Supporting Information for

Organic Monolayers by $B(C_6F_5)_3$-Catalyzed Hydrosilylation of Oxidized Silicon Surfaces.

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1. Equipment

X-ray Photoelectron Spectroscopy (XPS) Measurements. The XPS analysis of surfaces was performed using a JPS-9200 photoelectron spectrometer (JEOL, Japan). Survey and narrow-scan spectra were obtained under UHV conditions using monochromatic Al Kα X-ray radiation at 12 kV and 20 mA, and an analyzer pass energy of 50 eV for wide scans and 10 eV for narrow scans. The X–ray incidence angle and the electron acceptance angle was 10° to the surface normal. The take-off angle φ (angle between sample and detector) of 80° is defined to a precision of 1°. The intensity of the XPS core–level electron was measured as the peak area after standard background subtraction according to the linear procedure. All XPS spectra were evaluated using the Casa XPS software (version 2.3.15). The symmetrical GL(30) line shape was employed, which consists of a Gaussian (70%) and a Lorentzian (30%) component. The fwhm of each component was constrained to 1.0–1.1 eV. Atomic area ratios were determined after a baseline correction and normalizing the peak area ratios by the corresponding atomic sensitivity factors (1.00 for C1s, 2.93 for O1s and 4.43 for F1s). The binding energies were calibrated on the hydrocarbon (CH_2) peak with a binding energy of 285.0 eV. In all cases the assignment was supported by quantum chemical calculations of the C1s XPS energies.[i]

Static Water Contact Angle (SCA) Measurements. The wettability of the modified surfaces was determined by automated static water contact angle measurements with a Krüss DSA 100 goniometer (volume of the drop of deionized water was 3.0 μL). The reported values are the average of at least five droplets, and the relative error is less than ±2°.

Atomic Force Microscopy (AFM) Characterization. AFM images (1 × 1 μm^2, 5 × 5 μm^2, and 20 × 20 μm^2) were obtained with a MFP3D atomic force microscope (Asylum Research, Santa Barbara, CA) at a scan speed of 50.08 $\mu m \cdot s^{-1}$ at a resolution of 512 × 512 pixels. The imaging was performed in air in tapping mode using OLYMPUS OMCL-AC24OTS-R3 microcantilevers with a spring constant of 2 $N \cdot m^{-1}$. Images were flattened with a first-order correction using the MFP3D software. Micro-contact patterned images (height and phase) were obtained with a JSPM-5400 microscope (Jeol, Japan) with silicon cantilevers (BudgetSensors®, Tap300-G, 40 N/m) operating in the alternating current (AC) mode in air. The scan size was 20 × 20 μm^2 at a scan rate of 0.10 Hz.

Ellipsometry. The ellipsometric thickness of the modified surfaces was measured using a rotating Sentech Instruments (Type SE-400) ellipsometer, operating at 632.8 nm (He−Ne laser), and an angle of incidence of 70°. The thicknesses of the monolayers were determined with a planar three layer (ambient, monolayer, substrate) isotropic model, with assumed refractive indices of 1.00 and 1.44 for ambient and the monolayer, respectively. The reported values are the average of at least five measurements on three different samples.

^{1}H NMR Spectroscopy. ^{1}H NMR spectra were recorded on a Bruker AVB-400 spectrometer with ^{1}H operating frequency of 400 MHz. Unless stated otherwise all spectra were recorded at room temperature in $CDCl_3$ and all chemical shifts are given in δ units relative to the residual $CHCl_3$ (central line of singlet: δ_H = 7.27 ppm). Coupling constants (J) are given in Hertz (Hz).

^{13}C NMR Spectroscopy. ^{13}C NMR spectra were recorded at room temperature on a Bruker AVB-400 spectrometer with ^{13}C operating frequency of 101 MHz. Unless stated otherwise all

spectra were recorded at room temperature in $CDCl_3$ and all chemical shifts are given in δ units relative to the $CDCl_3$ (central line of triplet: δ_C = 77.0 ppm).

2. Supplementary Tables.

Table S1. ν_a-CH_2 Anti-symmetric and ν_s-CH_2 symmetric frequencies for monolayers derived from **1–4** onto oxidized Si(111).

	Wavenumbers (cm^{-1})	
Hydrosilane	**νa-CH_2 anti-symmetric**	**νs-CH_2 symmetric**
1	2927	2855
2	2927	2855
3	2926	2855
4	2927	2855

Table S2. RMS roughness (obtained from AFM) for monolayers derived from **1–4** onto oxidized Si(111). RMS values were obtained on at least five AFM images with area 1 × 1 μm.

Hydrosilane	RMS (nm)
Raw surface	0.42 ± 0.06
Plasma cleaned	0.10 ± 0.01
1	0.23 ± 0.02
2	0.25 ± 0.02
3	0.30 ± 0.01
4	0.27 ± 0.02

3. Supplementary XPS Figures.

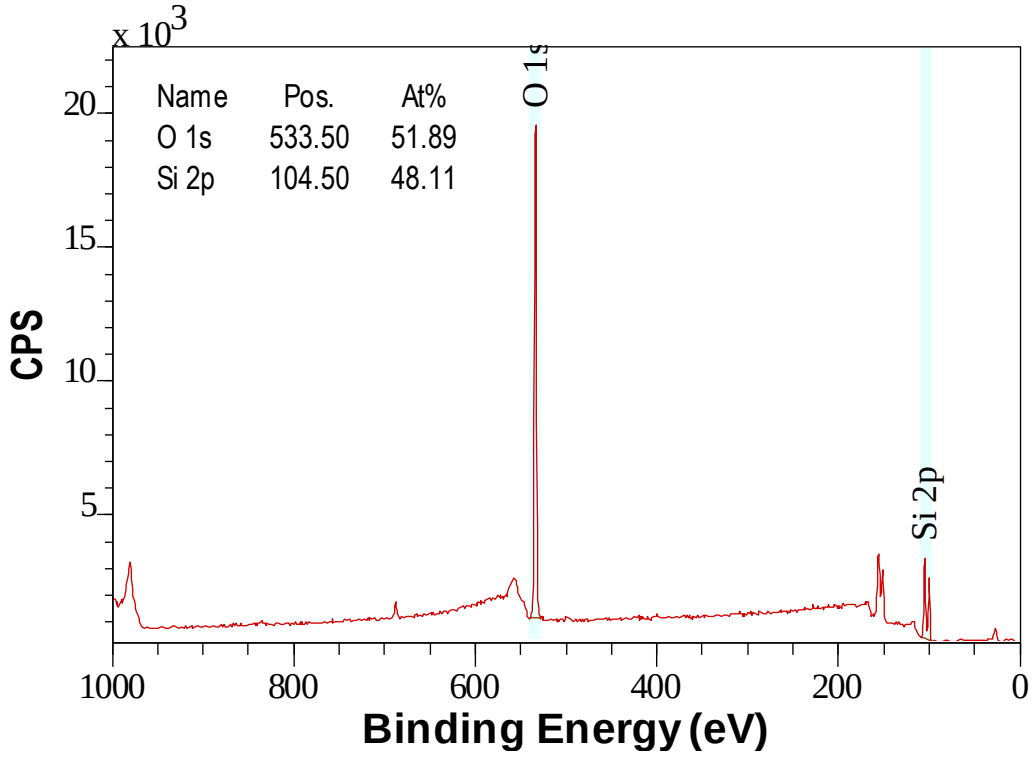


Figure S1. XPS survey scan for an oxidized Si (111) surface.

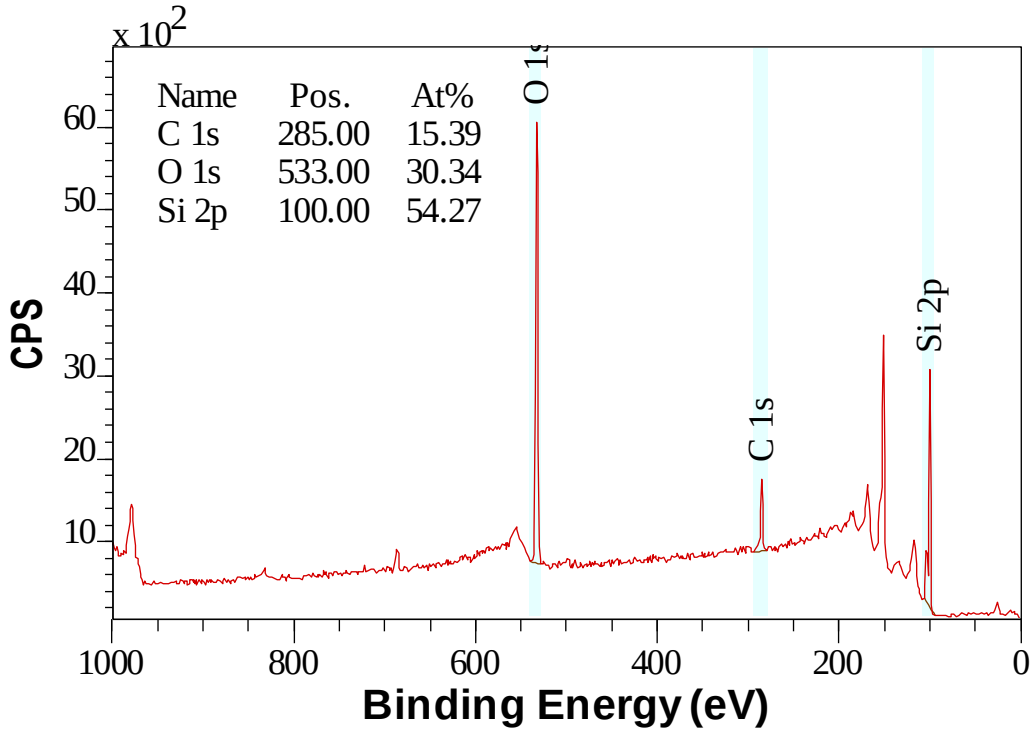


Figure S2. XPS survey scan for a **1**-modified Si (111) surface.

