148518	3.618229	0.224774	0.211140	-0.046142
H	0.563697	3.949186	0.440589	0.150231	-0.107592
H	-0.328598	4.811932	-0.783801	0.144533	-0.055192
B	0.033066	2.710844	-1.533738	0.997177	0.671941
C	-0.241987	-2.858399	-1.995834	-0.496902	0.069675
H	0.232301	-2.957894	-2.977794	0.187352	-0.036166
H	-0.010453	-3.759812	-1.419524	0.177541	-0.004077
H	-1.326327	-2.831005	-2.144175	0.176409	-0.007493
H	-0.069749	-0.708542	-1.871544	0.246753	-0.005641
C	-2.538858	-0.903408	0.195252	0.021582	-0.416445
C	-3.593656	-1.616119	0.781324	0.269918	-0.054249
C	-2.842182	0.205148	-0.611458	-0.911515	-0.083577
C	-4.918968	-1.232338	0.570841	-0.139887	-0.055394
H	-3.384843	-2.480645	1.407508	0.151910	0.033524
C	-4.165648	0.591206	-0.822221	0.023404	-0.057438
H	-2.041898	0.781058	-1.074677	-0.010986	0.102566
C	-5.205153	-0.127729	-0.230997	-0.042482	-0.015966
H	-5.725870	-1.794886	1.030745	0.159185	0.023126
H	-4.381969	1.451735	-1.448589	0.156198	0.042087
H	-6.235835	0.171424	-0.395636	0.154799	0.032630

11M

Electronic energy: -777.63283

Electronic energy + zero-point energy: -777.29445

Electronic energy + thermal energy correction: -777.26463

Electronic energy + thermal enthalpy correction: -777.26345

Electronic energy + thermal free energy correction: -777.36566

BSSE correction: 0.003379

Table S71. Cartesian coordinates, Mulliken and APT charges of all atoms at **11M** in the reaction between diphenylgermane and styrene.

Symbol	X	Y	Z	Mulliken	APT
H	0.109964	-0.815251	-1.895293	-0.081219	-0.376449
C	-0.217780	1.536865	-0.277632	-0.084448	-0.423844
C	-0.156550	2.180885	0.968047	-0.305583	-0.066319
C	-0.802332	2.224277	-1.349116	-0.033898	-0.056910
C	-0.658036	3.470544	1.138238	-0.042242	-0.039867
H	0.282053	1.671791	1.825417	0.203736	0.036780
C	-1.308251	3.514971	-1.185316	-0.312437	-0.030158
H	-0.872521	1.748094	-2.324149	0.180181	0.037227
C	-1.235686	4.139713	0.058524	-0.087711	-0.024550
H	-0.600838	3.951535	2.110084	0.162306	0.030827
H	-1.760755	4.030002	-2.027280	0.157047	0.029795
H	-1.629343	5.143158	0.188090	0.153690	0.035793
Ge	0.443647	-0.289934	-0.480275	0.270195	1.787908
C	-4.139687	-0.349505	0.735771	-0.086968	0.013121
C	-2.787753	-0.430053	1.059510	0.053337	-0.131455
C	-4.703764	-1.261992	-0.156267	-0.104297	-0.104618
C	-1.964561	-1.419895	0.502133	-0.415055	0.160645
C	-2.544615	-2.327663	-0.394423	0.005158	-0.132107
C	-3.899136	-2.251181	-0.718527	-0.104434	0.016462
H	-4.753742	0.426176	1.183302	0.159558	0.033145
H	-5.757859	-1.203239	-0.408075	0.145745	0.034639
H	-4.325186	-2.969150	-1.412994	0.154109	0.028624
H	-1.935934	-3.105924	-0.845739	0.108586	0.048436
H	-2.357356	0.288556	1.753141	0.137798	0.042780
C	-0.492536	-1.456373	0.829085	-0.327850	-0.411770
C	0.123113	-2.860476	0.860490	-0.597486	0.056830
H	-0.347500	-0.984482	1.809362	0.208987	-0.019427
H	-0.463341	-3.529546	1.500213	0.179019	-0.041120
H	1.144544	-2.823074	1.249709	0.178908	-0.005832
H	0.171026	-3.316068	-0.134928	0.216469	0.001220
C	2.384715	-0.353082	-0.204235	-0.137402	-0.428609
C	3.088835	0.731474	0.336919	0.187021	-0.077644
C	3.107845	-1.507944	-0.541917	-0.405816	-0.056520
C	4.467593	0.663020	0.544344	-0.154073	-0.040947
H	2.562254	1.648459	0.591068	0.109356	0.048459
C	4.485126	-1.582214	-0.337840	-0.151844	-0.052684
H	2.595217	-2.363331	-0.977926	0.129395	0.035041
C	5.167204	-0.495037	0.209358	-0.152910	-0.042461
H	4.994567	1.515380	0.962601	0.169523	0.026236
H	5.025689	-2.484208	-0.608607	0.164334	0.025599
H	6.239889	-0.549000	0.367929	0.151212	0.033726

6L

Electronic energy: -940.45982

Electronic energy + zero-point energy: -940.11776

Electronic energy + thermal energy correction: -940.08472

Electronic energy + thermal enthalpy correction: -940.08354

Electronic energy + thermal free energy correction: -940.19079

BSSE correction: 0.003697

Table S72. Cartesian coordinates, Mulliken and APT charges of all atoms at **6L** in the reaction between diphenylgermane and styrene.

Symbol	X	Y	Z	Mulliken	APT
H	1.591494	-1.770637	-2.828297	0.168168	-0.036290
C	1.672300	-2.742119	-2.307544	-0.625338	0.283670
C	1.340408	-2.607347	-0.844351	0.165304	-1.250520
C	2.202714	-1.910034	0.025377	-0.280592	0.533772
C	3.218569	-1.016922	-0.455917	-0.316988	-0.326923
H	3.407921	-0.959288	-1.523333	0.143997	0.047618
C	4.024270	-0.282061	0.413917	-0.174406	0.286500
H	4.809436	0.345425	-0.001213	0.169221	0.033559
C	3.842626	-0.333296	1.803550	-0.255883	-0.514782
H	4.488514	0.221164	2.474725	0.152328	0.044614
C	2.814504	-1.160919	2.301382	-0.111396	0.261167
H	2.649090	-1.225717	3.373959	0.165367	0.033696
C	2.010099	-1.903039	1.448556	-0.052172	-0.305344
H	1.238527	-2.545427	1.867361	0.146245	0.031110
Na	1.616012	0.791309	0.875252	0.441282	0.639355
H	0.971565	-3.420615	-2.801972	0.159400	-0.020125
H	2.688560	-3.117409	-2.493706	0.162320	-0.071291
H	0.725125	-3.386013	-0.396417	0.172364	0.049915
H	-1.585900	1.643006	1.104446	0.178102	0.042113
H	-0.714690	3.757129	2.033921	0.184606	0.030203
C	-0.810363	2.182872	0.563871	0.073273	-0.133692
C	-0.321246	3.382482	1.093221	-0.050837	0.020324
H	0.280607	-1.433936	-1.024179	-0.096361	0.717376
Ge	-0.861190	-0.143066	-1.324033	0.055255	1.071668
C	-0.325972	1.665088	-0.651817	-0.307121	-0.402895
C	0.661128	4.101952	0.412670	-0.341436	-0.106644
H	1.040021	5.033297	0.821343	0.170409	0.042605
H	-1.384343	0.143717	-2.760147	-0.108565	-0.455951
C	0.662797	2.413567	-1.320712	-0.235353	-0.125986
C	1.146396	3.617107	-0.805660	-0.034122	0.024926
H	1.068919	2.043253	-2.260898	0.179338	0.045757
H	1.903912	4.174002	-1.349352	0.185033	0.032170
C	-2.437451	-0.571617	-0.213072	0.642191	-0.383327
C	-2.292441	-1.483893	0.842712	-0.602135	-0.071667

C	-3.690226	0.037989	-0.382500	0.024075	-0.080454
C	-3.352977	-1.776363	1.703774	-0.444895	-0.033441
H	-1.334661	-1.981598	0.990537	0.025186	0.024505
C	-4.756372	-0.249762	0.469937	-0.126772	-0.046880
H	-3.836678	0.751501	-1.190858	0.154136	0.041551
C	-4.587761	-1.157087	1.517739	-0.224282	-0.045405
H	-3.217084	-2.488244	2.512907	0.163257	0.025027
H	-5.717762	0.232970	0.319564	0.159509	0.017450
H	-5.416619	-1.382456	2.182086	0.148287	0.030966

7L

Electronic energy: -940.51013

Electronic energy + zero-point energy: -940.16128

Electronic energy + thermal energy correction: -940.12739

Electronic energy + thermal enthalpy correction: -940.12621

Electronic energy + thermal free energy correction: -940.23939

BSSE correction: 0.002585

Table S73. Cartesian coordinates, Mulliken and APT charges of all atoms at **7L** in the reaction between diphenylgermane and styrene.

Symbol	X	Y	Z	Mulliken	APT
H	-1.863076	-1.551964	2.405226	0.166206	0.003159
C	-2.921506	-1.521858	2.686476	-0.559066	0.049495
C	-3.820684	-1.850294	1.496587	-0.263752	0.113826
C	-3.598202	-0.992282	0.267962	-0.060283	0.061891
C	-2.890090	0.213190	0.318379	-0.287998	-0.153822
H	-2.456878	0.553155	1.252799	0.155640	0.096574
C	-2.695408	0.989566	-0.828161	-0.241770	-0.030117
H	-2.122770	1.910844	-0.754320	0.148350	0.079568
C	-3.207503	0.566181	-2.054357	-0.292293	-0.088522
H	-3.057563	1.164781	-2.947109	0.186017	0.057229
C	-3.920103	-0.637435	-2.122957	-0.123627	-0.024739
H	-4.329846	-0.974023	-3.070571	0.176016	0.044859
C	-4.110507	-1.405727	-0.973531	0.296981	-0.098711
H	-4.665688	-2.339019	-1.035013	0.166550	0.048722
Na	-1.251463	-1.541272	-1.395037	0.512750	0.715750
H	-3.080837	-2.245632	3.489123	0.166698	-0.020465
H	-3.135257	-0.528587	3.091596	0.172547	-0.005529
H	-4.873191	-1.759006	1.793541	0.192330	-0.036166
H	1.261674	1.561823	-1.648936	0.142656	0.025611
H	0.594049	3.925235	-1.826218	0.154528	0.014975

C	0.761407	2.035012	-0.803361	-0.432292	-0.135147
C	0.382547	3.373275	-0.914095	-0.134595	0.018514
H	-3.682015	-2.899918	1.211744	0.158139	-0.029257
Ge	0.867702	-0.694869	0.379557	-0.016802	0.793133
C	0.518067	1.284515	0.360665	-0.333381	-0.291256
C	-0.275057	4.002589	0.145743	-0.068957	-0.110382
H	-0.581429	5.041085	0.062892	0.164393	0.027130
H	0.807381	-0.924180	1.946165	-0.132841	-0.447168
C	-0.119203	1.950666	1.419357	0.140392	-0.136817
C	-0.521958	3.285335	1.316730	-0.202378	0.000087
H	-0.308372	1.413891	2.348272	0.175599	0.030232
H	-1.020115	3.768012	2.153574	0.153593	0.012921
C	2.850849	-0.759413	0.062148	-0.054995	-0.324150
C	3.452620	-1.943020	-0.391965	-0.291009	-0.086540
C	3.693730	0.343087	0.276810	-0.046533	-0.140661
C	4.829620	-2.035807	-0.606776	-0.210683	-0.022731
H	2.832484	-2.818277	-0.583324	0.129389	0.023359
C	5.070006	0.266943	0.055862	-0.189067	-0.018608
H	3.267367	1.281770	0.624971	0.143986	0.040042
C	5.644333	-0.926079	-0.384783	-0.202044	-0.087368
H	5.264978	-2.969834	-0.952079	0.148423	0.005067
H	5.695805	1.137945	0.231906	0.152912	0.005239
H	6.715172	-0.988965	-0.555031	0.140269	0.020774

8L

Electronic energy: -629.74969

Electronic energy + zero-point energy: -629.56042

Electronic energy + thermal energy correction: -629.53974

Electronic energy + thermal enthalpy correction: -629.53856

Electronic energy + thermal free energy correction: -629.62198

BSSE correction: 0.000375

Table S74. Cartesian coordinates, Mulliken and APT charges of all atoms at **8L** in the reaction between diphenylgermane and styrene.

