Supporting Information for the manuscript "Organic Functionalization of Diamond(100) by Addition Reactions of Carbene, Silylene and Germylene: A Theoretical Prediction"

Table 1(Page S2): Cartesian coordinates of the product for the addition of singlet carbene to a C_9H_{12} cluster and calculated vibrational frequencies calculated at the B3LYP/6-31G(d).

Table 2(Page S3): Cartesian coordinates of the product for the addition of singlet silylene to a C_9H_{12} cluster and calculated vibrational frequencies calculated at the B3LYP/6-31G(d).

Table 3(Page S4): Cartesian coordinates of the product for the addition of singlet germylene to a C_9H_{12} cluster and calculated vibrational frequencies calculated at the B3LYP/6-31G(d).

Figure 1(Page S5): B3LYP/6-31G(d) optimized geometries (Units in Å for bond length) of the additions of singlet carbene, silylene and germylene to the C (100)-2x1 surface using larger clusters $C_{15}H_{16}$ and $C_{21}H_{20}$ respectively.

Table 1

(a) Cartesian coordinates.

Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
6	0	0.061792	-2.659450	-0.093422
6	0	-0.091086	-1.728897	-1.342513
6	0	0.099732	-1.891389	1.269711
6	0	-1.326448	-0.812069	-1.147023
6	0	1.018820	-0.646254	-1.309041
6	0	-1.142514	-0.968007	1.369612
6	0	1.202666	-0.803034	1.209505
6	0	0.664334	0.010487	0.028520
6	0	-0.886890	-0.098866	0.134995
1	0	-0.769543	-3.377714	-0.077861
1	0	0.981800	-3.250907	-0.197529
1	0	-0.112033	-2.332504	-2.261186
1	0	0.206251	-2.603627	2.100464
1	0	-2.266701	-1.358648	-1.013463
1	0	-1.454330	-0.138104	-2.004124
1	0	0.932645	0.032776	-2.167356
1	0	2.035987	-1.053998	-1.312307
1	0	-1.138667	-0.405151	2.312006
1	0	-2.097220	-1.502234	1.307438
1	0	1.246931	-0.235397	2.148123
1	0	2.205807	-1.199126	1.015600
6	0	-0.195879	1.238595	0.167259
1	0	-0.301475	1.891433	-0.699567
1	0	-0.167980	1.780085	1.113160

(b) Calculated frequencies(cm^{-1}) (NIMAGE=0).

302.5521	327.3380	339.6196	443.1411	445.2129	448.2146	518.1831	532.5459
567.6516	686.4515	709.6547	749.8917	791.5742	801.7518	860.6663	897.3773
901.4375	905.0587	911.5596	917.6526	922.5917	956.9975	959.8806	985.1415
1014.2247	1023.8699	1046.2733	1084.0953	1102.8187	1121.0414	1126.9305	
1163.9973	1181.5860	1230.4341	1254.4614	1273.6493	1277.3823	1300.0637	
1306.0441	1324.5449	1327.9492	1338.0273	1362.7958	1370.0096	1380.8876	
1401.7726	1496.2584	1510.7939	1512.1920	1527.7380	1529.9217	1549.8426	
3026.6249	3034.6079	3039.2221	3041.5547	3044.0243	3052.1097	3058.6891	3067.8868
3087.6211	3092.2324	3098.3133	3100.7472	3103.9183	3181.1772		

Table 2

(a) Cartesian coordinates.

Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
6	0	-0.005428	-2.634566	-0.019167
6	0	-0.010859	-1.755358	-1.304587
6	0	0.036885	-1.792543	1.290230
6	0	-1.171625	-0.735767	-1.229044
6	0	1.194170	-0.786013	-1.273047
6	0	-1.125503	-0.772264	1.286773
6	0	1.240339	-0.822015	1.242737
6	0	0.865885	0.012554	0.003024
6	0	-0.762537	0.046925	0.033405
1	0	-0.899463	-3.273197	-0.011694
1	0	0.860595	-3.310267	-0.044652
1	0	-0.040934	-2.390532	-2.200429
1	0	0.039343	-2.453398	2.167829
1	0	-2.158931	-1.197593	-1.114686
1	0	-1.203563	-0.121463	-2.137692
1	0	1.218318	-0.172742	-2.182542
1	0	2.164614	-1.289242	-1.194892
1	0	-1.124537	-0.184270	2.213213
1	0	-2.116374	-1.231507	1.195030
1	0	1.298204	-0.236038	2.168552
1	0	2.207032	-1.322237	1.114475
14	0	0.087280	1.697858	0.038237
1	0	0.081943	2.529610	-1.192754
1	0	0.129145	2.505068	1.284682

(b) Calculated frequencies(cm^{-1}) (NIMAGE=0).

203.0685	280.2669	281.1128	375.5600	402.1348	421.5872	496.8888	503.1121
508.2064	563.0388	574.0810	613.5062	678.3738	685.4539	700.2377	779.1205
784.7541	864.7599	896.2046	899.5818	911.6339	912.7102	932.0772	934.0797
959.4715	964.1934	995.4955	1004.1010	1017.9537	1070.9518	1100.3505	1106.5895
1148.8848	1161.4928	1182.0639	1206.9139	1213.2309	1264.7915	1273.5871	1287.7090
1298.3379	1329.0461	1334.6469	1335.4029	1348.7651	1385.3045	1390.4563	1513.5709
1514.1227	1532.2092	1532.8250	1553.3010	2231.8696	2259.2614	3028.3201	3041.4364
3043.3700	3045.4330	3047.7563	3057.4631	3062.6198	3066.3307	3085.9392	3090.8673
3096.3357	3098.8718						

Table 3

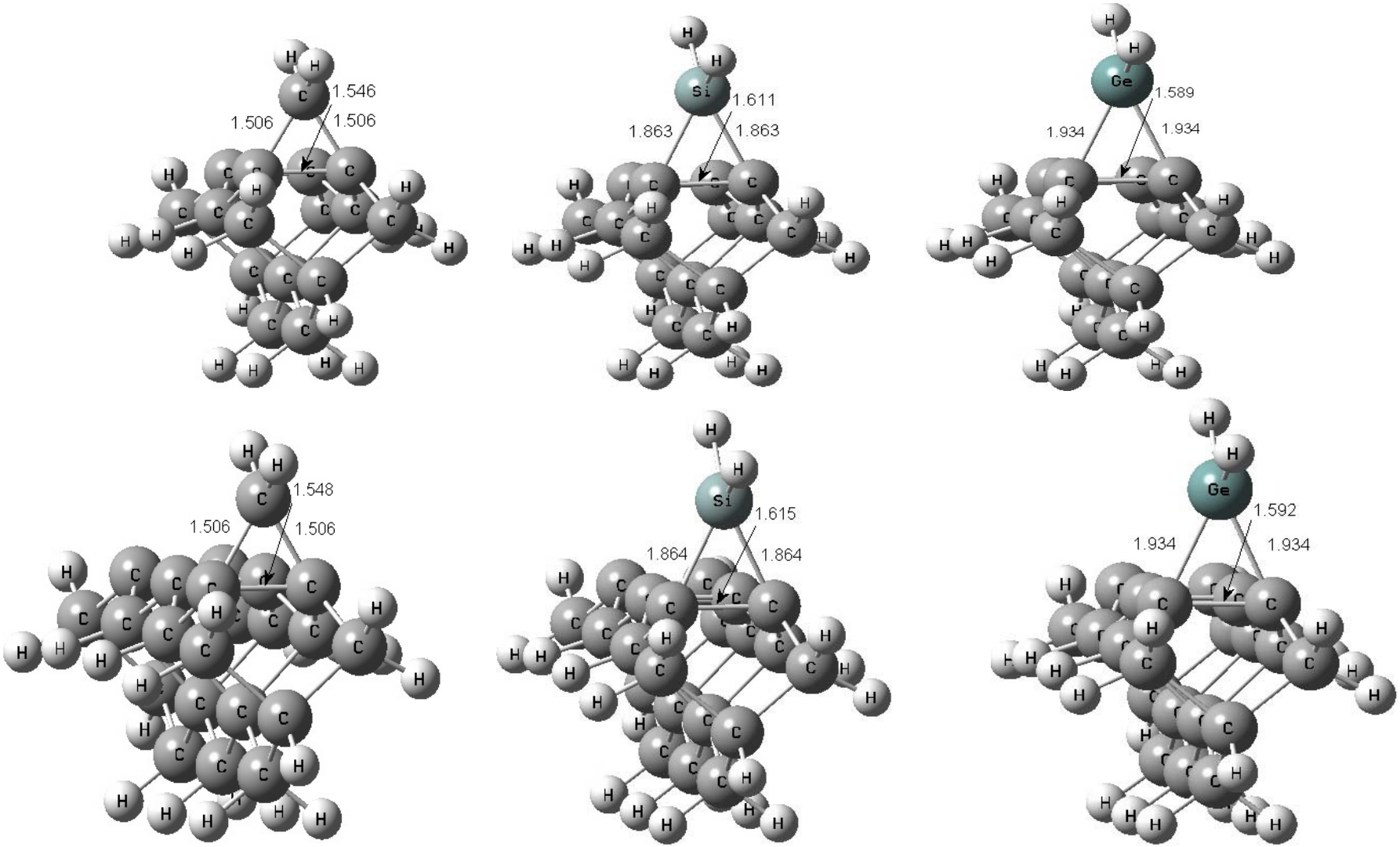
(a) Cartesian coordinates.

Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
6	0	0.017406	-2.691022	-0.012605
6	0	0.002231	-1.818509	-1.304786
6	0	0.043541	-1.846037	1.297498
6	0	-1.174454	-0.814312	-1.233986
6	0	1.193075	-0.829362	-1.271735
6	0	-1.134471	-0.841058	1.285214
6	0	1.232995	-0.856140	1.247824
6	0	0.835896	-0.048850	0.002362
6	0	-0.766664	-0.038529	0.027776
1	0	-0.866923	-3.343020	-0.005406
1	0	0.893343	-3.353977	-0.033411
1	0	-0.016063	-2.459038	-2.196705
1	0	0.053085	-2.505302	2.175801
1	0	-2.156947	-1.287159	-1.126479
1	0	-1.202353	-0.195368	-2.139250
1	0	1.200092	-0.210094	-2.177287
1	0	2.172592	-1.314372	-1.195529
1	0	-1.133580	-0.240800	2.203391
1	0	-2.119921	-1.312108	1.199005
1	0	1.268928	-0.256258	2.165718
1	0	2.209474	-1.339049	1.130362
32	0	0.046320	1.711649	0.035138
1	0	0.031855	2.560503	-1.251220
1	0	0.074544	2.526213	1.343312

(b) Calculated frequencies(cm^{-1}) (NIMAGE=0).

170.1164	244.7930	274.8929	298.2551	401.3883	404.4192	484.3566	484.7214
490.7432	515.7424	530.7379	551.0331	587.4328	686.3610	724.3447	777.6247
788.6393	830.4820	863.5167	888.9614	895.4956	910.5442	911.4260	934.0418
953.4450	959.2808	998.6020	1002.0248	1018.2135	1070.3634	1102.8891	1104.0335
1148.1538	1160.0015	1191.9632	1210.7429	1226.6886	1264.6734	1270.9769	
1282.04241300.4321	1327.8084	1336.1580	1336.4730	1349.1746	1384.0583	1388.4063	
1510.1472	1512.9520	1529.1245	1532.6417	1553.2276	2034.5723	2061.7366	3029.2175
3045.0737	3046.4924	3047.2409	3049.1238	3060.3485	3065.0336	3066.5708	3090.5201
3095.6020	3100.5552	3103.3270					

Figure 1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