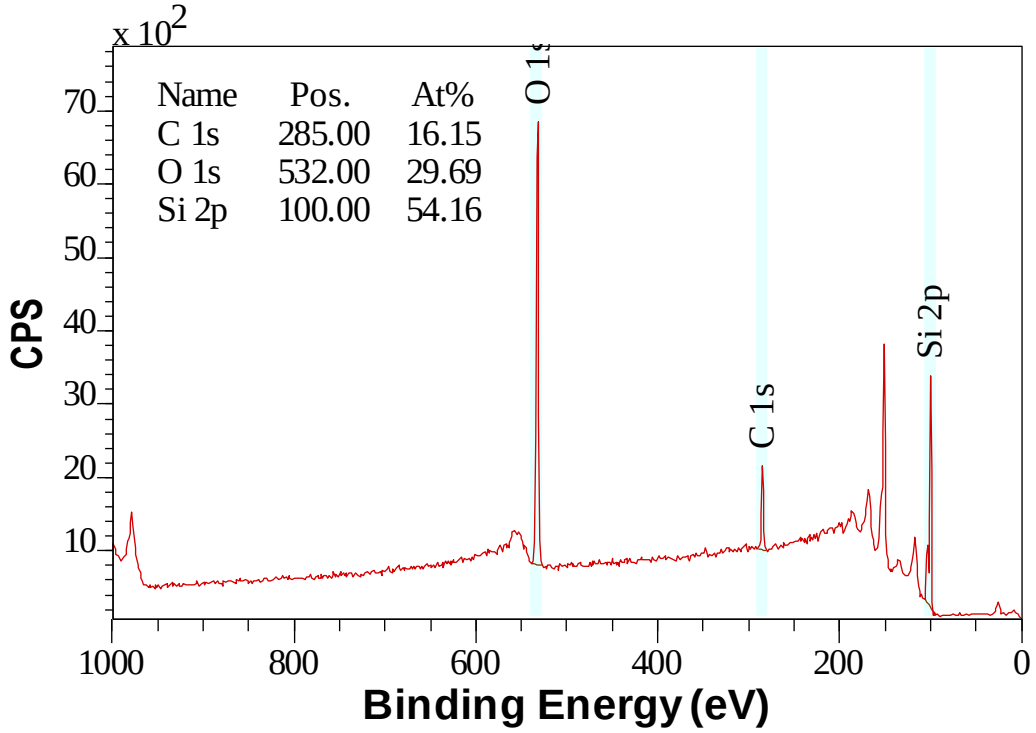


Figure S3. XPS survey scan for a **2**-modified Si (111) surface.

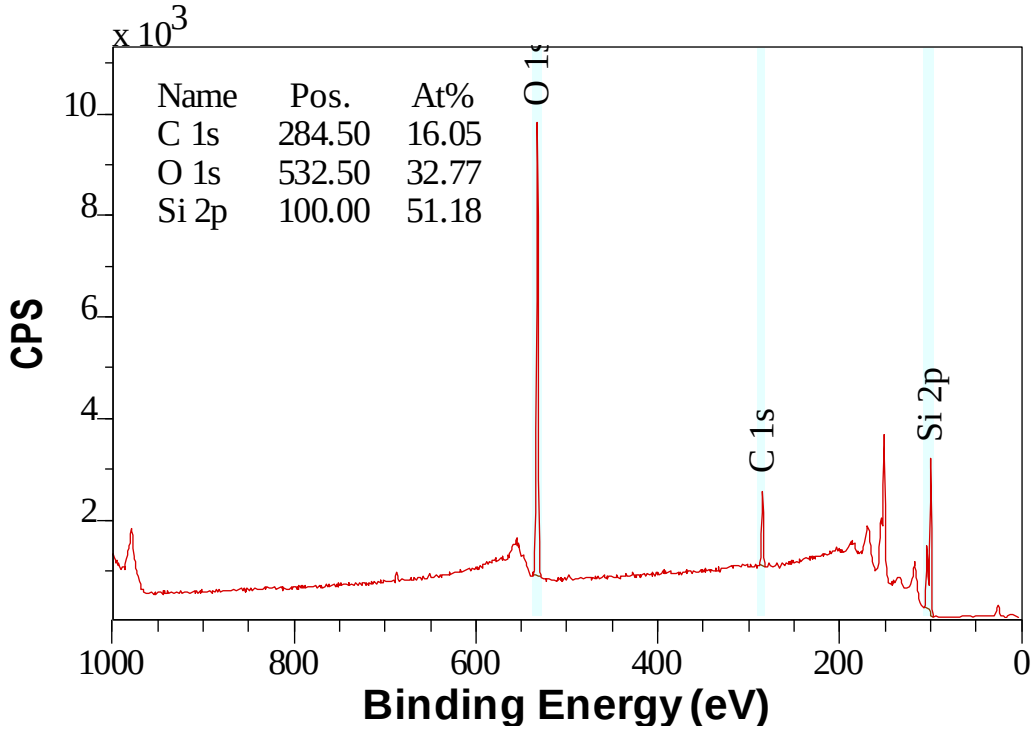


Figure S4. XPS survey scan for a **3**-modified Si (111) surface.

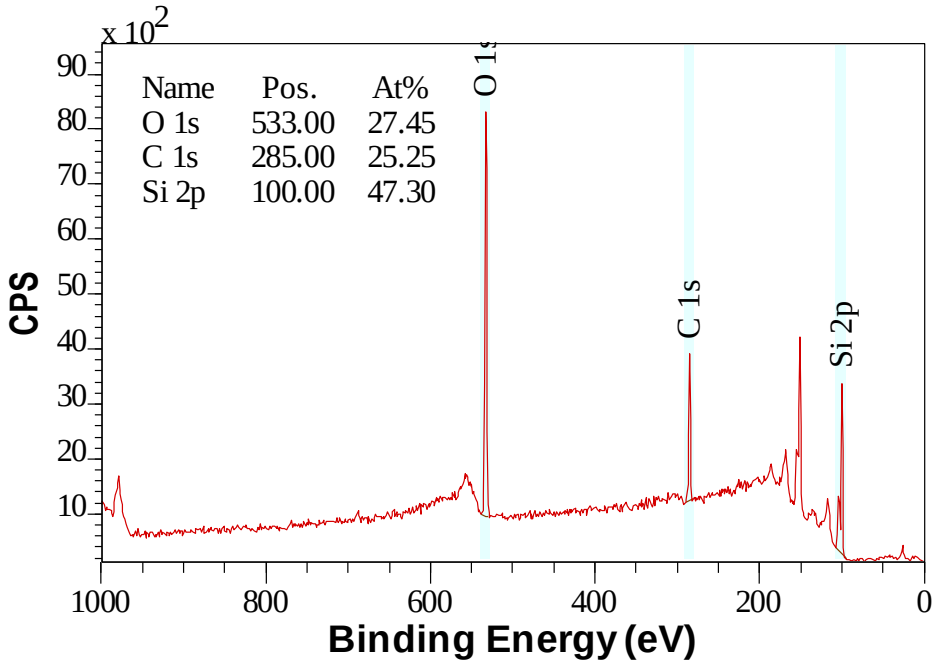


Figure S5. XPS survey scan for a **4**-modified Si (111) surface.