Symbol	X	Y	Z	Mulliken	APT
H	0.068371	1.193044	-2.058216	-0.169133	-0.453009
C	1.535186	-0.189295	-0.162222	0.197396	-0.305810
C	1.286668	-1.521375	0.201631	-0.008377	-0.143975
C	2.879626	0.197355	-0.286533	-0.480300	-0.091519
C	2.328211	-2.425183	0.426842	-0.371408	-0.002395
H	0.259732	-1.865964	0.305573	0.104875	0.036970

C	3.928437	-0.698323	-0.076040	-0.118353	-0.012221
H	3.118549	1.225214	-0.561066	0.097875	0.014516
C	3.654385	-2.017941	0.286750	-0.145867	-0.106252
H	2.102354	-3.451011	0.705999	0.153624	0.008486
H	4.957619	-0.368403	-0.191252	0.138319	0.005588
H	4.465501	-2.719730	0.457159	0.140007	0.022084
Ge	0.078295	1.160659	-0.477903	-0.094330	0.814338
Na	0.269816	3.627747	0.991469	0.664041	0.775527
C	-1.565152	0.057792	-0.174286	0.143495	-0.332030
C	-2.350186	-0.437591	-1.227222	0.004243	-0.120842
C	-1.983241	-0.250656	1.130960	-0.418662	-0.097239
C	-3.497513	-1.199475	-0.992167	-0.162044	-0.010974
H	-2.056218	-0.230389	-2.253794	0.157609	0.032407
C	-3.118894	-1.022526	1.379936	-0.182046	-0.009090
H	-1.402300	0.112257	1.979219	0.126393	0.018537
C	-3.884506	-1.497338	0.314021	-0.214733	-0.088192
H	-4.084608	-1.567474	-1.829367	0.150261	0.007935
H	-3.408290	-1.252017	2.402030	0.145997	0.011895
H	-4.772239	-2.094502	0.500425	0.141117	0.025266

9L

Electronic energy: -939.28351

Electronic energy + zero-point energy: -938.95831

Electronic energy + thermal energy correction: -938.92518

Electronic energy + thermal enthalpy correction: -938.924

Electronic energy + thermal free energy correction: -939.03419

BSSE correction: 0.002875

Table S75. Cartesian coordinates, Mulliken and APT charges of all atoms at **9L** in the reaction between diphenylgermane and styrene.

Symbol	X	Y	Z	Mulliken	APT
H	1.677835	0.171273	-2.732146	-0.170689	-0.456938
C	0.844680	1.653653	-0.559036	0.245066	-0.290657
C	1.482920	1.890141	0.667912	-0.069938	-0.160587
C	0.117449	2.720220	-1.112829	-0.508985	-0.111647
C	1.394179	3.125387	1.316520	-0.347557	0.005373
H	2.062507	1.093959	1.132081	0.153468	0.039361
C	0.029052	3.961502	-0.482265	-0.224662	-0.003105
H	-0.403730	2.578045	-2.059946	0.140426	0.021095
C	0.664395	4.167769	0.744770	-0.124963	-0.114839
H	1.899405	3.274723	2.267381	0.157820	0.012013

H	-0.537236	4.767132	-0.942704	0.149262	0.010209
H	0.594995	5.129466	1.244589	0.160110	0.024267
Ge	0.811109	-0.151910	-1.448760	-0.037762	0.814544
Na	-1.774624	-1.446844	-1.493102	0.613750	0.735661
C	-1.464284	0.177778	1.879034	-0.092966	-0.055396
C	-2.169478	-0.995316	1.614340	-0.034762	-0.068327
C	-1.862390	1.378304	1.295919	-0.110406	-0.023860
C	-3.277200	-0.990585	0.753333	-0.356304	-0.086217
C	-3.681218	0.230711	0.186152	-0.380363	-0.058349
C	-2.975076	1.400616	0.452814	0.069078	-0.065855
H	-0.590698	0.152789	2.523456	0.207456	0.062980
H	-1.295202	2.286918	1.475586	0.165989	0.079730
H	-3.291025	2.336128	0.001735	0.186434	0.052165
H	-4.561058	0.268080	-0.450080	0.096583	0.054390
H	-1.852285	-1.932415	2.066126	0.162078	0.057099
C	-3.937867	-2.272055	0.429498	-0.163547	0.163541
C	-4.731658	-2.503843	-0.623673	-0.185848	-0.231481
H	-3.712892	-3.095845	1.105570	0.153719	0.036268
H	-4.989785	-1.727504	-1.340355	0.167818	0.058783
H	-5.167178	-3.483271	-0.787075	0.176174	0.058054
C	2.193551	-1.119019	-0.360959	0.076241	-0.341212
C	3.559327	-1.115388	-0.687498	0.234034	-0.111691
C	1.820487	-1.818187	0.798454	-0.542532	-0.076200
C	4.505005	-1.776395	0.099544	-0.115943	-0.023712
H	3.892577	-0.579346	-1.573435	0.149812	0.036041
C	2.756060	-2.473468	1.601874	-0.270326	-0.012606
H	0.769144	-1.849616	1.086471	0.061663	0.012318
C	4.105848	-2.456702	1.250408	-0.234449	-0.082841
H	5.554444	-1.756288	-0.181992	0.150034	0.006554
H	2.433911	-2.999752	2.496684	0.152939	0.011920
H	4.838957	-2.968836	1.866619	0.142050	0.023154

10L

Electronic energy: -939.26173

Electronic energy + zero-point energy: -938.93694

Electronic energy + thermal energy correction: -938.90543

Electronic energy + thermal enthalpy correction: -938.90424

Electronic energy + thermal free energy correction: -939.00967

BSSE correction: 0.003362

Table S76. Cartesian coordinates, Mulliken and APT charges of all atoms at **10L** in the reaction between diphenylgermane and styrene.

Symbol	X	Y	Z	Mulliken	APT
H	-0.028434	0.877183	-0.950463	-0.100251	-0.468869
C	2.538818	0.632769	0.012608	0.123240	-0.221544
C	3.005616	1.735832	-0.720471	-0.413508	-0.170303
C	3.495353	-0.274401	0.494403	-0.069056	-0.153141
C	4.365264	1.922526	-0.972281	-0.206334	0.003106
H	2.293943	2.462307	-1.110183	0.136439	0.031238
C	4.857549	-0.097113	0.247246	-0.171291	0.011886
H	3.173431	-1.143452	1.066473	0.120514	0.035329
C	5.297310	1.003586	-0.488649	-0.181800	-0.120157
H	4.697747	2.781969	-1.547936	0.150880	0.007627
H	5.575659	-0.818405	0.627534	0.154196	0.006397
H	6.356212	1.143863	-0.683874	0.144961	0.023297
Ge	0.605955	0.464313	0.466866	0.203159	0.869164
Na	-1.847979	-0.428093	-1.223881	0.496446	0.677089
C	-4.327446	1.142613	-1.336888	-0.215025	0.174927
C	-3.359061	2.062836	-0.970872	-0.043254	-0.361268
C	-4.582233	0.006364	-0.540129	-0.202010	-0.305680
C	-2.577262	1.909994	0.212570	0.038986	0.689139
C	-2.853286	0.755285	1.002465	-0.508651	-0.184741
C	-3.845705	-0.160010	0.633086	-0.117581	0.126789
H	-4.896450	1.299583	-2.248902	0.163693	0.032876
H	-5.351271	-0.705406	-0.819655	0.165382	0.042537
H	-4.033495	-1.020394	1.270706	0.173239	0.044574
H	-2.311785	0.594395	1.927660	0.015842	0.042752
H	-3.169886	2.925472	-1.605218	0.165084	0.035893
C	-1.483871	2.781627	0.498381	-0.011261	-1.216066
C	-0.542552	2.470637	1.475431	-0.425205	1.063699
H	-1.226622	3.509986	-0.266587	0.151179	0.019735
H	-0.830782	1.963441	2.388155	0.280521	-0.094722
H	0.325480	3.115142	1.593200	0.182550	-0.003110
C	0.311177	-1.544629	0.256038	-0.416711	-0.463757
C	0.992196	-2.299571	-0.718301	0.087088	-0.085596
C	-0.658907	-2.214670	1.018410	-0.252090	-0.095337
C	0.708236	-3.649461	-0.929511	-0.223014	-0.065000
H	1.762927	-1.821643	-1.320804	0.155093	0.045456
C	-0.950626	-3.568874	0.818224	-0.090085	-0.038666
H	-1.198672	-1.669790	1.791820	0.212494	0.042521
C	-0.267504	-4.288412	-0.160133	-0.147422	-0.047521
H	1.249788	-4.205596	-1.689811	0.156557	0.014153
H	-1.701952	-4.059439	1.430823	0.160143	0.022022
H	-0.487052	-5.339769	-0.319711	0.156859	0.033272

11L

Electronic energy: -939.28897

Electronic energy + zero-point energy: -938.963

Electronic energy + thermal energy correction: -938.9313

Electronic energy + thermal enthalpy correction: -938.93011

Electronic energy + thermal free energy correction: -939.03518

BSSE correction: 0.004068

Table S77. Cartesian coordinates, Mulliken and APT charges of all atoms at **11L** in the reaction between diphenylgermane and styrene.

Symbol	X	Y	Z	Mulliken	APT
H	-0.499199	-0.301364	-1.018651	-0.161138	-0.443488
C	1.415271	1.627846	-0.112900	0.390893	-0.392581
C	1.084689	2.780043	0.614646	-0.480303	-0.084598
C	2.447970	1.718389	-1.058405	-0.101115	-0.061775
C	1.759980	3.983359	0.405310	-0.269631	-0.028121
H	0.287703	2.742646	1.353768	0.137031	0.057562
C	3.126494	2.918218	-1.273570	-0.233630	-0.056906
H	2.737038	0.838257	-1.630169	0.140683	0.040872
C	2.782030	4.054227	-0.540778	-0.192286	-0.052731
H	1.489801	4.863369	0.981435	0.169341	0.026360
H	3.924959	2.965628	-2.008152	0.159935	0.024347
H	3.310018	4.988865	-0.703818	0.153002	0.033316
Ge	0.472902	-0.068943	0.182803	0.234085	1.765143
Na	-2.719291	0.312713	-1.675869	0.666326	0.748272
C	-5.108792	0.379187	-0.316490	-0.074279	0.355481
C	-4.134907	0.927703	0.491419	0.200954	-0.433662
C	-5.017361	-0.947083	-0.811083	-0.340145	-0.739968
C	-2.932755	0.196656	0.866369	-0.610672	0.683388
C	-2.933884	-1.199279	0.450023	-0.398891	-0.534577
C	-3.937146	-1.723102	-0.356721	0.024649	0.527809
H	-5.973052	0.985960	-0.578673	0.144222	0.012914
H	-5.802013	-1.374023	-1.423908	0.133345	0.035417
H	-3.875008	-2.770310	-0.646628	0.155226	0.023251
H	-2.129354	-1.851522	0.775476	0.063795	0.029235
H	-4.242489	1.949856	0.847413	0.140038	0.009979
C	-1.865191	0.795266	1.507359	-0.143327	-0.830571
C	-0.598664	0.056247	1.832282	-0.487529	-0.053393
H	-1.952813	1.835465	1.810651	0.084426	-0.013018
H	-0.764885	-0.946872	2.246157	0.264764	-0.072038
H	0.005814	0.598360	2.567312	0.220711	-0.009771
C	1.777843	-1.531230	0.048461	0.369630	-0.442658
C	3.102124	-1.382830	0.485872	-0.158876	-0.071888
C	1.379125	-2.784694	-0.437760	-0.300271	-0.085775
C	3.999729	-2.449822	0.436154	-0.233104	-0.033408
H	3.443480	-0.420978	0.863882	0.150171	0.040574
C	2.271076	-3.856111	-0.490434	-0.309598	-0.033223

H	0.356604	-2.930446	-0.783333	0.137501	0.036941
C	3.584906	-3.688659	-0.052937	-0.111835	-0.055541
H	5.021952	-2.314539	0.776938	0.159444	0.021857
H	1.943055	-4.818353	-0.872441	0.155744	0.023991
H	4.282493	-4.519645	-0.093293	0.150714	0.032979

12L

Electronic energy: -1407.3749

Electronic energy + zero-point energy: -1406.8498

Electronic energy + thermal energy correction: -1406.7973

Electronic energy + thermal enthalpy correction: -1406.7961

Electronic energy + thermal free energy correction: -1406.9510

BSSE correction: 0.007030

Table S78. Cartesian coordinates, Mulliken and APT charges of all atoms at **12L** in the reaction between diphenylgermane and styrene.