4. Micro-contact patterned images by AFM

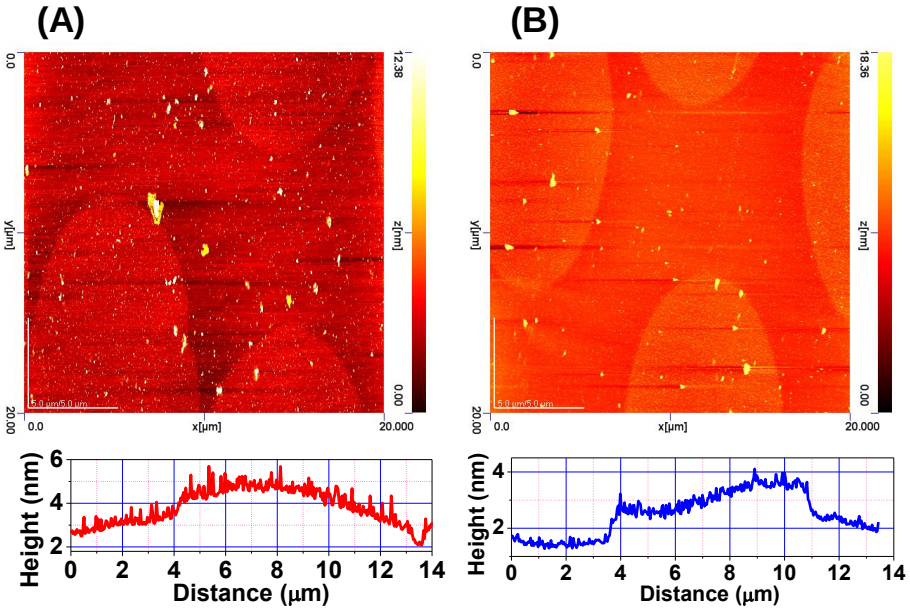


Figure S6. AFM height image of the patterned silicon monolayer with hydrosilane **4** and **5** (B) and, corresponding height profiles.

5. Characterization of the alkyl(dimethyl)silanes.

Dimethyl(octyl)silane (1). This compound was synthesized from chloro(dimethyl)octylsilane following the general procedure in the main text, and was obtained in in 98% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm): 3.73–3.63 (m, J = 7.0 Hz, 1H), 1.35–1.27 (m, 10H), 1.20–1.17 (t, J = 6.9 Hz, 2H), 0.90–0.86 (t, J = 6.7 Hz, 3H), 0.61–0.56 (dq, J = 10.5, 3.6 Hz, 2H), 0.09-0.08 (d, J = 3.9 Hz, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ (ppm): 33.2, 31.9, 29.7, 29.3, 29.2, 14.2, 14.1, -4.5. ESI-MS calcd for $C_{10}H_{24}Si$, 171.1569 $[M-H]^+$, found 171.1567.

Decyldimethylsilane (2). This compound was synthesized from chloro(decyl)dimethylsilane following the general procedure in the main text, and was obtained in in 97% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm): 3.83–3.77 (m, 1H), 1.37–1.29 (m, 16H), 0.92–0.84 (m, 3H), 0.63–0.57 (m, 2H), 0.09-0.08 (d, J = 3.7 Hz, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ (ppm): 33.1, 31.9, 29.6, 29.5, 29.3, 29.2, 24.3, 22.6, 14.1, 13.9, -4.5. ESI-MS calcd for $C_{12}H_{28}Si$, 199.1882 $[M-H]^+$, found 199.1887.

Dodecyldimethylsilane (3). This compound was synthesized from chloro(dodecyl)dimethylsilane following the general procedure in the main text, and was obtained in 95% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm): ^{1}H NMR (400 MHz, $CDCl_3$) δ, 3.81–3.76 (m, 1H), 1.89–1.77 (m, 2H), 1.36–1.24 (m, 18H), 0.86 (t, J = 6.7 Hz, 3H), 0.56 (ddd, J = 9.8, 6.9, 3.2 Hz, 2H), 0.09-0.08 (d, J = 3.9 Hz, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ (ppm): 33.2, 31.9, 29.7, 29.8, 29.7, 29.6, 29.4, 29.3, 24.4, 22.7, 14.2, 14.1, -4.4. ESI-MS calcd for $C_{14}H_{32}Si$, 227.2195 $[M-H]^+$, found 227.2198.

Dimethyl(octadecyl)silane (4). This compound was synthesized from chloro(dimethyl) octadecylsilane following the general procedure in the main text, and was obtained in 97% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm): 3.83-3.77 (m, 1H), 1.32–1.21 (m, 19H), 0.85-0.82 (t, 3H), 0.56-0.41 (m, 2H), 0.12-0.11 (d, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ (ppm): 33.1, 31.9, 29.6, 29.5, 29.3, 29.2, 24.3, 22.6, 14.2, 13.9, -4.5. ESI-MS calcd for $C_{20}H_{44}Si$, 311.3134 $[M-H]^+$, found 311.3108.

(Heptadecafluoro-1,1,2,2-tetrahydrodecyl)dimethylsilane (5). This compound was synthesized from (heptadecafluoro-1,1,2,2-tetrahydrodecyl)dimethylchlorosilane following the general procedure in the main text, and was obtained in 98% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm): 3.94-3.89 (sept, J = 3.6 Hz, 1H), 2.13-2.00 (m, 2H), 0.86-0.81 (dt, J = 12.7, 3.5 Hz, 2H), 0.13-0.12 (d, J = 3.6 Hz, 6H);^{13}C NMR (101 MHz, $CDCl_3$) δ (ppm): δ 120.9, 118.7, 115.8, 113.6, 112.9, 110.9, 108.3, 105.7, 26.4, 3.7, -5.0. ESI-MS calcd for $C_{12}H_{11}F_{17}Si$, 505.0280 $[M-H]^+$; experimental, 505.0275.

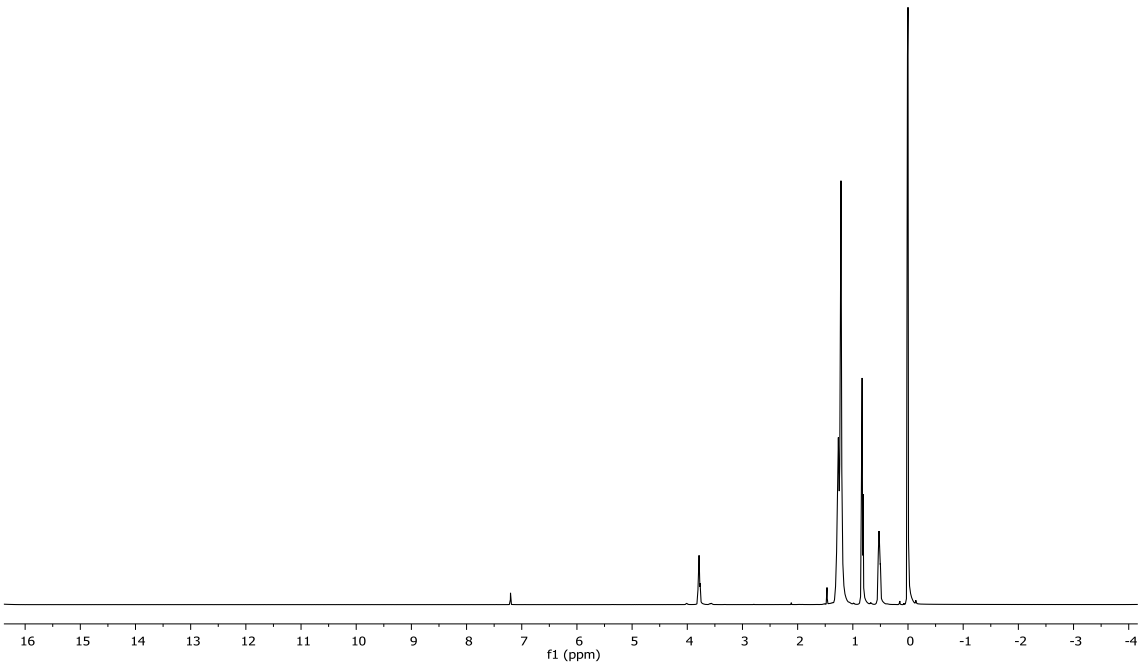


Figure S7. ^{1}H NMR spectrum of hydrosilane **1**.

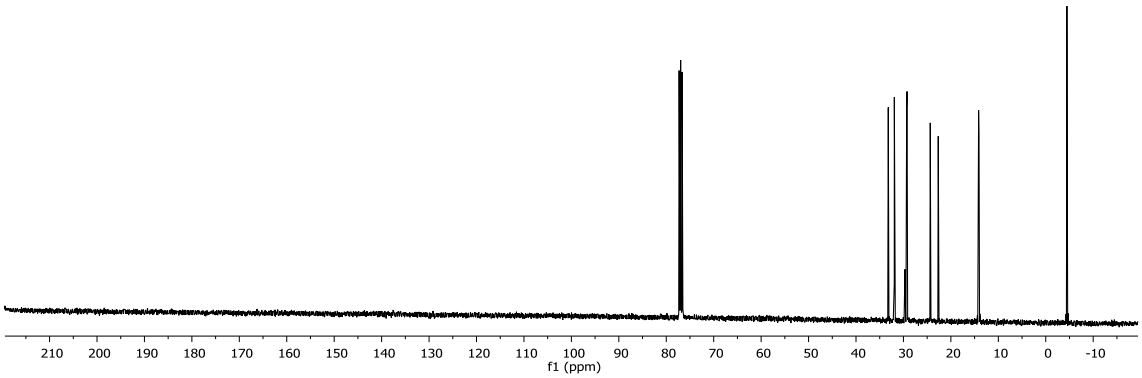


Figure S8. ^{13}C NMR spectrum of hydrosilane **1**.

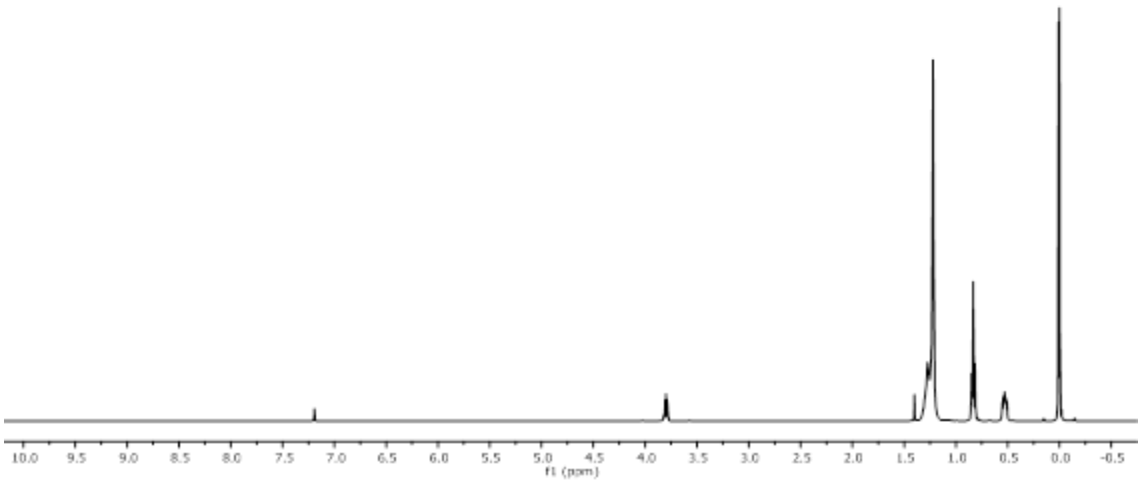


Figure S9. ^{1}H NMR spectrum of hydrosilane **2**.

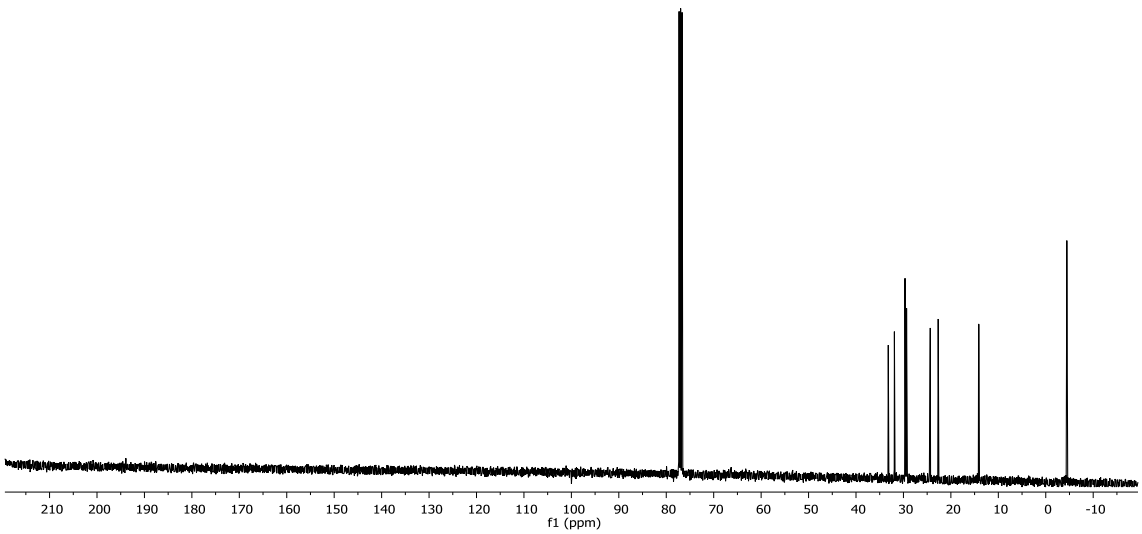


Figure S10. ^{13}C NMR spectrum of hydrosilane **2**.

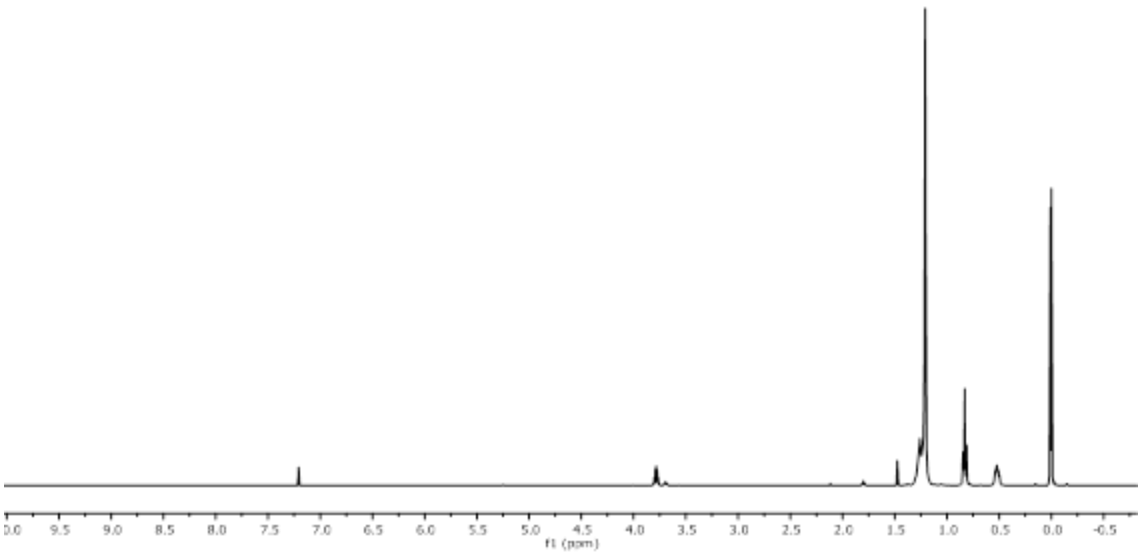


Figure S11. ^{1}H NMR spectrum of hydrosilane **3**.

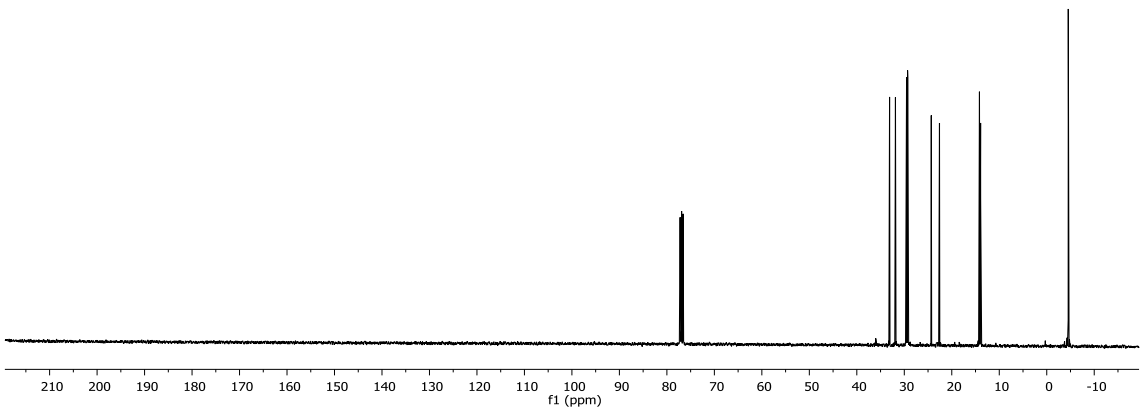


Figure S12. ^{13}C NMR spectrum of hydrosilane **3**.