Symbol	X	Y	Z	Mulliken	APT
H	1.876351	0.916934	0.568183	-0.148121	-0.419030
C	1.646229	-1.809182	-0.315837	-0.344812	-0.398259
C	1.020473	-2.433984	-1.403857	0.264606	-0.091158
C	1.717348	-2.517394	0.894388	-0.499264	-0.071803
C	0.488444	-3.719564	-1.291609	-0.082318	-0.024071
H	0.940290	-1.912524	-2.354978	0.189662	0.061590
C	1.180631	-3.799252	1.017792	-0.078892	-0.059452
H	2.212885	-2.068680	1.754913	0.166554	0.044573
C	0.567147	-4.404299	-0.079629	-0.248653	-0.052579
H	0.010021	-4.183837	-2.148963	0.170246	0.034367
H	1.247558	-4.327040	1.964599	0.172277	0.030089
H	0.151497	-5.403241	0.010666	0.165793	0.039372
Ge	2.498073	-0.046431	-0.490299	0.285317	1.729853
Na	-0.177048	2.328403	0.767494	0.073021	0.648289
C	-1.717043	3.639840	-1.081085	0.111787	0.342826
C	-1.227331	2.513149	-1.706371	-0.000488	-0.456078
C	-0.861477	4.615367	-0.510166	-0.279620	-0.733049
C	0.198470	2.231578	-1.803876	-0.544417	0.633933
C	1.050442	3.291665	-1.279481	-0.375600	-0.507619
C	0.522244	4.425855	-0.673969	0.163271	0.496942
H	-2.795106	3.775957	-1.020068	0.161397	0.020928
H	-1.258633	5.509969	-0.045972	0.135057	0.039238
H	1.210435	5.184731	-0.306359	0.158348	0.021357
H	2.128119	3.203911	-1.376351	0.086276	0.030068

H	-1.920620	1.788864	-2.129378	0.078359	0.018041
C	0.683897	1.041305	-2.308161	-0.304490	-0.808465
C	2.137095	0.667392	-2.288824	-0.418760	-0.076895
H	-0.025290	0.313037	-2.690948	0.100927	0.005167
H	2.815427	1.499583	-2.510771	0.231963	-0.057006
H	2.368461	-0.119317	-3.014912	0.194475	-0.006900
H	-4.144396	-0.251389	-2.235628	0.184286	0.040480
H	-1.613027	-0.723394	-1.382173	-0.095625	-0.300506
H	-6.598646	-0.159407	-2.477157	0.166368	0.030244
C	-4.773806	-0.613660	-1.425541	-0.318561	-0.066134
C	-6.161993	-0.559785	-1.567274	-0.176301	-0.038154
H	-1.718933	-2.499567	0.439018	-0.084204	-0.310909
Ge	-2.244932	-1.136955	-0.045471	0.202679	1.584174
C	-4.187462	-1.126998	-0.260903	0.068307	-0.377186
C	-6.984256	-1.020610	-0.540717	-0.275681	-0.026356
H	-8.063794	-0.981245	-0.649005	0.153629	0.035052
C	-5.030736	-1.583098	0.763448	-0.151193	-0.063669
C	-6.417067	-1.533421	0.627106	-0.063430	-0.047483
H	-4.604392	-1.982382	1.681745	0.163474	0.038279
H	-7.054515	-1.893726	1.428905	0.169834	0.027204
C	4.381095	-0.239804	0.048561	0.101577	-0.427846
C	5.048637	-1.471689	-0.001698	0.188561	-0.091376
C	5.112129	0.891872	0.439552	-0.542074	-0.089085
C	6.400731	-1.571502	0.330157	-0.129906	-0.029311
H	4.507420	-2.368455	-0.297173	0.140500	0.043004
C	6.463446	0.800121	0.772400	-0.218428	-0.034715
H	4.621743	1.863479	0.487711	0.145665	0.038347
C	7.110124	-0.435041	0.717812	-0.171017	-0.063304
H	6.899627	-2.535220	0.287098	0.163519	0.017662
H	7.011026	1.688317	1.073770	0.162386	0.020774
H	8.161907	-0.510921	0.976405	0.150949	0.029479
C	-1.830462	0.167025	1.373072	0.206335	-0.392813
C	-0.726625	-0.013558	2.221804	-0.433083	-0.045008
C	-2.645329	1.294205	1.574699	0.060332	-0.056907
C	-0.436761	0.906953	3.234805	-0.164761	-0.083450
H	-0.083072	-0.880690	2.090376	0.129530	0.066945
C	-2.360821	2.219997	2.582695	-0.077335	-0.047217
H	-3.510751	1.455279	0.935604	0.201876	0.062902
C	-1.253488	2.026051	3.414792	-0.027326	-0.036989
H	0.421680	0.749735	3.880752	0.199685	0.051254
H	-2.997751	3.088520	2.717260	0.191368	0.054141
H	-1.032057	2.741418	4.200510	0.194162	0.054208

13L

Electronic energy: -1407.3486

Electronic energy + zero-point energy: -1406.8263

Electronic energy + thermal energy correction: -1406.7744

Electronic energy + thermal enthalpy correction: -1406.7732

Electronic energy + thermal free energy correction: -1406.9289

BSSE correction: 0.006668

Table S79. Cartesian coordinates, Mulliken and APT charges of all atoms at **13L** in the reaction between diphenylgermane and styrene.

Symbol	X	Y	Z	Mulliken	APT
H	-2.005056	0.399092	-1.840653	-0.123574	-0.406540
C	-3.654268	-1.451639	-0.481542	0.263442	-0.428762
C	-4.516270	-1.790195	0.572514	-0.362815	-0.067296
C	-3.492771	-2.373271	-1.524572	0.001496	-0.063696
C	-5.193003	-3.009083	0.586712	-0.118767	-0.034400
H	-4.666566	-1.092472	1.394748	0.151933	0.041674
C	-4.167011	-3.596126	-1.517443	-0.190237	-0.035458
H	-2.833148	-2.136474	-2.356858	0.168652	0.035963
C	-5.018133	-3.915007	-0.460554	-0.238439	-0.034213
H	-5.856032	-3.252499	1.411632	0.161460	0.026416
H	-4.029468	-4.296669	-2.335895	0.161325	0.025428
H	-5.544716	-4.864573	-0.452505	0.147109	0.030927
Ge	-2.669117	0.242236	-0.451111	0.233863	1.878350
Na	3.413412	-0.721328	1.219490	0.391086	0.698632
C	2.333756	-2.731888	2.702098	-0.055681	0.229463
C	1.311187	-2.486679	1.802479	-0.007288	-0.337746
C	2.764829	-1.736254	3.608781	-0.201124	-0.472836
C	0.615587	-1.233238	1.752792	-0.135114	0.623255
C	1.095567	-0.232287	2.656774	-0.288307	-0.369273
C	2.123859	-0.494542	3.568676	0.050228	0.261773
H	2.806840	-3.710535	2.712716	0.163703	0.031184
H	3.545396	-1.941420	4.332741	0.159370	0.042509
H	2.424092	0.287880	4.261932	0.167266	0.033942
H	0.599829	0.733154	2.685455	0.116547	0.057409
H	0.998631	-3.274879	1.121413	0.152675	0.035468
C	-0.382927	-0.963606	0.784282	-0.337788	-1.233154
C	-1.304725	0.218653	0.950846	-1.007768	-0.151176
H	-0.773554	-1.838964	0.262442	0.174188	0.023745
H	-0.742482	1.168578	0.857171	0.403497	-0.038253
H	-1.805132	0.255402	1.931899	0.242632	-0.070164
H	1.391952	-2.353697	-1.444202	0.170792	0.043553
H	0.528419	-0.180502	-0.286790	0.111398	0.612052
H	2.875229	-4.323440	-1.457323	0.176353	0.034735
C	2.471378	-2.207883	-1.439157	-0.527108	-0.081866
C	3.305243	-3.326226	-1.435577	-0.199867	-0.005958
H	1.349387	0.966715	-2.761101	-0.141329	-0.423058

Ge	1.689014	0.628389	-1.282845	0.113282	1.107455
C	2.989145	-0.899595	-1.409209	-0.104663	-0.392021
C	4.691113	-3.164573	-1.386391	-0.283941	-0.062713
H	5.342605	-4.032864	-1.375041	0.164146	0.038005
C	4.388901	-0.763521	-1.370880	0.207323	-0.108346
C	5.233397	-1.879742	-1.355284	0.016950	-0.014022
H	4.831328	0.232062	-1.357357	0.154554	0.042273
H	6.310894	-1.743964	-1.328841	0.179067	0.026176
C	-3.945604	1.691845	-0.104719	0.288066	-0.431385
C	-3.541736	2.853659	0.568959	-0.366668	-0.051344
C	-5.285917	1.593095	-0.504802	-0.211905	-0.063819
C	-4.442261	3.887425	0.828453	-0.218877	-0.048300
H	-2.510604	2.958255	0.900603	0.048606	0.034535
C	-6.192112	2.622573	-0.248452	-0.140761	-0.049128
H	-5.631961	0.697135	-1.016407	0.137625	0.041555
C	-5.770295	3.772694	0.418490	-0.188966	-0.044134
H	-4.109125	4.778763	1.351884	0.171583	0.024195
H	-7.226294	2.526110	-0.565644	0.161303	0.021190
H	-6.474066	4.574430	0.620848	0.149446	0.028906
C	2.873449	2.104602	-0.674033	0.076018	-0.457204
C	2.960839	2.458165	0.681640	-0.534160	-0.121535
C	3.707591	2.786997	-1.575932	0.167645	-0.082805
C	3.856035	3.435369	1.126952	-0.236823	-0.021670
H	2.300243	1.979943	1.405185	0.029975	0.044007
C	4.598751	3.768758	-1.142041	-0.123377	-0.040252
H	3.662673	2.547591	-2.636482	0.178316	0.044273
C	4.679107	4.091595	0.213932	-0.148662	-0.055606
H	3.898404	3.692791	2.181622	0.167915	0.028454
H	5.230793	4.282683	-1.860538	0.161052	0.017797
H	5.371062	4.856504	0.552814	0.152122	0.032835

14L

Electronic energy: -1407.4082

Electronic energy + zero-point energy: -1406.8784

Electronic energy + thermal energy correction: -1406.8265

Electronic energy + thermal enthalpy correction: -1406.8253

Electronic energy + thermal free energy correction: -1406.9766

BSSE correction: 0.009000

Table S80. Cartesian coordinates, Mulliken and APT charges of all atoms at **14L** in the reaction between diphenylgermane and styrene.

Symbol	X	Y	Z	Mulliken	APT
H	3.705616	1.758824	-2.019988	-0.083708	-0.395579
C	2.194976	1.910899	0.398352	0.553073	-0.424748
C	1.901042	1.356073	1.652325	-0.694765	-0.095519
C	1.868309	3.257538	0.182587	0.164115	-0.057690
C	1.281730	2.110517	2.649591	-0.122917	-0.056532
H	2.159032	0.319630	1.863612	0.144643	0.052035
C	1.245010	4.017603	1.172689	-0.043652	-0.045348
H	2.099355	3.725370	-0.772831	0.164030	0.039468
C	0.944607	3.441778	2.407061	-0.263404	-0.038392
H	1.053396	1.657108	3.609879	0.187350	0.047292
H	0.989770	5.055154	0.979735	0.176939	0.037278
H	0.450092	4.026518	3.176166	0.174679	0.051225
Ge	2.957823	0.823539	-1.044408	0.228574	1.799688
Na	-3.274815	-1.098213	-0.550337	0.364118	0.714710
C	-2.161880	-3.402028	-1.807906	-0.110202	-0.018512
C	-1.053791	-2.764863	-1.242276	-0.145888	-0.120885
C	-2.899252	-2.767392	-2.811647	-0.198641	-0.079706
C	-0.654770	-1.489221	-1.667283	0.166742	0.080898
C	-1.410936	-0.857802	-2.665906	-0.259287	-0.131257
C	-2.520130	-1.489046	-3.234375	-0.071175	-0.010540
H	-2.446509	-4.391433	-1.463222	0.202155	0.052407
H	-3.755059	-3.261913	-3.259755	0.186499	0.055906
H	-3.090061	-0.977468	-4.004125	0.203600	0.053638
H	-1.146675	0.143928	-2.991308	0.051913	0.094508
H	-0.496329	-3.258169	-0.450084	0.122614	0.079461
C	0.534131	-0.809972	-1.022082	-0.165549	0.027591
C	1.479766	-0.082748	-1.984814	-0.445191	-0.368811
H	1.078108	-1.570838	-0.451296	0.159105	-0.009102
H	0.937386	0.696060	-2.534639	0.237355	-0.001828
H	1.892931	-0.775919	-2.726510	0.204408	-0.015936
H	-0.533614	0.172295	2.007658	0.014063	0.054574
H	0.153759	-0.093673	-0.283184	-0.790744	0.011714
H	0.875521	-1.790463	2.434698	0.139927	0.016043
C	-1.004880	-0.807048	2.061702	-0.525159	-0.147964
C	-0.198292	-1.917570	2.310931	0.123548	0.022368
H	-4.762435	-0.090585	1.000828	-0.233023	-0.429403
Ge	-3.581742	0.766534	1.733820	0.076854	0.607268
C	-2.399151	-0.911649	1.901247	0.024360	-0.240591
C	-0.764741	-3.189287	2.419699	-0.122705	-0.121116
H	-0.140828	-4.054916	2.621614	0.158568	0.036573
C	-2.939664	-2.207205	2.023970	-0.141973	-0.170732
C	-2.144580	-3.329445	2.277317	-0.108905	0.007890
H	-4.018392	-2.344381	1.938079	0.133397	0.020766
H	-2.604629	-4.309863	2.369718	0.155788	0.014457
C	4.261813	-0.451600	-0.327950	0.165457	-0.420798
C	3.898061	-1.534410	0.488613	-0.383521	-0.045100
C	5.623432	-0.280254	-0.618439	-0.007760	-0.055481
C	4.855918	-2.411499	0.996683	-0.209896	-0.054512

H	2.854333	-1.707493	0.740584	-0.110810	0.023140
C	6.587270	-1.154179	-0.114193	-0.131621	-0.036083
H	5.941661	0.548008	-1.247401	0.155455	0.037385
C	6.204259	-2.222099	0.695529	0.081042	-0.031527
H	4.549878	-3.240835	1.627329	0.179137	0.035692
H	7.635268	-1.000244	-0.352821	0.163394	0.026212
H	6.951692	-2.903145	1.090497	0.157505	0.034742
C	-2.889088	1.459321	-0.080911	-0.098804	-0.238614
C	-3.762165	1.616345	-1.176758	-0.116478	-0.175827
C	-1.584119	1.964699	-0.253821	-0.157942	-0.140576
C	-3.367538	2.221275	-2.373799	-0.097816	0.008088
H	-4.793221	1.272056	-1.086240	0.120810	0.023572
C	-1.176001	2.564951	-1.446245	-0.079480	-0.009313
H	-0.865768	1.918725	0.566132	0.250943	0.048324
C	-2.065350	2.696713	-2.514933	-0.319709	-0.110816
H	-4.078972	2.326032	-3.188933	0.159321	0.014855
H	-0.162292	2.946324	-1.533116	0.131387	0.034123
H	-1.748617	3.172892	-3.438262	0.157857	0.034946

15L

Electronic energy: -777.63256

Electronic energy + zero-point energy: -777.29391

Electronic energy + thermal energy correction: -777.26431

Electronic energy + thermal enthalpy correction: -777.26313

Electronic energy + thermal free energy correction: -777.36574

BSSE correction: 0.002699

Table S81. Cartesian coordinates, Mulliken and APT charges of all atoms at **15L** in the reaction between diphenylgermane and styrene.

Symbol	X	Y	Z	Mulliken	APT
H	1.464629	-0.039154	-2.661913	-0.120584	-0.427901
C	1.431528	1.701502	-0.334598	0.180762	-0.437621
C	2.682589	1.878395	0.273764	-0.141145	-0.052105
C	0.525129	2.770911	-0.303591	-0.237014	-0.046479
C	3.021501	3.085419	0.885602	-0.292152	-0.043946
H	3.402414	1.062357	0.278284	0.156525	0.041191
C	0.856930	3.980824	0.307219	-0.134964	-0.053580
H	-0.458100	2.665322	-0.758748	0.143340	0.029703
C	2.108047	4.139272	0.902217	-0.165289	-0.034104
H	3.995641	3.202455	1.350824	0.160273	0.029170
H	0.140370	4.796612	0.320314	0.161447	0.029947

H	2.368948	5.078831	1.379616	0.154317	0.035153
Ge	0.959429	0.007014	-1.202665	0.213153	1.831828
C	-5.124797	-1.544038	0.218415	-0.060571	-0.005966
C	-3.731106	-1.513767	0.233587	-0.128627	-0.103167
C	-5.851629	-0.356694	0.307066	-0.199779	-0.086362
C	-3.041520	-0.301201	0.336690	0.043289	0.089270
C	-3.780983	0.882598	0.425358	-0.552077	-0.099605
C	-5.174944	0.858416	0.411406	-0.096795	-0.006306
H	-5.643670	-2.494777	0.141471	0.151800	0.030088
H	-6.936813	-0.378603	0.298787	0.141451	0.034866
H	-5.732629	1.787133	0.485929	0.156907	0.030927
H	-3.255936	1.831844	0.510868	0.107053	0.034615
H	-3.167933	-2.442058	0.167178	0.137501	0.038912
C	-1.532604	-0.263125	0.296200	-0.274694	0.096391
C	-0.995705	-0.184300	-1.144459	-0.512708	-0.396072
H	-1.128593	-1.157509	0.785625	0.167908	-0.026931
H	-1.454577	0.662390	-1.670159	0.193921	-0.008485
H	-1.282640	-1.084797	-1.699880	0.214865	-0.004559
H	-1.178325	0.600702	0.873306	0.237694	-0.023541
C	1.823099	-1.449069	-0.218612	0.462840	-0.434129
C	1.874114	-1.433018	1.183902	-0.545190	-0.071762
C	2.371096	-2.552227	-0.887759	0.002750	-0.039342
C	2.448310	-2.486253	1.895216	-0.186608	-0.041432
H	1.468450	-0.584151	1.731984	0.177944	0.041819
C	2.948073	-3.609166	-0.181989	-0.222039	-0.045953
H	2.354436	-2.589375	-1.974926	0.160098	0.033106
C	2.985909	-3.577148	1.211410	-0.127434	-0.031129
H	2.478744	-2.454927	2.980194	0.167485	0.031098
H	3.369812	-4.453701	-0.718633	0.152422	0.027056
H	3.435814	-4.397032	1.762896	0.151926	0.035340

Triethylgermane + styrene

5M

Electronic energy: -714.32089

Electronic energy + zero-point energy: -713.96925

Electronic energy + thermal energy correction: -713.93676

Electronic energy + thermal enthalpy correction: -713.93558

Electronic energy + thermal free energy correction: -714.04034

BSSE correction: 0.004106

Table S82. Cartesian coordinates, Mulliken and APT charges of all atoms at **5M** in the reaction between triethylgermane and styrene.

Symbol	X	Y	Z	Mulliken	APT
H	-0.542861	2.568460	-1.454820	0.159030	-0.082056
C	-0.918563	2.992433	-0.508102	-0.623293	0.297448
C	-1.282946	1.932005	0.491741	-0.465204	-0.751405
C	-2.205455	0.949149	0.219810	-0.040632	0.577576
C	-2.853227	0.806430	-1.081194	-0.088879	-0.505694
H	-2.635890	1.534850	-1.856197	0.134064	0.038455
C	-3.788843	-0.187235	-1.335207	-0.149819	0.465440
H	-4.258504	-0.217654	-2.316794	0.147324	0.017896
C	-4.142682	-1.155297	-0.373941	-0.423449	-0.765156
H	-4.895315	-1.907222	-0.577886	0.135211	0.041640
C	-3.545113	-1.037304	0.905483	0.016007	0.406402
H	-3.822690	-1.739379	1.689346	0.159850	0.020624
C	-2.617796	-0.054895	1.195532	-0.056970	-0.456720
H	-2.211665	0.011446	2.202548	0.091462	0.024202
Na	-1.550306	-1.454711	-0.804147	0.383794	0.764873
H	-0.133583	3.648554	-0.118080	0.141817	-0.030461
H	-1.769839	3.636320	-0.783322	0.157269	-0.103790
H	-0.892237	2.013491	1.503309	0.074675	0.006911
Ge	1.654561	-0.190582	-0.070161	0.458583	1.519468
H	0.484966	-0.429484	-1.094824	-0.090261	-0.442879
C	2.302094	1.662260	-0.211979	-0.350155	-0.291088
H	1.652393	2.202163	-0.905803	0.197717	0.007677
H	3.298241	1.632619	-0.669633	0.202351	-0.053075
C	1.019941	-0.667928	1.728243	-0.228018	-0.314797
H	1.718191	-0.238497	2.456571	0.224431	-0.019812
H	0.061201	-0.163016	1.883188	0.390564	0.001353
C	3.072468	-1.440674	-0.634453	-0.437187	-0.317054
H	2.718577	-2.469749	-0.499449	0.164452	-0.035580
H	3.922727	-1.316332	0.048363	0.193899	-0.032179
C	2.360125	2.396276	1.133310	-0.608760	0.078175
H	3.046871	1.906452	1.831964	0.144392	-0.028426
H	2.702546	3.428523	1.006584	0.161329	-0.047650
H	1.373186	2.428098	1.605395	0.239719	0.014237
C	0.887716	-2.177238	1.965063	-0.786472	0.088513
H	1.855964	-2.682556	1.893137	0.182328	-0.017940
H	0.473722	-2.393044	2.955109	0.166331	-0.037192
H	0.223804	-2.656871	1.233658	0.168353	-0.043175
C	3.518771	-1.220525	-2.085006	-0.611134	0.090790
H	3.899202	-0.205202	-2.238129	0.159398	-0.011643
H	4.313852	-1.914002	-2.377278	0.163812	-0.054819
H	2.685607	-1.362261	-2.781972	0.142071	-0.019088

6M

Electronic energy: -714.30942

Electronic energy + zero-point energy: -713.95789

Electronic energy + thermal energy correction: -713.9275

Electronic energy + thermal enthalpy correction: -713.92632

Electronic energy + thermal free energy correction: -714.02322

BSSE correction: 0.004873

Table S83. Cartesian coordinates, Mulliken and APT charges of all atoms at **6M** in the reaction between triethylgermane and styrene.

Symbol	X	Y	Z	Mulliken	APT
H	0.372635	1.936306	-1.943725	0.185879	-0.016046
C	0.273825	2.471015	-0.986976	-0.550550	0.149586
C	-0.152194	1.531299	0.133386	-0.563032	-0.864160
C	-1.531074	1.063560	0.065126	-0.357505	0.474758
C	-2.263489	1.032454	-1.146807	0.011245	-0.233514
H	-1.830229	1.469566	-2.040064	0.153517	0.054554
C	-3.544382	0.472764	-1.220022	-0.261380	0.099766
H	-4.077998	0.487419	-2.166552	0.168850	0.034994
C	-4.139762	-0.100629	-0.095076	-0.239578	-0.286748
H	-5.135058	-0.528809	-0.149764	0.161181	0.044456
C	-3.434734	-0.080215	1.118875	0.072894	0.133944
H	-3.883907	-0.504807	2.012514	0.184290	0.038882
C	-2.168028	0.489379	1.194075	0.170873	-0.232333
H	-1.641631	0.496974	2.145710	0.126696	0.047120
Na	-1.771590	-1.586974	-0.766683	0.466694	0.760717
H	1.249518	2.915302	-0.772260	0.101049	-0.008285
H	-0.438014	3.293129	-1.151224	0.166511	-0.076517
H	0.063558	1.934994	1.127032	0.197749	0.001200
Ge	1.230498	-0.205921	0.017227	0.570626	1.951156
H	0.073029	-0.677652	-1.168915	-0.235017	-0.478623
C	2.802057	0.999536	0.480131	-0.460966	-0.392736
H	3.152423	1.509930	-0.426754	0.195373	-0.041578
H	3.593392	0.282648	0.737516	0.162169	-0.096377
C	0.825197	-1.198434	1.700156	-0.379702	-0.354189
H	1.810903	-1.541452	2.041899	0.195926	-0.033612
H	0.459169	-0.511722	2.472323	0.224813	-0.031176
C	2.409623	-1.546707	-0.979709	-0.429076	-0.379590
H	1.850460	-2.493730	-1.023825	0.167126	-0.078033
H	3.337280	-1.740575	-0.423762	0.162938	-0.074808
C	2.636352	2.004496	1.622883	-0.531263	0.077204
H	2.174746	1.538975	2.502647	0.158386	-0.024242
H	3.599837	2.418521	1.944384	0.154729	-0.083971
H	2.004452	2.851315	1.338205	0.167502	-0.018368
C	-0.109945	-2.409040	1.588584	-0.583076	0.092886

H	0.117942	-3.014342	0.701622	0.126687	-0.026532
H	-0.037301	-3.077953	2.453371	0.165875	-0.056584
H	-1.160910	-2.094820	1.541697	0.126714	-0.047901
C	2.733653	-1.076083	-2.399308	-0.595272	0.113721
H	3.344285	-0.165069	-2.383398	0.174195	-0.028659
H	3.279419	-1.820397	-2.992127	0.143031	-0.082941
H	1.810957	-0.837957	-2.946221	0.122896	-0.027421

7M

Electronic energy: -714.31407

Electronic energy + zero-point energy: -713.96253

Electronic energy + thermal energy correction: -713.93109

Electronic energy + thermal enthalpy correction: -713.92990

Electronic energy + thermal free energy correction: -714.03039

BSSE correction: 0.005084

Table S84. Cartesian coordinates, Mulliken and APT charges of all atoms at **7M** in the reaction between triethylgermane and styrene.

Symbol	X	Y	Z	Mulliken	APT
H	-0.320137	-2.780891	-0.086664	0.213589	-0.006528
C	-0.415959	-2.376365	0.927320	-0.504006	0.093530
C	-0.014908	-0.902361	0.993531	-0.962544	-0.581535
C	1.428612	-0.637079	0.764868	-0.022236	0.303267
C	2.282573	-1.533902	0.098035	0.290174	-0.185127
H	1.898174	-2.494139	-0.230016	0.155543	0.061693
C	3.621865	-1.216528	-0.154210	-0.214249	0.042819
H	4.255572	-1.937009	-0.663335	0.173238	0.038403
C	4.147639	0.013564	0.245171	-0.245260	-0.186752
H	5.187936	0.257617	0.056453	0.165099	0.047874
C	3.314673	0.917320	0.918423	0.101250	0.057757
H	3.707652	1.873980	1.250445	0.189599	0.044057
C	1.984676	0.591783	1.173868	-0.152472	-0.173363
H	1.345867	1.304545	1.691848	0.160593	0.053486
Na	2.074775	0.598833	-1.678203	0.599451	0.754649
H	-1.463015	-2.496713	1.223199	0.137900	-0.000373
H	0.194937	-3.000665	1.593053	0.162277	-0.061242
H	-0.261959	-0.506692	1.985291	0.207575	-0.016985
Ge	-1.284726	0.208850	-0.206473	0.554597	2.001706
H	0.124503	0.153751	-1.512524	-0.441682	-0.658324
C	-2.873897	0.026914	1.098706	-0.477615	-0.412398
H	-3.355786	-0.947082	0.926321	0.194501	-0.066172

H	-3.599982	0.772606	0.739846	0.169397	-0.091568
C	-1.094337	2.192001	-0.022867	-0.433387	-0.347745
H	-2.090359	2.575072	-0.283278	0.183571	-0.046637
H	-0.972319	2.408528	1.046903	0.208459	-0.038201
C	-2.339173	-0.403193	-1.795680	-0.523216	-0.353699
H	-2.093513	0.291621	-2.608576	0.201283	-0.060643
H	-3.408713	-0.297178	-1.572784	0.164375	-0.069968
C	-2.640095	0.225399	2.599258	-0.534179	0.088587
H	-2.024605	1.112319	2.801494	0.150473	-0.033213
H	-3.573096	0.349899	3.163718	0.153248	-0.097452
H	-2.118090	-0.631689	3.040693	0.148113	-0.033626
C	-0.036348	2.935936	-0.834858	-0.561172	0.102320
H	-0.100672	2.677085	-1.897465	0.152204	-0.022759
H	-0.138129	4.023975	-0.746310	0.152907	-0.071374
H	0.974717	2.682623	-0.490246	0.101616	-0.056478
C	-2.036250	-1.837591	-2.233067	-0.460907	0.103326
H	-2.345434	-2.560632	-1.469160	0.167255	-0.027304
H	-2.549857	-2.107956	-3.163237	0.145037	-0.076866
H	-0.959408	-1.968729	-2.399301	0.129603	-0.017140

8M

Electronic energy: -858.85154

Electronic energy + zero-point energy: -858.38380

Electronic energy + thermal energy correction: -858.34090

Electronic energy + thermal enthalpy correction: -858.33971

Electronic energy + thermal free energy correction: -858.46569

BSSE correction: 0.006228

Table S85. Cartesian coordinates, Mulliken and APT charges of all atoms at **8M** in the reaction between triethylgermane and styrene.