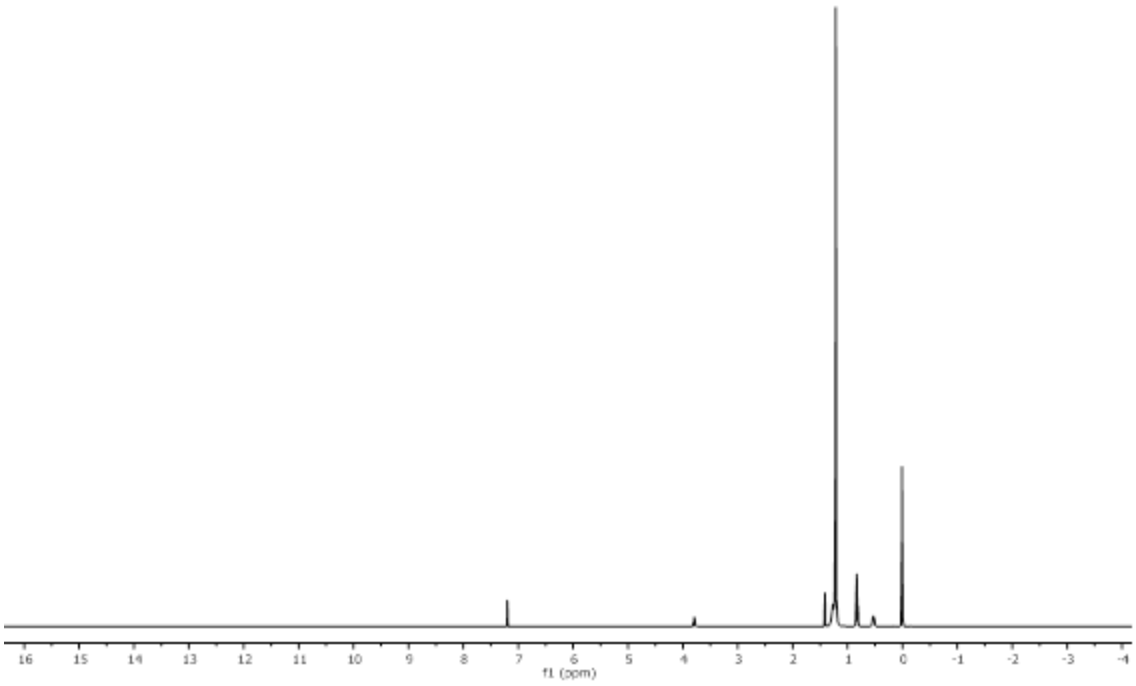


Figure S13. ^{1}H NMR spectrum of hydrosilane **4**.

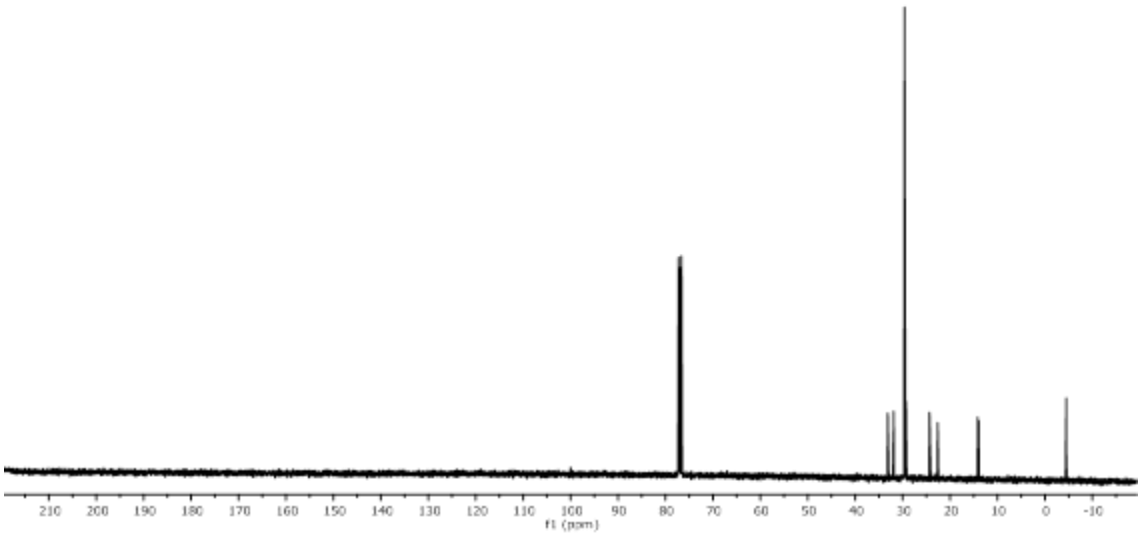


Figure S14. ^{13}C NMR spectrum of hydrosilane **4**.

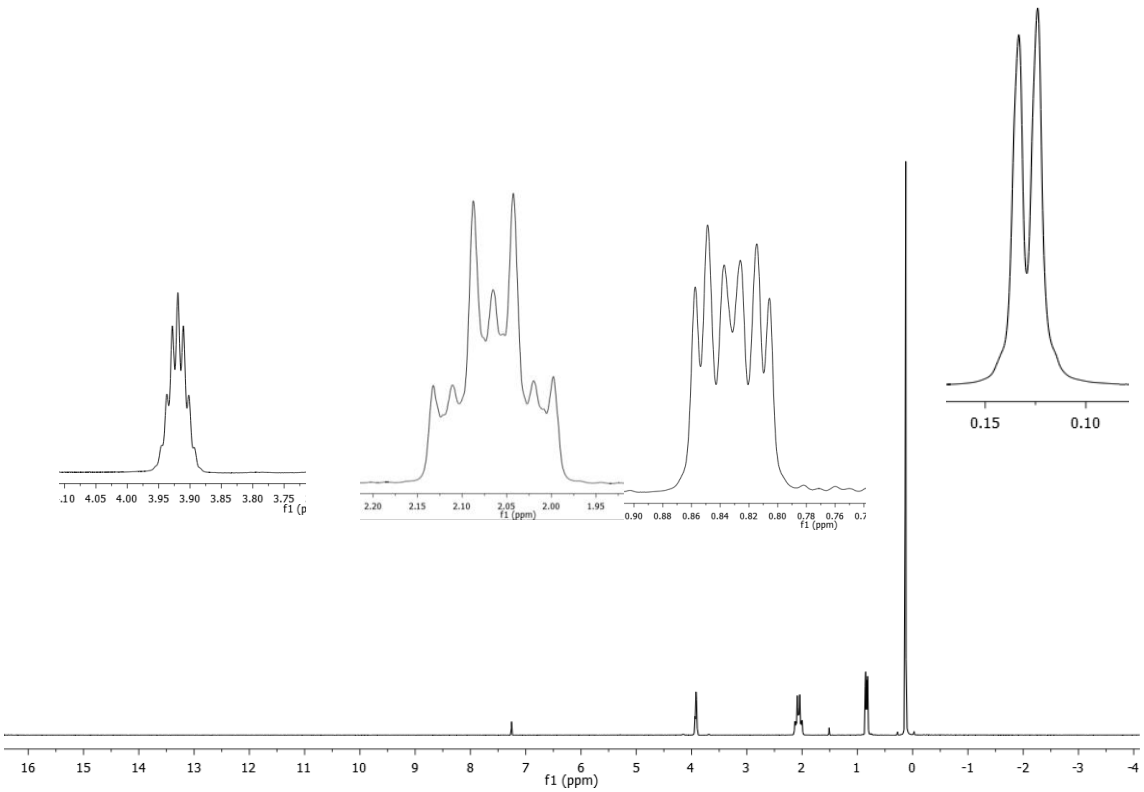


Figure S15. ^{1}H NMR spectrum of hydrosilane **5**.

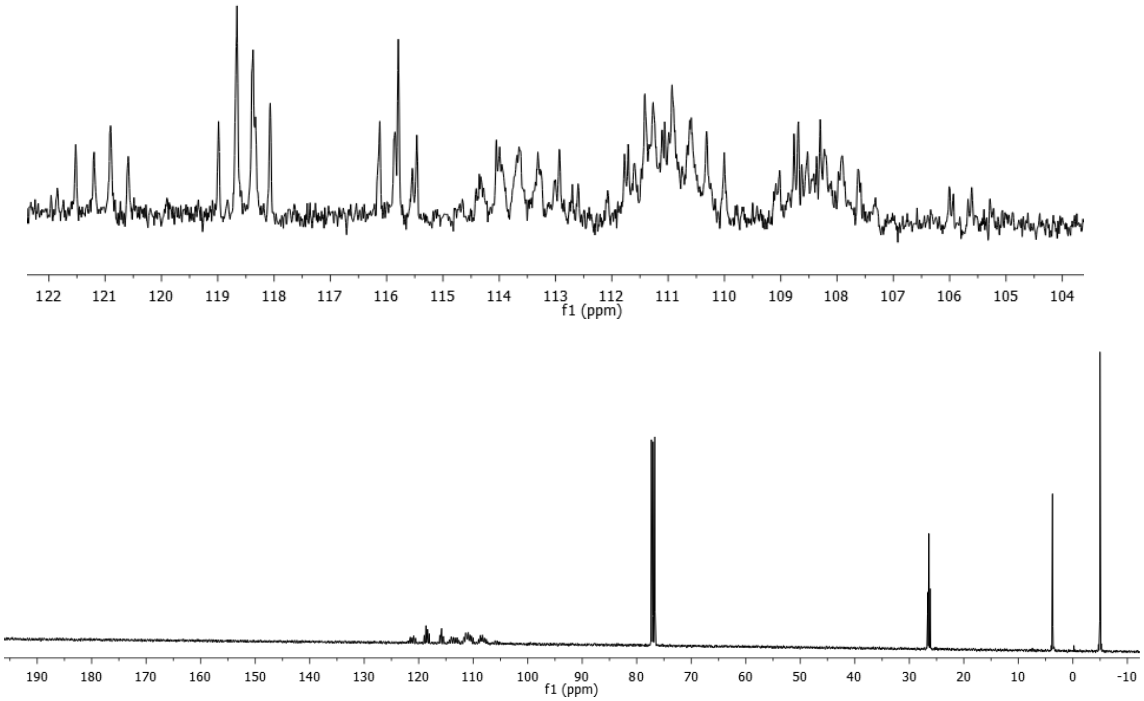
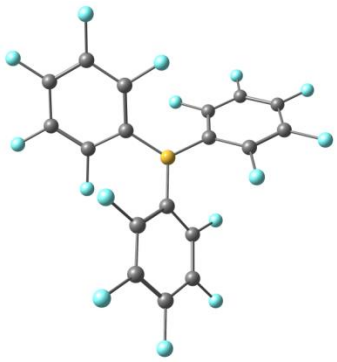


Figure S16. ^{13}C NMR spectrum of hydrosilane **5**.

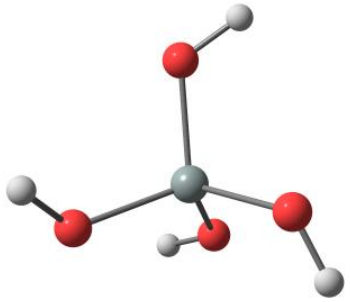
6. Cartesian coordinates of stationary points at the M11/6-311+G(d,p) level of theory.

$B(C_6F_5)_3$



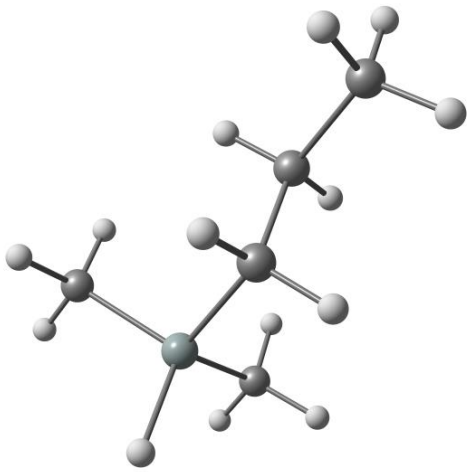
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	0.000223	-0.002704	0.003068
2	6	0	-0.194729	1.551788	0.002620
3	6	0	-1.252938	2.166826	-0.664259
4	6	0	0.678567	2.409962	0.668973
5	6	0	-1.435111	3.537039	-0.685297
6	6	0	0.516222	3.782825	0.688590
7	6	0	-0.545621	4.348072	0.001103
8	6	0	-1.248591	-0.948744	0.004007
9	6	0	-1.252778	-2.173944	-0.660741
10	6	0	-2.429313	-0.618241	0.667369
11	6	0	-2.351119	-3.013718	-0.684963
12	6	0	-3.539903	-1.441715	0.683553
13	6	0	-3.499847	-2.644584	-0.003327
14	6	0	1.444096	-0.610348	0.001295
15	6	0	1.755166	-1.791975	0.671811
16	6	0	2.502166	-0.002526	-0.672699
17	6	0	3.026996	-2.334369	0.690550
18	6	0	3.781475	-0.526347	-0.694870
19	6	0	4.044258	-1.698021	-0.003173
20	9	0	-4.560380	-3.441575	-0.008232
21	9	0	-2.314643	-4.168414	-1.348717
22	9	0	-0.168210	-2.581984	-1.336501
23	9	0	2.305019	1.132462	-1.360136
24	9	0	4.757097	0.082378	-1.367832
25	9	0	5.268392	-2.209980	-0.004527
26	9	0	3.280681	-3.456957	1.361868
27	9	0	0.809623	-2.449814	1.358983
28	9	0	-2.523743	0.533324	1.348680
29	9	0	-4.641662	-1.090462	1.345309
30	9	0	1.725501	1.918465	1.348293
31	9	0	-2.144095	1.431396	-1.345788
32	9	0	1.369216	4.562270	1.352014
33	9	0	-0.709758	5.664558	-0.000682
34	9	0	-2.452492	4.081183	-1.351464

Oxidized Si surface model



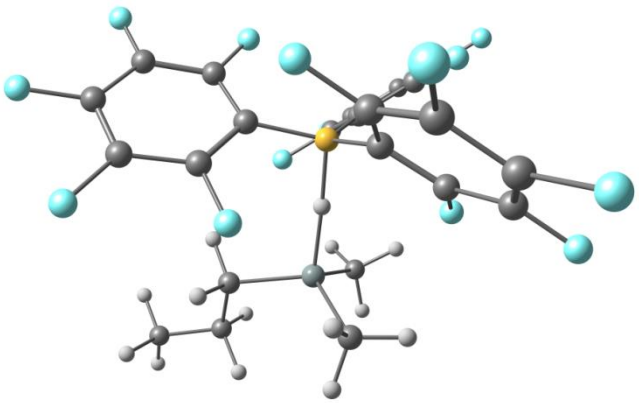
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	0.559388	-0.211550	0.021838
2	1	0	-0.143147	-0.854001	-0.084940
3	14	0	2.133958	-0.669976	0.078577
4	8	0	2.953148	0.556791	0.797295
5	8	0	2.847718	-0.919925	-1.377689
6	8	0	2.175622	-2.105264	0.872839
7	1	0	3.196048	-0.191736	-1.893544
8	1	0	2.919236	-2.702597	0.783749
9	1	0	2.563010	1.067854	1.507441

Hydrosilane compound model



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	14	0	1.121782	-1.214119	-0.013894
2	1	0	1.631041	-0.493036	1.198607
3	6	0	-0.756472	-1.210070	0.013964
4	1	0	-1.157218	-0.190057	-0.033682
5	1	0	-1.161243	-1.768993	-0.839738
6	1	0	-1.143221	-1.677882	0.927434
7	6	0	1.753283	-2.983034	0.014146
8	1	0	1.361235	-3.551541	-0.839167
9	1	0	2.848549	-3.019896	-0.034166
10	1	0	1.442155	-3.503641	0.927937
11	6	0	1.742797	-0.335338	-1.558562
12	1	0	1.408161	0.713322	-1.536997
13	1	0	2.842987	-0.300147	-1.536647
14	6	0	1.274852	-0.998310	-2.865445
15	1	0	0.175549	-1.029934	-2.891406
16	1	0	1.612645	-2.044913	-2.891071
17	6	0	1.789087	-0.270614	-4.109409
18	1	0	2.886535	-0.251796	-4.121295
19	1	0	1.448736	-0.752820	-5.033855
20	1	0	1.439847	0.769948	-4.121632