Symbol	X	Y	Z	Mulliken	APT
H	0.457634	-0.251274	-2.710639	0.214968	0.000631
C	1.259705	0.472243	-2.525630	-0.514537	0.083725
C	1.213644	1.011314	-1.095454	-0.725098	-0.559538
C	0.026339	1.853951	-0.787345	-0.013116	0.274373
C	-1.156599	1.822671	-1.546933	0.284969	-0.184640
H	-1.210551	1.192697	-2.428781	0.154320	0.068512
C	-2.276516	2.579622	-1.185181	-0.104139	0.027377
H	-3.172599	2.533726	-1.797582	0.167582	0.045808
C	-2.251863	3.385193	-0.045151	-0.219317	-0.165804
H	-3.119091	3.974240	0.234380	0.177062	0.051398

C	-1.077242	3.441414	0.717158	0.164944	0.047429
H	-1.031304	4.075130	1.598013	0.198039	0.046704
C	0.038133	2.692218	0.346472	-0.382592	-0.163990
H	0.942351	2.738035	0.950775	0.164262	0.055457
Na	-1.820013	0.660132	0.858114	0.323243	0.738403
H	2.208572	-0.043275	-2.706148	0.155343	-0.001740
H	1.165801	1.272734	-3.271460	0.159658	-0.056708
H	2.100738	1.628251	-0.914487	0.229705	-0.019088
Ge	1.521261	-0.551030	0.212634	0.552054	2.006700
H	-0.458851	-0.699093	0.262243	-0.795179	-0.681073
C	3.564144	-0.560760	-0.044973	-0.483748	-0.412403
H	3.793752	-1.076140	-0.989495	0.193286	-0.063243
H	3.930714	-1.234272	0.744808	0.164850	-0.082361
C	1.577372	-0.082738	2.157660	-0.492135	-0.351737
H	2.166353	-0.904155	2.588349	0.187315	-0.043722
H	2.208663	0.809063	2.261893	0.208782	-0.038841
C	1.302278	-2.503355	-0.155606	-0.383923	-0.347831
H	0.693105	-2.886668	0.673718	0.215250	-0.055913
H	2.286419	-2.984696	-0.088879	0.194640	-0.068957
C	4.332829	0.763154	0.017614	-0.571201	0.086512
H	3.997209	1.391865	0.853434	0.143427	-0.031921
H	5.414108	0.622116	0.140578	0.152376	-0.096018
H	4.196068	1.350976	-0.897195	0.140588	-0.033111
C	0.291798	0.087739	2.963790	-0.416232	0.091048
H	-0.401041	-0.741791	2.782245	0.176849	-0.026565
H	0.484215	0.132274	4.041921	0.176743	-0.068063
H	-0.214586	1.027977	2.706281	0.073048	-0.051814
C	0.640163	-2.847384	-1.490312	-0.589497	0.089729
H	1.283885	-2.576275	-2.334864	0.160419	-0.030243
H	0.416235	-3.917527	-1.578768	0.135347	-0.068352
H	-0.305452	-2.302192	-1.599644	0.225738	-0.010366
C	-3.338290	-1.227878	-1.318670	-0.761027	-0.337368
H	-3.520379	-0.151438	-1.223417	0.176531	-0.020593
H	-2.527337	-1.388886	-2.036335	0.210475	0.024853
H	-4.243942	-1.658630	-1.775446	0.152242	-0.000362
C	-3.666756	-1.439099	1.409936	-0.811603	-0.345799
H	-2.970691	-1.592936	2.243730	0.197950	0.027417
H	-4.024032	-0.400402	1.407342	0.100332	-0.030049
H	-4.548028	-2.046806	1.662210	0.185799	0.013472
C	-2.504925	-3.458620	0.026638	-0.842308	-0.301093
H	-2.514822	-3.941612	-0.955464	0.147474	-0.010121
H	-1.450175	-3.354441	0.317765	0.259797	0.038793
H	-2.968666	-4.124049	0.763176	0.137990	-0.017599
B	-3.113954	-2.007825	0.033623	1.042255	0.958685

9M

Electronic energy: -858.85194

Electronic energy + zero-point energy: -858.38495

Electronic energy + thermal energy correction: -858.34273

Electronic energy + thermal enthalpy correction: -858.34154

Electronic energy + thermal free energy correction: -858.46624

BSSE correction: 0.006315

Table S86. Cartesian coordinates, Mulliken and APT charges of all atoms at **9M** in the reaction between triethylgermane and styrene.

Symbol	X	Y	Z	Mulliken	APT
H	-0.758594	-0.102456	-2.789109	0.202863	0.001635
C	-1.448480	-0.857446	-2.398901	-0.418917	0.084616
C	-1.171294	-1.189005	-0.930190	-1.038927	-0.556914
C	0.113407	-1.900580	-0.690495	-0.003668	0.275013
C	1.233449	-1.767648	-1.530449	0.302384	-0.178043
H	1.167162	-1.144775	-2.416687	0.153529	0.066956
C	2.439949	-2.413578	-1.243752	-0.138182	0.029852
H	3.284204	-2.290510	-1.916079	0.168795	0.047295
C	2.567144	-3.209323	-0.102546	-0.168575	-0.167290
H	3.501148	-3.716544	0.115657	0.179217	0.051194
C	1.460946	-3.360211	0.742904	0.089843	0.045244
H	1.533980	-3.986778	1.626977	0.194603	0.044855
C	0.258920	-2.716888	0.448916	-0.218871	-0.168085
H	-0.593377	-2.839636	1.114576	0.160965	0.052852
Na	1.967172	-0.537459	0.837251	0.297975	0.738121
H	-2.460736	-0.456098	-2.511648	0.142826	-0.000585
H	-1.365400	-1.746382	-3.037707	0.162610	-0.056021
H	-1.967732	-1.846953	-0.563560	0.206060	-0.024295
Ge	-1.501569	0.474964	0.234440	0.565131	2.014302
H	0.519289	0.734479	0.229195	-0.774373	-0.708995
C	-3.548024	0.381402	0.033187	-0.450744	-0.405665
H	-3.824700	0.855858	-0.920037	0.192470	-0.063060
H	-3.925720	1.062330	0.811223	0.172502	-0.082892
C	-1.484101	0.136383	2.203031	-0.505630	-0.345879
H	-2.094299	0.956351	2.605353	0.189877	-0.042737
H	-2.075735	-0.773327	2.370785	0.207252	-0.040500
C	-1.381866	2.382713	-0.327538	-0.368416	-0.358239
H	-0.640924	2.863943	0.319999	0.300545	-0.042725
H	-2.356435	2.853099	-0.141710	0.212588	-0.067079
C	-4.255026	-0.971805	0.155718	-0.541730	0.089251
H	-3.891440	-1.545203	1.018980	0.146104	-0.032961
H	-5.341650	-0.874659	0.273266	0.154518	-0.096245
H	-4.088899	-1.593284	-0.732036	0.147569	-0.032396
C	-0.171918	0.057955	2.979088	-0.402934	0.092902

H	0.471426	0.914371	2.751485	0.166888	-0.024895
H	-0.334960	0.038667	4.062864	0.176747	-0.070674
H	0.376410	-0.861980	2.735258	0.061783	-0.052597
C	-0.989632	2.568196	-1.794669	-0.584126	0.090333
H	-1.754147	2.162489	-2.467420	0.169914	-0.025884
H	-0.853054	3.624739	-2.056231	0.129120	-0.065674
H	-0.046561	2.049988	-2.009979	0.194352	-0.015980
C	3.220699	1.419842	-1.302041	-0.688107	-0.347165
H	3.628117	0.415150	-1.133062	0.196309	-0.024939
H	2.414411	1.350489	-2.038715	0.230211	0.018964
H	4.026875	2.000179	-1.777766	0.155905	-0.006892
C	3.359230	1.849124	1.428953	-0.762458	-0.349052
H	2.591246	1.893744	2.209529	0.210461	0.019444
H	3.917130	0.906773	1.513652	0.130597	-0.039640
H	4.078076	2.638473	1.693351	0.167140	0.005344
C	2.063596	3.612057	-0.166370	-0.895765	-0.338633
H	1.351091	3.644182	-0.994607	0.191277	0.023593
H	1.565647	3.957000	0.745225	0.148758	0.005644
H	2.849057	4.349414	-0.397405	0.132414	-0.009649
B	2.781684	2.218588	-0.006908	0.949318	1.044872

10M

Electronic energy: -858.91345

Electronic energy + zero-point energy: -858.44100

Electronic energy + thermal energy correction: -858.39885

Electronic energy + thermal enthalpy correction: -858.39767

Electronic energy + thermal free energy correction: -858.52194

BSSE correction: 0.006504

Table S87. Cartesian coordinates, Mulliken and APT charges of all atoms at **10M** in the reaction between triethylgermane and styrene.

Symbol	X	Y	Z	Mulliken	APT
H	1.235865	0.347080	-2.764220	0.185323	0.013492
C	1.822973	1.095332	-2.225934	-0.491794	0.063957
C	1.425271	1.199861	-0.745483	-0.543479	-0.461901
C	0.058650	1.791682	-0.531454	-0.809827	0.226609
C	-0.995812	1.600333	-1.439701	1.000951	-0.147729
H	-0.853433	0.962906	-2.306489	0.204839	0.073207
C	-2.234823	2.217228	-1.253781	-0.360457	0.013609
H	-3.028696	2.049409	-1.974504	0.165689	0.062320
C	-2.459901	3.036387	-0.144431	-0.134973	-0.146098

H	-3.418820	3.526073	-0.008845	0.185939	0.061373
C	-1.427589	3.225957	0.781639	0.052960	0.017551
H	-1.578897	3.868674	1.643650	0.185362	0.049712
C	-0.189210	2.612950	0.583496	-0.241943	-0.141769
H	0.613889	2.787324	1.296741	0.165496	0.049657
Na	-2.299581	0.530939	0.951103	0.246672	0.788241
H	2.874452	0.807409	-2.321867	0.119898	-0.005479
H	1.689215	2.056015	-2.736836	0.174314	-0.037445
H	2.134715	1.882962	-0.256035	0.209069	-0.026840
Ge	1.826924	-0.520660	0.215662	0.561752	1.622322
H	-1.807127	-1.024193	-0.285854	-0.615095	-0.420059
C	3.750383	-0.817772	-0.113552	-0.409000	-0.339269
H	3.884753	-1.154971	-1.148738	0.192286	-0.025148
H	4.048028	-1.662783	0.520360	0.170094	-0.046259
C	1.591775	-0.298377	2.165413	-0.443767	-0.345274
H	2.107588	-1.156387	2.615393	0.170942	-0.023611
H	2.137247	0.591721	2.501943	0.200821	-0.025335
C	0.855427	-2.126916	-0.370842	-0.306927	-0.334109
H	-0.075265	-2.224851	0.196905	0.291172	0.007553
H	1.501466	-2.964031	-0.072085	0.167105	-0.041328
C	4.641774	0.395817	0.173932	-0.546041	0.083291
H	4.506192	0.758597	1.198989	0.167735	-0.013303
H	5.703471	0.159529	0.049556	0.166474	-0.057856
H	4.415211	1.229706	-0.499534	0.170295	-0.016271
C	0.142245	-0.255643	2.666269	-0.524927	0.082039
H	-0.466811	-1.048520	2.215742	0.145845	0.005097
H	0.079459	-0.377049	3.752344	0.176092	-0.052592
H	-0.309456	0.715462	2.432680	0.120595	-0.046892
C	0.543731	-2.211256	-1.868558	-0.691710	0.071710
H	1.436558	-2.055279	-2.485041	0.146432	-0.027306
H	0.124340	-3.187753	-2.129643	0.161180	-0.035078
H	-0.204224	-1.460864	-2.146475	0.240929	0.000567
C	-4.159147	-0.737681	-0.576193	-0.676139	-0.180497
H	-4.379796	0.198560	-0.026800	0.152807	-0.109339
H	-4.081402	-0.448536	-1.633791	0.175166	-0.048154
H	-5.079018	-1.332407	-0.478474	0.145986	-0.058919
C	-3.006959	-2.058845	1.513665	-0.743190	-0.182390
H	-2.172818	-2.688100	1.856976	0.165704	-0.050319
H	-3.095544	-1.247230	2.262651	0.170662	-0.113890
H	-3.921421	-2.654034	1.650722	0.154875	-0.055471
C	-2.781118	-3.013761	-0.984594	-0.902740	-0.158200
H	-2.673907	-2.805331	-2.058743	0.125049	-0.059018
H	-1.931775	-3.651379	-0.698043	0.134455	-0.057912
H	-3.688754	-3.626125	-0.868263	0.117985	-0.076476
B	-2.871500	-1.656516	-0.087411	0.953058	0.675230

11M

Electronic energy: -551.48530

Electronic energy + zero-point energy: -551.13989

Electronic energy + thermal energy correction: -551.11127

Electronic energy + thermal enthalpy correction: -551.11009

Electronic energy + thermal free energy correction: -551.20539

BSSE correction: 0.003096

Table S88. Cartesian coordinates, Mulliken and APT charges of all atoms at **11M** in the reaction between triethylgermane and styrene.