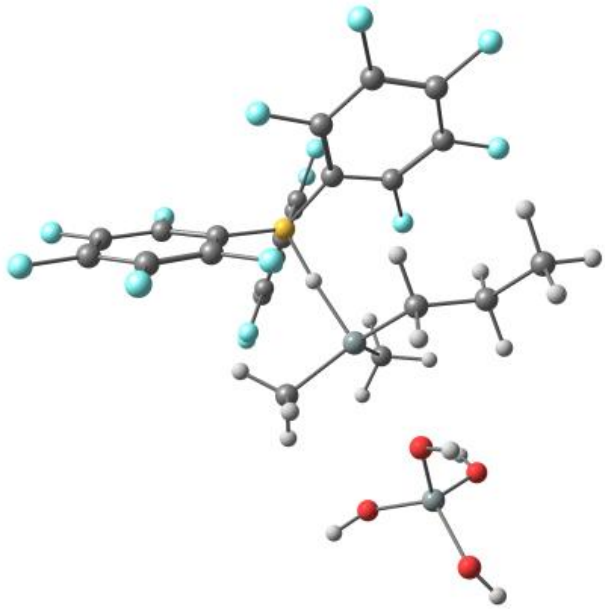
Intermediate I



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	14	0	0.508597	-0.062710	2.542072
2	6	0	-0.434390	-1.527059	3.189719
3	1	0	-0.386517	-2.363267	2.481610
4	1	0	0.018490	-1.865071	4.132004
5	1	0	-1.484572	-1.285487	3.387558
6	6	0	-0.048041	1.581593	3.204839
7	1	0	-0.088082	1.545487	4.301973
8	1	0	0.635564	2.388712	2.918142
9	1	0	-1.055359	1.822571	2.843513
10	6	0	2.356289	-0.287460	2.489065
11	1	0	2.591867	-1.335906	2.257353
12	1	0	2.778615	0.325694	1.678925
13	6	0	3.000216	0.106389	3.835580
14	1	0	2.544367	-0.471044	4.654938
15	1	0	2.791800	1.164181	4.049782
16	6	0	4.511585	-0.128050	3.834002
17	1	0	4.993009	0.460280	3.043014
18	1	0	4.963415	0.156582	4.791153
19	1	0	4.740469	-1.185253	3.651094
20	1	0	0.087268	0.011890	1.035140
21	5	0	-0.241135	0.008517	-0.312532
22	6	0	1.171410	-0.435672	-0.932395
23	6	0	1.767612	-1.609060	-0.491404
24	6	0	1.903903	0.282682	-1.865793
25	6	0	3.000903	-2.057569	-0.919536
26	6	0	3.142923	-0.133162	-2.332779
27	6	0	3.695480	-1.307992	-1.856106
28	6	0	-0.669698	1.548054	-0.456763
29	6	0	0.201728	2.542337	-0.034731
30	6	0	-1.883568	1.995765	-0.954580
31	6	0	-0.085419	3.891634	-0.087529
32	6	0	-2.212183	3.341286	-1.037125
33	6	0	-1.309010	4.293551	-0.600453
34	6	0	-1.417983	-1.081529	-0.288965
35	6	0	-2.458118	-0.934748	0.618144
36	6	0	-1.486468	-2.209834	-1.091989
37	6	0	-3.497341	-1.834109	0.751286
38	6	0	-2.517704	-3.133769	-1.003099
39	6	0	-3.526162	-2.946309	-0.075002
40	9	0	-1.611273	5.588532	-0.669294
41	9	0	0.793520	4.801497	0.341489
42	9	0	3.804825	0.594974	-3.234423
43	9	0	4.885502	-1.716233	-2.292142

44	9	0	3.524516	-3.190301	-0.443181
45	9	0	1.125159	-2.367190	0.428682
46	9	0	1.435121	1.435324	-2.373754
47	9	0	-2.811016	1.126966	-1.393555
48	9	0	-3.391336	3.722094	-1.533147
49	9	0	1.408813	2.185661	0.465150
50	9	0	-4.462283	-1.643419	1.655048
51	9	0	-4.517417	-3.829621	0.025488
52	9	0	-2.466995	0.144617	1.436390
53	9	0	-0.538602	-2.459128	-2.012430
54	9	0	-2.543063	-4.202198	-1.802420

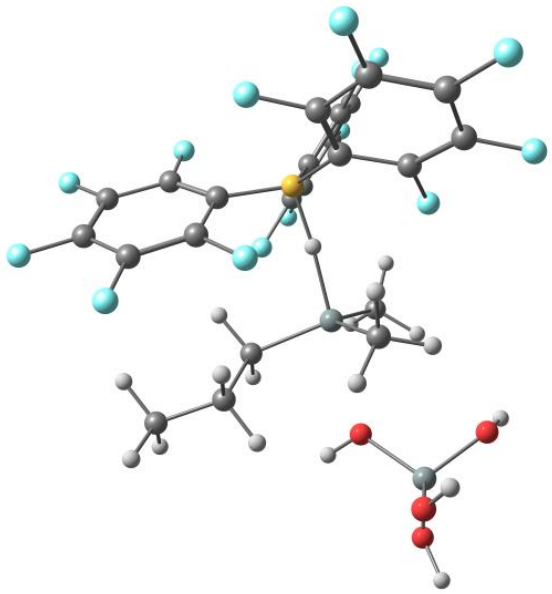
Intermediate II



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	14	0	1.731701	-0.057516	0.649576
2	1	0	0.169320	-0.084905	0.204128
3	6	0	1.565698	-1.094447	2.185121
4	6	0	2.448158	-0.867672	-0.867759
5	6	0	1.956247	1.793474	0.819824
6	1	0	2.274533	-1.927845	2.124429
7	1	0	0.559416	-1.515816	2.283685
8	1	0	1.793833	-0.504340	3.080080
9	1	0	1.690540	-0.992769	-1.648958
10	1	0	3.244212	-0.232349	-1.276422
11	1	0	2.855485	-1.856065	-0.615958
12	1	0	0.968522	2.275340	0.840866
13	1	0	2.377743	1.983248	1.820507
14	5	0	-1.114777	-0.001736	-0.174696
15	6	0	-1.142767	-1.072608	-1.375086
16	6	0	-1.196061	1.556865	-0.571229
17	6	0	-1.867280	-0.458400	1.174237
18	6	0	-1.680635	-0.852253	-2.632561
19	6	0	-0.597839	-2.332194	-1.175279
20	6	0	-1.687855	-1.817268	-3.628743
21	6	0	-0.577312	-3.323430	-2.138056
22	6	0	-1.135112	-3.060800	-3.378750
23	9	0	-2.229998	0.336345	-2.943277
24	9	0	-0.028759	-2.620251	0.020185
25	9	0	-2.221360	-1.557141	-4.825430
26	9	0	-0.030123	-4.517514	-1.888394
27	9	0	-1.131779	-3.998388	-4.327034
28	6	0	-1.986605	2.518532	0.037778
29	6	0	-0.308738	2.042225	-1.522302
30	6	0	-1.893405	3.872127	-0.261144
31	6	0	-0.170612	3.377208	-1.844091
32	6	0	-0.975765	4.304889	-1.200703
33	9	0	-2.895215	2.181114	0.969946
34	9	0	0.518699	1.172130	-2.147215
35	9	0	-2.678001	4.758064	0.357738
36	9	0	0.737447	3.780847	-2.739060

37	9	0	-0.863014	5.601821	-1.487079
38	6	0	-2.851547	-1.431877	1.250277
39	6	0	-1.520953	0.125490	2.384621
40	6	0	-3.451254	-1.804541	2.445690
41	6	0	-2.083642	-0.216176	3.598056
42	6	0	-3.064238	-1.195550	3.625352
43	9	0	-3.288130	-2.064853	0.146028
44	9	0	-0.566958	1.087153	2.395066
45	9	0	-4.398333	-2.746314	2.464892
46	9	0	-1.697425	0.379064	4.730839
47	9	0	-3.628022	-1.547609	4.780774
48	6	0	2.832145	2.454021	-0.261091
49	1	0	3.836439	2.004892	-0.258033
50	1	0	2.421310	2.247589	-1.258648
51	6	0	2.935691	3.966658	-0.059111
52	1	0	3.390667	4.205818	0.911090
53	1	0	3.538508	4.437235	-0.844046
54	1	0	1.939927	4.429753	-0.076746
55	14	0	5.376548	-1.106623	0.935927
56	8	0	4.757409	-2.616464	1.062245
57	8	0	6.632286	-0.767912	1.927217
58	8	0	5.833970	-0.905854	-0.618478
59	1	0	4.548484	-3.045389	1.893241
60	1	0	7.545217	-0.927123	1.682781
61	1	0	5.485585	-1.446176	-1.329932
62	8	0	4.187353	-0.038934	1.395165
63	1	0	4.461334	0.782965	1.813093

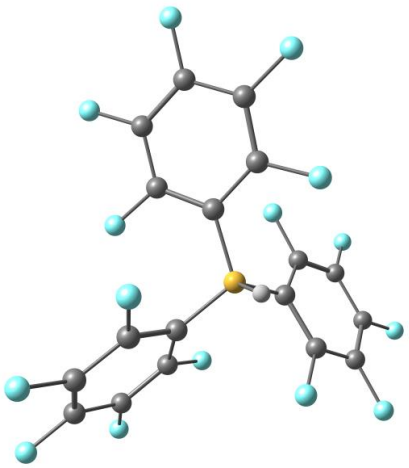
Intermediate III



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	14	0	1.729247	-0.085074	0.651701
2	1	0	0.168284	-0.091248	0.201259
3	6	0	1.545425	-1.121721	2.185114
4	6	0	2.435052	-0.900575	-0.867148
5	6	0	1.981216	1.761882	0.829025
6	1	0	2.324454	-1.891274	2.189235
7	1	0	0.572246	-1.624819	2.213209
8	1	0	1.651326	-0.509565	3.088268
9	1	0	1.672452	-1.027342	-1.643217
10	1	0	3.229678	-0.268156	-1.282656
11	1	0	2.842863	-1.887892	-0.613313
12	1	0	0.999603	2.256217	0.854520
13	1	0	2.406207	1.941340	1.829991
14	5	0	-1.118094	0.008941	-0.168346
15	6	0	-1.167048	-1.046825	-1.381668
16	6	0	-1.183773	1.571506	-0.550393
17	6	0	-1.866139	-0.454657	1.180985
18	6	0	-1.709385	-0.802542	-2.633074
19	6	0	-0.639337	-2.316623	-1.202200
20	6	0	-1.735977	-1.754032	-3.641866
21	6	0	-0.637761	-3.295124	-2.178066
22	6	0	-1.198828	-3.008226	-3.411909
23	9	0	-2.244518	0.397340	-2.925072
24	9	0	-0.070265	-2.629490	-0.013019
25	9	0	-2.273531	-1.470559	-4.831442
26	9	0	-0.106054	-4.499795	-1.947255
27	9	0	-1.213320	-3.933183	-4.372339
28	6	0	-1.963190	2.536433	0.067212
29	6	0	-0.294118	2.053992	-1.500924
30	6	0	-1.857223	3.891149	-0.222846
31	6	0	-0.143918	3.389505	-1.814453
32	6	0	-0.938137	4.320761	-1.162383
33	9	0	-2.872145	2.200968	0.999709
34	9	0	0.522312	1.179290	-2.133759
35	9	0	-2.631007	4.780903	0.404099
36	9	0	0.764957	3.790410	-2.709887
37	9	0	-0.812875	5.618409	-1.440360
38	6	0	-2.848764	-1.429631	1.258695

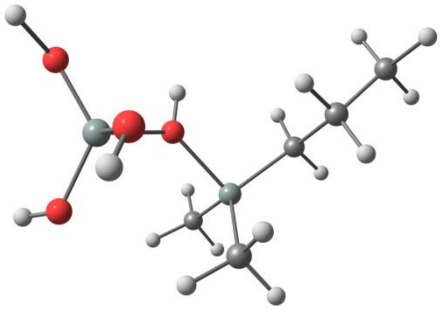
39	6	0	-1.510976	0.121024	2.392745
40	6	0	-3.438735	-1.810648	2.456448
41	6	0	-2.063636	-0.228682	3.608266
42	6	0	-3.043305	-1.209040	3.636944
43	9	0	-3.293200	-2.057178	0.154453
44	9	0	-0.558139	1.084055	2.402303
45	9	0	-4.384574	-2.753676	2.476466
46	9	0	-1.669441	0.360316	4.741561
47	9	0	-3.598308	-1.568475	4.794345
48	6	0	2.861921	2.417053	-0.251186
49	1	0	3.861901	1.958347	-0.253179
50	1	0	2.446360	2.218215	-1.248254
51	6	0	2.980899	3.927948	-0.045528
52	1	0	3.437738	4.160314	0.925460
53	1	0	3.589487	4.393410	-0.829074
54	1	0	1.990287	4.402024	-0.063527
55	14	0	5.379065	-1.151393	0.899769
56	8	0	4.761310	-2.664267	0.994760
57	8	0	6.647515	-0.842359	1.883401
58	8	0	5.816420	-0.909338	-0.654695
59	1	0	4.576332	-3.130117	1.811315
60	1	0	7.558144	-0.993347	1.626319
61	1	0	5.479658	-1.443879	-1.375667
62	8	0	4.196023	-0.094998	1.395952
63	1	0	4.472336	0.719727	1.826149

Intermediate III anionc



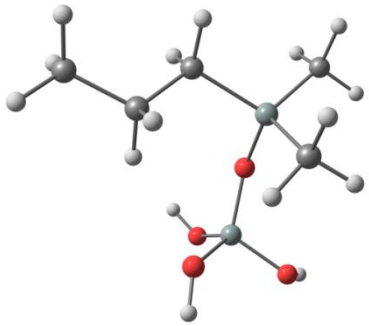
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	0.000000	0.000000	0.770067
2	6	0	-0.070881	1.573336	0.330894
3	6	0	-1.327108	-0.848052	0.330894
4	6	0	1.397989	-0.725283	0.330894
5	6	0	0.826047	2.461171	0.913285
6	6	0	0.843153	3.820752	0.662994
7	6	0	-0.078706	4.358194	-0.218576
8	6	0	-0.986930	3.519253	-0.831191
9	6	0	-0.962755	2.158918	-0.551815
10	9	0	1.769330	1.997017	1.761618
11	9	0	1.741532	4.627223	1.256429
12	9	0	-0.083424	5.676963	-0.477861
13	9	0	-1.881815	4.026595	-1.697804
14	9	0	-1.876270	1.418331	-1.221481
15	6	0	-1.388300	-1.913230	-0.551815
16	6	0	-2.554298	-2.614333	-0.831191
17	6	0	-3.734954	-2.247258	-0.218576
18	6	0	-3.730445	-1.180184	0.662994
19	6	0	-2.544460	-0.515207	0.913285
20	9	0	-0.290175	-2.334063	-1.221481
21	9	0	-2.546226	-3.642997	-1.697804
22	9	0	-4.874682	-2.910728	-0.477861
23	9	0	-4.878059	-0.805401	1.256429
24	9	0	-2.614132	0.533777	1.761618
25	6	0	1.718413	-1.945963	0.913285
26	6	0	2.887292	-2.640568	0.662994
27	6	0	3.813660	-2.110936	-0.218576
28	6	0	3.541228	-0.904920	-0.831191
29	6	0	2.351056	-0.245688	-0.551815
30	9	0	0.844802	-2.530793	1.761618
31	9	0	3.136527	-3.821823	1.256429
32	9	0	4.958106	-2.766235	-0.477861
33	9	0	4.428041	-0.383598	-1.697804
34	9	0	2.166445	0.915732	-1.221481
35	1	0	0.000000	0.000000	1.991402

Intermediate III cationic



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	14	0	-1.807961	0.683142	-1.176227
2	6	0	-1.019635	-0.427768	-2.420866
3	6	0	-2.350883	-0.131050	0.388874
4	6	0	-1.116321	2.388597	-0.989573
5	1	0	-0.865776	0.070341	-3.385341
6	1	0	-1.623879	-1.328576	-2.583364
7	1	0	-0.034861	-0.755901	-2.063665
8	1	0	-1.469517	-0.392381	0.989673
9	1	0	-2.973679	0.540536	0.991535
10	1	0	-2.899381	-1.062160	0.199249
11	1	0	-0.054547	2.315643	-0.709170
12	1	0	-1.112229	2.896773	-1.968357
13	6	0	-1.877508	3.233952	0.054212
14	1	0	-2.960340	3.211310	-0.149339
15	1	0	-1.748179	2.782312	1.047016
16	6	0	-1.391596	4.683065	0.085212
17	1	0	-1.539357	5.169501	-0.886938
18	1	0	-1.929842	5.266579	0.839391
19	1	0	-0.322107	4.729786	0.323025
20	14	0	-5.000794	0.311960	-1.704455
21	8	0	-4.685730	-1.271267	-1.772693
22	8	0	-5.804328	0.966056	-2.941271
23	8	0	-5.466208	0.763909	-0.231472
24	1	0	-4.807608	-1.866575	-2.516036
25	1	0	-6.730815	1.205088	-3.015286
26	1	0	-5.808476	0.209093	0.472941
27	8	0	-3.457399	1.092489	-1.951425
28	1	0	-3.480810	1.846138	-2.561721

Product (IV)



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	14	0	-2.222153	-0.832895	-1.512520
2	6	0	-2.756069	0.919784	-1.867022
3	1	0	-2.108775	1.399658	-2.612583
4	1	0	-3.784130	0.926572	-2.252379
5	1	0	-2.737204	1.535536	-0.958811
6	6	0	-0.570903	-0.906918	-0.650787
7	1	0	-0.589268	-0.332491	0.283562
8	1	0	-0.304708	-1.941821	-0.402996
9	1	0	0.227719	-0.496298	-1.281618
10	6	0	-2.239452	-1.860249	-3.073945
11	1	0	-1.401557	-1.570567	-3.727587
12	1	0	-2.056839	-2.911032	-2.797532
13	6	0	-3.567979	-1.746728	-3.842436
14	1	0	-3.690051	-0.716166	-4.205555
15	1	0	-4.411017	-1.921453	-3.158268
16	6	0	-3.647458	-2.714487	-5.024308
17	1	0	-3.562071	-3.754066	-4.681758
18	1	0	-4.594750	-2.614864	-5.568058
19	1	0	-2.829297	-2.532044	-5.733484
20	8	0	-3.360490	-1.508214	-0.472398
21	14	0	-4.864650	-1.346236	0.114515
22	8	0	-5.015191	-0.248222	1.328545
23	1	0	-4.911264	-0.517594	2.242033
24	8	0	-5.368250	-2.783301	0.742609
25	1	0	-5.101025	-3.614803	0.349714
26	8	0	-5.788729	-0.810695	-1.138594
27	1	0	-6.654593	-0.432982	-0.978656

[i] Giesbers, M.; Marcelis, A.T.M.; Zuilhof, H. Simulation of XPS C1s Spectra of Organic Monolayers by Quantum Chemical Methods. *Langmuir* **2013,** *29,* 4782-4788.