Symbol	X	Y	Z	Mulliken	APT
Ge	1.135633	-0.149942	-0.207373	0.568403	1.585372
C	1.376844	1.466470	-1.314489	-0.414835	-0.335774
H	0.425779	2.012481	-1.353550	0.220698	-0.021779
H	1.575571	1.137077	-2.341791	0.155506	-0.032653
C	2.874372	-0.724739	0.523685	-0.402562	-0.346956
H	3.583532	-0.800856	-0.310311	0.184169	-0.048243
H	3.262344	0.059403	1.185260	0.206502	-0.025408
C	0.370835	-1.604872	-1.295732	-0.430529	-0.333653
H	-0.048934	-2.362725	-0.622313	0.179961	-0.018609
H	1.203816	-2.089594	-1.821685	0.169879	-0.034626
C	2.510584	2.384433	-0.836900	-0.627559	0.102599
H	3.472672	1.862076	-0.849971	0.186132	-0.020571
H	2.608629	3.269621	-1.473921	0.162684	-0.057989
H	2.347798	2.734072	0.187683	0.156412	-0.013344
C	2.790950	-2.061958	1.270682	-0.630461	0.090473
H	2.425280	-2.860559	0.616273	0.181208	-0.013077
H	3.766238	-2.375171	1.657140	0.165653	-0.057182
H	2.107345	-2.001307	2.124448	0.158865	-0.016596
C	-0.693913	-1.147025	-2.302737	-0.559040	0.097070
H	-0.294141	-0.393116	-2.989273	0.161320	-0.020910
H	-1.055584	-1.983754	-2.909853	0.157332	-0.058919
H	-1.560510	-0.706386	-1.798832	0.160255	-0.007248
C	-3.511268	-1.128340	0.420087	0.015114	0.024652
C	-2.223626	-1.011157	0.936799	-0.186110	-0.136626
C	-4.122544	-0.035408	-0.196036	-0.084041	-0.114082
C	-1.508078	0.192618	0.848395	-0.748100	0.177221
C	-2.143141	1.286555	0.242867	0.341503	-0.151145
C	-3.433172	1.173566	-0.275449	-0.410188	0.030406
H	-4.039467	-2.073835	0.500191	0.160929	0.032029
H	-5.125431	-0.123435	-0.601323	0.164220	0.036962
H	-3.899764	2.035242	-0.743649	0.155618	0.031823
H	-1.625707	2.238770	0.167376	0.128458	0.046811
H	-1.755067	-1.869731	1.413093	0.140708	0.034879
C	-0.082583	0.261678	1.325810	0.078234	-0.413112

H	0.068482	-0.551396	2.047930	0.204700	-0.030762
C	0.297810	1.588826	1.993989	-0.588481	0.075398
H	1.316287	1.545148	2.394071	0.162985	-0.015116
H	0.263135	2.427876	1.291279	0.180683	-0.000752
H	-0.380971	1.824360	2.821852	0.173775	-0.040565

6L

Electronic energy: -714.29742

Electronic energy + zero-point energy: -713.94863

Electronic energy + thermal energy correction: -713.91642

Electronic energy + thermal enthalpy correction: -713.91524

Electronic energy + thermal free energy correction: -714.02083

BSSE correction: 0.003063

Table S89. Cartesian coordinates, Mulliken and APT charges of all atoms at **6L** in the reaction between triethylgermane and styrene.

Symbol	X	Y	Z	Mulliken	APT
H	0.140327	2.343095	1.031885	0.173942	-0.030156
C	0.524215	2.794969	0.099858	-0.618953	0.254560
C	1.018161	1.737104	-0.853583	-0.043307	-1.194061
C	2.172404	0.984644	-0.537764	-0.023472	0.555220
C	2.676118	0.897901	0.802929	-0.276236	-0.326759
H	2.289422	1.573770	1.559083	0.110074	0.041738
C	3.694323	0.005201	1.147417	-0.112906	0.313407
H	4.060011	-0.003391	2.171364	0.173323	0.029337
C	4.247580	-0.871633	0.208651	-0.268817	-0.532144
H	5.041203	-1.557256	0.482719	0.161527	0.039355
C	3.756212	-0.822875	-1.110514	-0.108423	0.278396
H	4.172502	-1.487290	-1.863597	0.170265	0.029201
C	2.752929	0.064691	-1.474799	-0.238926	-0.301779
H	2.400882	0.085396	-2.503552	0.136487	0.028270
Na	1.378409	-1.333985	0.329638	0.394238	0.657307
H	-0.301887	3.362273	-0.338821	0.139978	-0.011312
H	1.303074	3.512098	0.395339	0.164354	-0.067950
H	0.808442	1.880326	-1.912745	0.196354	0.041196
H	-0.021235	0.588031	-0.494741	0.002562	0.586549
Ge	-1.543247	-0.203031	0.030905	0.337894	1.124111
C	-2.331993	-1.529867	-1.232567	-0.419933	-0.384427
H	-2.266581	-1.132490	-2.252155	0.183989	-0.029511
H	-3.402566	-1.598628	-0.994719	0.190125	-0.090848
C	-1.867432	-0.962755	1.855928	-0.329323	-0.456022

H	-2.938038	-1.203403	1.918922	0.180486	-0.096408
H	-1.335474	-1.916909	1.974120	0.118134	-0.031182
C	-2.743731	1.375964	-0.093080	-0.418248	-0.287679
H	-2.406006	2.139061	0.617526	0.215666	-0.020124
H	-3.748511	1.069387	0.228203	0.189087	-0.085399
C	-1.698342	-2.923071	-1.173549	-0.633174	0.098669
H	-1.742305	-3.340297	-0.160640	0.177482	-0.019628
H	-2.198836	-3.636461	-1.837533	0.158231	-0.061473
H	-0.643877	-2.895261	-1.478160	0.147562	-0.030589
C	-1.479665	0.000708	2.982498	-0.624256	0.077625
H	-2.044546	0.936503	2.911010	0.189020	-0.012613
H	-1.667537	-0.421141	3.975969	0.146694	-0.060774
H	-0.416398	0.268369	2.931948	0.185594	-0.019799
C	-2.794931	1.961366	-1.509453	-0.650169	0.092615
H	-3.217518	1.242283	-2.219489	0.185946	-0.023503
H	-3.406563	2.869063	-1.560483	0.158109	-0.064981
H	-1.791683	2.219619	-1.868253	0.179021	-0.008436

7L

Electronic energy: -714.34674

Electronic energy + zero-point energy: -713.99145

Electronic energy + thermal energy correction: -713.95837

Electronic energy + thermal enthalpy correction: -713.95719

Electronic energy + thermal free energy correction: -714.06692

BSSE correction: 0.002025

Table S90. Cartesian coordinates, Mulliken and APT charges of all atoms at **7L** in the reaction between triethylgermane and styrene.

Symbol	X	Y	Z	Mulliken	APT
H	0.801220	2.311567	0.950605	0.147881	0.008166
C	1.520878	2.815283	0.296355	-0.733033	0.031546
C	2.004507	1.876531	-0.802444	-0.132472	0.090098
C	2.675835	0.606955	-0.325045	-0.861811	0.042499
C	2.962830	0.358738	1.022360	-0.148701	-0.140926
H	2.699896	1.094020	1.775773	0.170748	0.078313
C	3.577006	-0.834999	1.419046	-0.015993	-0.012466
H	3.791370	-1.004019	2.469793	0.199905	0.053350
C	3.912594	-1.803312	0.472959	-0.327150	-0.087378
H	4.392000	-2.727127	0.780046	0.176021	0.055774
C	3.635436	-1.566294	-0.878003	0.090145	-0.019424
H	3.895290	-2.309447	-1.625440	0.193162	0.052761

C	3.024187	-0.375602	-1.266416	0.558954	-0.122986
H	2.803544	-0.200277	-2.316806	0.192633	0.062849
Na	0.868927	-1.545465	0.387338	0.396703	0.675791
H	1.018333	3.679871	-0.144576	0.152368	-0.000949
H	2.348327	3.186037	0.909455	0.153303	-0.019992
H	2.702735	2.403621	-1.464582	0.183939	-0.039938
H	1.150458	1.588280	-1.427647	0.128037	-0.001561
Ge	-1.666997	-0.195731	0.030131	0.221084	0.758574
C	-3.192551	-1.294394	-0.710921	-0.393645	-0.307072
H	-2.908334	-1.696993	-1.691965	0.168953	-0.048292
H	-4.041139	-0.616314	-0.885358	0.169834	-0.110756
C	-2.580308	0.636142	1.628130	-0.348302	-0.303132
H	-3.552293	1.027426	1.293058	0.159011	-0.109690
H	-2.796845	-0.146458	2.366902	0.151732	-0.048304
C	-1.699687	1.358984	-1.262261	-0.427878	-0.304469
H	-1.023133	2.147711	-0.906360	0.248392	-0.046490
H	-2.711379	1.790416	-1.246904	0.151236	-0.114406
C	-3.621243	-2.437541	0.213556	-0.671109	0.115283
H	-3.952986	-2.054772	1.185621	0.183891	-0.025270
H	-4.443406	-3.035931	-0.198202	0.141495	-0.080617
H	-2.785301	-3.121876	0.408228	0.124148	-0.033299
C	-1.767095	1.754833	2.285107	-0.684837	0.117390
H	-1.572979	2.569494	1.576970	0.174860	-0.023409
H	-2.267941	2.194160	3.156794	0.143293	-0.083096
H	-0.790081	1.383948	2.623132	0.154740	-0.034455
C	-1.331077	0.954293	-2.693101	-0.648671	0.117944
H	-2.057957	0.240424	-3.096787	0.182071	-0.029037
H	-1.290249	1.804894	-3.385022	0.141459	-0.074522
H	-0.351327	0.457130	-2.727578	0.133603	-0.038402

8L

Electronic energy: -403.58852

Electronic energy + zero-point energy: -403.39288

Electronic energy + thermal energy correction: -403.37291

Electronic energy + thermal enthalpy correction: -403.37173

Electronic energy + thermal free energy correction: -403.45120

BSSE correction: 0.000469

Table S91. Cartesian coordinates, Mulliken and APT charges of all atoms at **8L** in the reaction between triethylgermane and styrene.

Symbol	X	Y	Z	Mulliken	APT

Na	-0.030093	-0.153987	-2.971095	0.510721	0.713407
Ge	0.001405	0.000328	-0.094677	0.263150	0.782444
C	0.031720	1.831876	0.749729	-0.367541	-0.320276
H	0.931867	2.366850	0.420354	0.138141	-0.047624
H	0.128835	1.697747	1.837162	0.160384	-0.112510
C	-1.556589	-0.837242	0.874552	-0.367991	-0.321393
H	-1.427018	-0.640258	1.948646	0.160922	-0.112704
H	-2.484817	-0.333406	0.575175	0.137928	-0.048146
C	1.549930	-0.877669	0.853815	-0.368174	-0.321254
H	1.566004	-1.947653	0.609069	0.137507	-0.047642
H	1.361273	-0.807214	1.935341	0.160148	-0.112681
C	-1.212502	2.667885	0.436876	-0.639352	0.117624
H	-2.121808	2.170341	0.793060	0.180175	-0.025158
H	-1.184657	3.663168	0.897014	0.141532	-0.077048
H	-1.329788	2.811509	-0.645023	0.128414	-0.033005
C	-1.684409	-2.343959	0.632479	-0.637553	0.118656
H	-0.783322	-2.874587	0.960736	0.179635	-0.026104
H	-2.535734	-2.790372	1.160876	0.141399	-0.076516
H	-1.813246	-2.562200	-0.435702	0.127875	-0.034228
C	2.905165	-0.248250	0.517350	-0.636584	0.119467
H	2.926946	0.812273	0.793492	0.179996	-0.025020
H	3.741987	-0.735545	1.032508	0.141529	-0.077192
H	3.109661	-0.303138	-0.559792	0.127739	-0.033092

9L

Electronic energy: -713.11817

Electronic energy + zero-point energy: -712.78692

Electronic energy + thermal energy correction: -712.75429

Electronic energy + thermal enthalpy correction: -712.75311

Electronic energy + thermal free energy correction: -712.86294

BSSE correction: 0.002083

Table S92. Cartesian coordinates, Mulliken and APT charges of all atoms at **9L** in the reaction between triethylgermane and styrene.

Symbol	X	Y	Z	Mulliken	APT
Na	0.846416	-0.983536	-1.021130	0.469353	0.679927
Ge	-1.756316	-0.203623	-0.084583	0.229643	0.775498
C	-3.463494	-0.586198	-1.089795	-0.390107	-0.313387
H	-3.414350	-0.110746	-2.078201	0.161297	-0.048612
H	-4.289411	-0.100764	-0.549567	0.157624	-0.113755
C	-2.287981	-0.793292	1.773498	-0.312818	-0.306037

H	-3.260651	-0.337898	2.010862	0.148579	-0.109706
H	-2.443594	-1.880053	1.772457	0.155366	-0.047270
C	-1.887230	1.803608	0.120368	-0.355495	-0.311650
H	-1.165942	2.132327	0.881369	0.221358	-0.051844
H	-2.885408	2.043316	0.515318	0.149444	-0.112728
C	-3.751053	-2.082308	-1.247502	-0.656399	0.114429
H	-3.834196	-2.572918	-0.270646	0.171422	-0.026749
H	-4.681520	-2.284095	-1.792569	0.137580	-0.081331
H	-2.939037	-2.583976	-1.788741	0.132736	-0.029166
C	-1.262459	-0.420003	2.847935	-0.740435	0.120361
H	-1.131833	0.667469	2.904222	0.204950	-0.022536
H	-1.545030	-0.764994	3.850359	0.136801	-0.083530
H	-0.278075	-0.849461	2.618124	0.155743	-0.039862
C	-1.645890	2.560303	-1.188410	-0.736319	0.120014
H	-2.379626	2.271674	-1.950099	0.167637	-0.029670
H	-1.706434	3.650380	-1.074859	0.143478	-0.077928
H	-0.654224	2.327129	-1.599162	0.187581	-0.034339
C	1.782633	1.298944	1.311034	-0.260046	-0.036930
C	2.556145	0.138298	1.317894	-0.044924	-0.107256
C	1.755681	2.113874	0.181693	-0.008322	-0.090980
C	3.315265	-0.232211	0.197389	-0.171062	0.026637
C	3.287643	0.605349	-0.932580	-0.167308	-0.093014
C	2.511861	1.763008	-0.939815	-0.133149	-0.051595
H	1.188832	1.554997	2.182580	0.149862	0.071343
H	1.141990	3.008726	0.167400	0.176863	0.074165
H	2.502346	2.397781	-1.820457	0.192413	0.056945
H	3.891992	0.363933	-1.801977	0.116229	0.059084
H	2.566259	-0.497015	2.199763	0.155623	0.065302
C	4.095470	-1.486367	0.241698	-0.226812	0.098834
C	4.685914	-2.090879	-0.794118	-0.192880	-0.188963
H	4.166708	-1.947417	1.225537	0.155478	0.032474
H	4.649265	-1.693095	-1.804469	0.151303	0.057608
H	5.238431	-3.013209	-0.653890	0.167711	0.056217

10L

Electronic energy: -713.09815

Electronic energy + zero-point energy: -712.76662

Electronic energy + thermal energy correction: -712.73609

Electronic energy + thermal enthalpy correction: -712.73491

Electronic energy + thermal free energy correction: -712.83592

BSSE correction: 0.002742

Table S93. Cartesian coordinates, Mulliken and APT charges of all atoms at **10L** in the reaction between triethylgermane and styrene.

Symbol	X	Y	Z	Mulliken	APT
Na	0.888602	-0.312618	1.702541	0.635805	0.607157
Ge	-1.579610	0.070133	0.024603	0.275893	1.094665
C	-3.007267	-1.136062	-0.667387	-0.404068	-0.326117
H	-2.649948	-1.647669	-1.570211	0.179387	-0.038132
H	-3.854136	-0.510158	-0.980638	0.204820	-0.098180
C	-2.506328	1.008912	1.557173	-0.468452	-0.513000
H	-3.540161	1.184359	1.225547	0.216586	-0.170586
H	-2.571354	0.342690	2.426053	0.166202	-0.018855
C	-1.479150	1.526487	-1.351155	-0.457141	-0.394500
H	-0.739440	2.275986	-1.042318	0.197324	-0.028641
H	-2.456798	2.030017	-1.314562	0.207916	-0.083063
C	-3.467191	-2.162952	0.372747	-0.628390	0.109820
H	-3.877720	-1.668342	1.260347	0.178625	-0.017037
H	-4.241227	-2.834930	-0.014457	0.152554	-0.075251
H	-2.631412	-2.789162	0.709555	0.136980	-0.020251
C	-1.859966	2.340645	1.949143	-0.543665	0.055965
H	-1.869911	3.044499	1.110537	0.206681	-0.013631
H	-2.372639	2.823405	2.788700	0.170721	-0.055800
H	-0.807974	2.219363	2.242770	0.131127	-0.013942
C	-1.194254	1.072454	-2.788407	-0.651427	0.078018
H	-1.882314	0.279062	-3.101371	0.184622	-0.018656
H	-1.298089	1.895347	-3.504753	0.156148	-0.056023
H	-0.176688	0.682661	-2.900252	0.150174	-0.015684
C	4.761822	-0.219894	0.433419	-0.190389	0.187051
C	3.774354	-1.186972	0.372292	-0.022932	-0.420888
C	4.529480	1.079967	-0.049189	-0.031870	-0.300724
C	2.494251	-0.918290	-0.194850	-0.006838	0.700733
C	2.271356	0.413481	-0.650279	-0.544708	-0.165495
C	3.280261	1.379831	-0.581816	-0.275385	0.116025
H	5.729992	-0.472928	0.856957	0.141874	0.016432
H	5.309106	1.832820	-0.004538	0.147486	0.031180
H	3.077709	2.378800	-0.959292	0.163900	0.032050
H	1.316191	0.678380	-1.094608	0.001946	0.026445
H	3.976588	-2.189860	0.742572	0.136087	0.021253
C	1.449223	-1.896954	-0.177100	0.227387	-1.217691
C	0.157159	-1.643988	-0.661770	-0.605968	1.134634
H	1.623112	-2.802029	0.402815	0.148961	-0.028618
H	0.051583	-1.042336	-1.563778	0.172823	-0.105648
H	-0.564065	-2.455410	-0.607232	0.139204	-0.015019

11L

Electronic energy: -713.13052

Electronic energy + zero-point energy: -712.79851

Electronic energy + thermal energy correction: -712.76772

Electronic energy + thermal enthalpy correction: -712.76654

Electronic energy + thermal free energy correction: -712.86747

BSSE correction: 0.004268

Table S94. Cartesian coordinates, Mulliken and APT charges of all atoms at **11L** in the reaction between triethylgermane and styrene.

Symbol	X	Y	Z	Mulliken	APT
Na	1.683123	-2.267101	0.617663	0.764330	0.796428
Ge	-1.634463	0.132384	0.044139	0.486558	1.546821
C	-3.516897	-0.110938	-0.509579	-0.402814	-0.340524
H	-3.697459	0.498100	-1.404203	0.170058	-0.028529
H	-4.168795	0.291360	0.275928	0.174421	-0.059103
C	-1.237493	-1.183899	1.468074	-0.257422	-0.362634
H	-2.130921	-1.346529	2.081994	0.199691	-0.026972
H	-1.038297	-2.139760	0.963737	0.174981	-0.024293
C	-1.472371	1.952925	0.798219	-0.363512	-0.352116
H	-0.530639	2.046714	1.351454	0.202095	-0.024502
H	-2.277375	2.069247	1.535741	0.181102	-0.043857
C	-3.868261	-1.577397	-0.790919	-0.626051	0.093907
H	-3.742727	-2.193534	0.106261	0.174698	-0.020519
H	-4.903844	-1.696072	-1.127003	0.156682	-0.065104
H	-3.223191	-2.001142	-1.568826	0.157667	-0.013640
C	-0.060656	-0.758072	2.358886	-0.725738	0.079667
H	-0.366978	0.032014	3.050702	0.192074	-0.001826
H	0.322819	-1.581232	2.977226	0.133156	-0.071716
H	0.767862	-0.322886	1.780809	0.174429	-0.017156
C	-1.575226	3.051716	-0.267890	-0.642600	0.099527
H	-2.510374	2.971974	-0.833513	0.172998	-0.022291
H	-1.543740	4.053536	0.173222	0.154168	-0.058225
H	-0.753706	2.986295	-0.989390	0.170914	-0.010720
C	4.415172	-0.229616	-0.351936	0.063420	0.285495
C	3.307625	-0.832469	-0.930026	0.316883	-0.409312
C	4.317432	1.006441	0.303677	-0.244414	-0.588202
C	1.991491	-0.245839	-0.878440	0.150904	0.753126
C	1.943263	1.046506	-0.254095	-0.941969	-0.452415
C	3.064478	1.631827	0.319350	-0.354570	0.409171
H	5.382381	-0.721885	-0.431964	0.130556	0.006620
H	5.186806	1.475395	0.750465	0.134373	0.025199
H	2.961129	2.611752	0.781287	0.146411	0.015672
H	1.002247	1.588153	-0.242612	0.070826	0.023269
H	3.435583	-1.767286	-1.479155	0.110624	-0.012191

C	0.845077	-0.927196	-1.343990	-0.533256	-0.870147
C	-0.478674	-0.214081	-1.532045	-0.302695	-0.079826
H	1.043715	-1.739649	-2.046962	0.038289	-0.022421
H	-0.360977	0.750825	-2.060068	0.185365	-0.112737
H	-1.114799	-0.823010	-2.187590	0.207366	-0.043926

12L

Electronic energy: -955.06081

Electronic energy + zero-point energy: -954.52302

Electronic energy + thermal energy correction: -954.47215

Electronic energy + thermal enthalpy correction: -954.47096

Electronic energy + thermal free energy correction: -954.62143

BSSE correction: 0.005602

Table S95. Cartesian coordinates, Mulliken and APT charges of all atoms at **12L** in the reaction between triethylgermane and styrene.

Symbol	X	Y	Z	Mulliken	APT
Na	1.307717	1.948605	-1.819945	0.698996	0.784536
Ge	-2.738799	-0.944439	0.045722	0.522556	1.582742
C	-2.445595	-2.264268	1.492740	-0.438223	-0.381052
H	-1.854814	-3.100286	1.096912	0.187297	-0.026607
H	-3.411623	-2.683333	1.802378	0.172754	-0.058368
C	-3.614812	0.645313	0.821240	-0.356422	-0.329590
H	-4.331869	0.282537	1.570670	0.174044	-0.045375
H	-2.864885	1.234011	1.361526	0.238177	-0.009005
C	-3.940819	-1.733432	-1.310799	-0.404996	-0.340819
H	-3.966759	-1.061400	-2.178163	0.202264	-0.024498
H	-4.961584	-1.757738	-0.908674	0.167835	-0.053270
C	-1.730810	-1.630094	2.692317	-0.568939	0.093960
H	-2.337954	-0.836204	3.140486	0.174058	-0.014685
H	-1.505161	-2.359250	3.478811	0.152610	-0.059723
H	-0.780799	-1.173028	2.389637	0.141577	-0.027344
C	-4.331704	1.531345	-0.205943	-0.616047	0.102680
H	-5.079172	0.964296	-0.772559	0.164560	-0.032892
H	-4.849590	2.368119	0.275769	0.153022	-0.062195
H	-3.617449	1.951962	-0.920609	0.210182	0.001250
C	-3.505951	-3.140315	-1.739418	-0.659447	0.106394
H	-3.529709	-3.835905	-0.893587	0.184287	-0.019719
H	-4.151729	-3.552971	-2.522213	0.159017	-0.071335
H	-2.481406	-3.140144	-2.129240	0.138544	-0.019409
C	-0.681580	4.505132	-0.440467	0.093560	0.329080

C	-1.039353	3.369857	-1.144898	0.422957	-0.407395
C	-0.086334	4.429333	0.833293	-0.299140	-0.630115
C	-0.812512	2.034292	-0.637899	-0.768422	0.702384
C	-0.246888	1.996200	0.690292	-0.728542	-0.491647
C	0.099123	3.154884	1.378292	-0.485838	0.413684
H	-0.882716	5.479328	-0.881828	0.137893	0.006792
H	0.183596	5.323662	1.383064	0.128653	0.027312
H	0.524823	3.056295	2.375503	0.141333	0.018662
H	-0.101554	1.036725	1.180335	0.033898	0.027697
H	-1.517088	3.471455	-2.118984	0.137745	0.001241
C	-1.014102	0.892707	-1.432071	0.091847	-0.814468
C	-1.017209	-0.495550	-0.836711	-0.392466	-0.204996
H	-1.583675	1.032876	-2.352245	0.093090	-0.001514
H	-0.837814	-1.258933	-1.606809	0.221692	-0.031670
H	-0.204189	-0.620192	-0.108317	-0.048829	-0.057233
Ge	3.084924	-0.742340	0.013806	0.419992	1.509310
H	2.098101	-0.091847	-1.017279	0.025415	-0.424291
C	4.075419	-2.134059	-0.956272	-0.329746	-0.314527
H	3.355928	-2.857382	-1.356175	0.180672	-0.016926
H	4.692538	-2.678050	-0.230721	0.178650	-0.032069
C	4.295094	0.667512	0.658721	-0.440019	-0.315274
H	5.080404	0.182819	1.251916	0.170096	-0.021594
H	4.801891	1.128741	-0.197404	0.144743	-0.035033
C	2.055976	-1.499786	1.504112	-0.072970	-0.314092
H	1.346131	-0.740355	1.853045	0.309488	-0.016400
H	2.755887	-1.666831	2.332863	0.249463	-0.031931
C	4.949091	-1.570012	-2.082922	-0.711906	0.090749
H	5.703428	-0.877921	-1.694565	0.171205	-0.014351
H	5.478153	-2.362471	-2.621344	0.166490	-0.050403
H	4.346355	-1.023973	-2.817298	0.138506	-0.021448
C	3.574791	1.731068	1.497515	-0.554693	0.088545
H	3.097887	1.285996	2.377462	0.197175	-0.001943
H	4.263155	2.504977	1.851604	0.173451	-0.052464
H	2.777726	2.229260	0.933407	0.221171	-0.022491
C	1.329056	-2.803886	1.152865	-0.852345	0.068248
H	2.038043	-3.584720	0.858857	0.164656	-0.024669
H	0.751892	-3.182569	2.003058	0.182430	-0.032861
H	0.629414	-2.662731	0.321279	0.290941	0.002427

13L

Electronic energy: -955.03890

Electronic energy + zero-point energy: -954.50244

Electronic energy + thermal energy correction: -954.45281

Electronic energy + thermal enthalpy correction: -954.45163

Electronic energy + thermal free energy correction: -954.59729

BSSE correction: 0.006036

Table S96. Cartesian coordinates, Mulliken and APT charges of all atoms at **13L** in the reaction between triethylgermane and styrene.

Symbol	X	Y	Z	Mulliken	APT
Na	2.374897	2.221438	0.307793	0.519848	0.678925
Ge	-2.889496	-0.536014	0.005239	0.529979	1.641089
C	-3.633747	-2.049594	1.034476	-0.371806	-0.367542
H	-3.287183	-2.989236	0.587111	0.160394	-0.027675
H	-4.726510	-2.040878	0.935568	0.174114	-0.060837
C	-3.589515	1.136886	0.795879	-0.410056	-0.337252
H	-4.600452	0.911540	1.161746	0.167865	-0.045850
H	-2.995185	1.389809	1.681515	0.195366	-0.021801
C	-3.451106	-0.655666	-1.880662	-0.329967	-0.353160
H	-3.110631	0.251123	-2.395526	0.206544	-0.016520
H	-4.547409	-0.646851	-1.925238	0.183630	-0.042882
C	-3.232955	-1.991391	2.514896	-0.628314	0.095700
H	-3.582513	-1.065010	2.984526	0.175456	-0.014603
H	-3.648594	-2.826272	3.089208	0.161984	-0.062996
H	-2.143752	-2.024531	2.631837	0.166634	-0.021665
C	-3.639892	2.329687	-0.168072	-0.587306	0.096953
H	-4.273635	2.109724	-1.033884	0.175571	-0.028817
H	-4.046343	3.223409	0.318131	0.151481	-0.061567
H	-2.643485	2.582713	-0.544426	0.190097	-0.000264
C	-2.895041	-1.900224	-2.583629	-0.660683	0.109154
H	-3.216923	-2.821015	-2.084672	0.177537	-0.019684
H	-3.220066	-1.962387	-3.627689	0.159604	-0.065089
H	-1.798965	-1.896611	-2.582465	0.179592	-0.020267
C	0.623246	3.978720	-1.044712	-0.050518	0.277669
C	0.353591	2.671257	-1.422208	-0.141272	-0.315596
C	0.477518	4.399761	0.293069	-0.179804	-0.520330
C	-0.107711	1.685209	-0.486153	-0.370904	0.510221
C	-0.201117	2.128458	0.875642	-0.002963	-0.322693
C	0.060767	3.453090	1.234670	0.016703	0.317410
H	0.943706	4.691378	-1.800526	0.166299	0.027550
H	0.667645	5.428024	0.578339	0.163715	0.038299
H	-0.063286	3.747907	2.274040	0.176362	0.031527
H	-0.544800	1.437253	1.638270	0.082605	0.044169
H	0.459179	2.381266	-2.465092	0.155446	0.031034
C	-0.215669	0.323498	-0.849757	-0.003770	-1.119159
C	-0.918018	-0.682724	0.031142	-1.239758	-0.234517
H	-0.249294	0.125048	-1.922669	0.204920	0.032029
H	-0.682913	-1.700636	-0.312504	0.131074	-0.006078
H	-0.540980	-0.635733	1.064172	0.434621	-0.008409
Ge	2.666318	-1.019285	0.063529	0.368417	1.112411
H	1.264751	-0.036331	-0.492788	-0.257926	0.597288

C	4.429929	-0.793895	-0.853532	-0.401590	-0.397974
H	4.328574	-1.113620	-1.897259	0.194918	-0.037717
H	5.131156	-1.493902	-0.379814	0.195463	-0.089993
C	3.126472	-1.243000	1.996239	-0.346222	-0.413837
H	3.689478	-2.182777	2.083572	0.196220	-0.094346
H	3.816182	-0.444291	2.300460	0.145118	-0.036249
C	2.036604	-2.814362	-0.518199	-0.244901	-0.286608
H	1.234345	-3.140173	0.155289	0.229460	-0.027237
H	2.865159	-3.522783	-0.382053	0.221299	-0.088335
C	4.997386	0.626999	-0.801287	-0.571838	0.072822
H	5.047436	1.000923	0.231025	0.117519	-0.023469
H	6.011578	0.696748	-1.209685	0.169981	-0.062413
H	4.374356	1.316372	-1.387163	0.125523	-0.031072
C	1.908286	-1.273609	2.924470	-0.605931	0.075785
H	1.205860	-2.062364	2.630373	0.177280	-0.010457
H	2.184185	-1.452710	3.969737	0.159274	-0.066705
H	1.355991	-0.326636	2.883225	0.158589	-0.023012
C	1.551547	-2.838997	-1.971741	-0.733753	0.101156
H	2.350709	-2.546588	-2.662312	0.167289	-0.027589
H	1.203326	-3.831816	-2.278186	0.148512	-0.063233
H	0.723709	-2.136963	-2.123679	0.156978	-0.015688

14L

Electronic energy: -955.08781

Electronic energy + zero-point energy: -954.54501

Electronic energy + thermal energy correction: -954.49453

Electronic energy + thermal enthalpy correction: -954.49334

Electronic energy + thermal free energy correction: -954.64266

BSSE correction: 0.005866

Table S97. Cartesian coordinates, Mulliken and APT charges of all atoms at **14L** in the reaction between triethylgermane and styrene.

Symbol	X	Y	Z	Mulliken	APT
Na	2.297808	2.117600	0.137660	0.473897	0.687579
Ge	-3.359796	-0.584618	0.028529	0.557229	1.588182
C	-4.509352	-2.091982	0.562527	-0.443899	-0.331332
H	-4.298971	-2.949914	-0.087196	0.165876	-0.028774
H	-5.555722	-1.814053	0.385736	0.178453	-0.044318
C	-3.819044	0.977109	1.155428	-0.306957	-0.326331
H	-4.818792	0.793158	1.569545	0.177771	-0.040278
H	-3.134884	1.007312	2.012027	0.184979	-0.025569

C	-3.615831	-0.150903	-1.876818	-0.251800	-0.340956
H	-2.941173	0.676394	-2.135058	0.215137	-0.029010
H	-4.633821	0.230398	-2.021496	0.168965	-0.029984
C	-4.301682	-2.479947	2.033000	-0.551430	0.089795
H	-4.507051	-1.635880	2.700997	0.176415	-0.014810
H	-4.956382	-3.303424	2.336109	0.165669	-0.057497
H	-3.269723	-2.798155	2.216703	0.169786	-0.013822
C	-3.804349	2.321413	0.416436	-0.603093	0.101056
H	-4.525442	2.327112	-0.407672	0.168190	-0.024605
H	-4.060973	3.151015	1.084247	0.161775	-0.054730
H	-2.819889	2.537107	-0.011442	0.103675	-0.020276
C	-3.365335	-1.355924	-2.793058	-0.747002	0.097429
H	-4.074902	-2.163774	-2.586458	0.186654	-0.019459
H	-3.466283	-1.093603	-3.851233	0.158094	-0.052239
H	-2.358839	-1.766597	-2.652775	0.147279	-0.016813
C	-0.231980	3.431407	-0.917251	-0.009172	-0.009950
C	-0.324038	2.069681	-1.220405	0.825340	-0.115002
C	-0.224193	3.853174	0.413949	-0.340810	-0.078811
C	-0.405242	1.104211	-0.207597	-1.682882	0.013718
C	-0.392321	1.543449	1.125034	0.215611	-0.127197
C	-0.307065	2.901667	1.434972	0.197611	-0.018932
H	-0.178356	4.160112	-1.720107	0.201077	0.052818
H	-0.166992	4.909996	0.653552	0.182296	0.055373
H	-0.308246	3.217913	2.473550	0.198361	0.055243
H	-0.449488	0.816030	1.929790	0.205543	0.078798
H	-0.334752	1.748504	-2.259175	0.212420	0.064802
C	-0.453505	-0.367230	-0.544885	-1.023161	0.076743
C	-1.481928	-1.177718	0.257347	0.011688	-0.360073
H	-0.653536	-0.468716	-1.618433	0.102177	-0.021487
H	-1.425862	-2.226497	-0.061903	0.188118	-0.020052
H	-1.223798	-1.183098	1.323628	0.244812	-0.001556
Ge	3.601144	-0.469825	0.024623	0.275501	0.758870
H	0.555005	-0.774953	-0.385547	0.032853	-0.025225
C	5.600662	-0.595151	-0.214826	-0.443587	-0.300765
H	5.850204	-0.262882	-1.231792	0.180291	-0.054829
H	5.879474	-1.657205	-0.157512	0.166333	-0.112391
C	3.330163	-1.716345	1.592382	-0.536898	-0.296241
H	3.791259	-2.684532	1.349125	0.166388	-0.107950
H	3.879663	-1.317139	2.455260	0.168579	-0.052556
C	2.976608	-1.650284	-1.500328	-0.290723	-0.296528
H	2.099423	-2.226331	-1.174310	0.220437	-0.066745
H	3.767910	-2.386909	-1.699565	0.182843	-0.107790
C	6.401535	0.212000	0.810254	-0.647084	0.112603
H	6.168811	-0.107585	1.833163	0.164286	-0.026647
H	7.486431	0.115043	0.678897	0.135889	-0.082692
H	6.158083	1.279900	0.746527	0.136612	-0.031105
C	1.858401	-1.919137	1.965644	-0.469570	0.119481
H	1.299476	-2.383990	1.143781	0.195031	-0.019680
H	1.721804	-2.556332	2.848353	0.157619	-0.083797

H	1.370456	-0.957145	2.176098	0.092274	-0.038312
C	2.645081	-0.878754	-2.780434	-0.708417	0.133515
H	3.508908	-0.296711	-3.125201	0.156718	-0.033782
H	2.337188	-1.528273	-3.609695	0.121890	-0.076359
H	1.831238	-0.162133	-2.603864	0.158040	-0.048748

15L

Electronic energy: -551.48448

Electronic energy + zero-point energy: -551.13885

Electronic energy + thermal energy correction: -551.11054

Electronic energy + thermal enthalpy correction: -551.10936

Electronic energy + thermal free energy correction: -551.20423

BSSE correction: 0.002989

Table S98. Cartesian coordinates, Mulliken and APT charges of all atoms at **15L** in the reaction between triethylgermane and styrene.

Symbol	X	Y	Z	Mulliken	APT
Ge	-1.314591	-0.074754	0.157818	0.545969	1.565560
C	-3.229414	-0.510379	-0.021312	-0.437969	-0.324435
H	-3.747067	0.334649	-0.491259	0.164387	-0.034456
H	-3.657187	-0.619832	0.983042	0.180972	-0.042500
C	-0.421722	-1.576190	1.084601	-0.316011	-0.316280
H	-1.201865	-2.161674	1.588211	0.177726	-0.042366
H	0.020759	-2.235958	0.328495	0.196889	-0.026900
C	-1.092604	1.602892	1.167770	-0.313611	-0.339503
H	-0.020422	1.830528	1.225431	0.260578	-0.023403
H	-1.426631	1.441728	2.199846	0.165017	-0.029090
C	-3.457003	-1.789269	-0.838704	-0.575297	0.092509
H	-2.946627	-2.647212	-0.386798	0.174300	-0.015449
H	-4.519034	-2.044434	-0.916185	0.163179	-0.059769
H	-3.071595	-1.681112	-1.858514	0.170147	-0.015189
C	0.646649	-1.145474	2.097085	-0.601832	0.095475
H	0.214779	-0.521969	2.887352	0.161018	-0.025382
H	1.116465	-2.009891	2.578970	0.164003	-0.056595
H	1.440657	-0.564660	1.617782	0.067206	-0.006134
C	-1.860670	2.773211	0.539631	-0.721718	0.098368
H	-2.939403	2.585468	0.542285	0.181245	-0.020949
H	-1.690192	3.711357	1.078004	0.159935	-0.055615
H	-1.564247	2.936056	-0.503082	0.151687	-0.016326
C	3.673850	0.769751	0.572009	-0.081479	-0.011937
C	2.579021	1.281204	-0.126150	0.163528	-0.091548

C	4.044458	-0.563591	0.408768	-0.131518	-0.070119
C	1.838698	0.477832	-0.999563	-0.909452	0.035489
C	2.226252	-0.858718	-1.157718	0.045181	-0.095810
C	3.315240	-1.376931	-0.460054	0.005987	-0.011462
H	4.231844	1.412281	1.246317	0.171029	0.036784
H	4.891548	-0.967344	0.954224	0.162565	0.040402
H	3.596032	-2.417236	-0.594653	0.164728	0.036469
H	1.670365	-1.502899	-1.834482	0.134670	0.048174
H	2.292604	2.321740	0.009102	0.149472	0.040370
C	0.665148	1.046346	-1.768365	-0.317438	0.151407
C	-0.621940	0.209205	-1.677779	-0.390077	-0.339093
H	0.470063	2.059543	-1.397240	0.130900	-0.032395
H	-1.411913	0.704633	-2.257143	0.200293	-0.040458
H	-0.475813	-0.770140	-2.150010	0.199999	-0.015999
H	0.957999	1.159163	-2.821200	0.183791	-0.081841