Supporting Information-SII

Reactivity and Selectivity of Organotin Reagents in Allylation and Arylation: Nucleophilicity Parameter as a Guide

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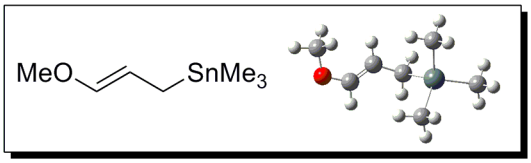
Electronic energies, electronic states and geometries in Cartesian coordinates (Angstroms), the structures of the following 56 organotin compounds:

- **List of Compounds with page number**

3-Methoxy allyltrimethyl stannane (*1*)

E(RB+HF-LYP/6-311+G(d,p) -354.939507 Hartree
Electronic state: 1-A
Cartesian Coordinates (Angstroms):

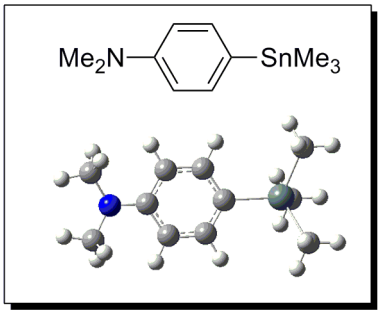
C	-0.466041	-0.732205	-1.187494
Sn	1.179567	0.025550	0.027538
C	-1.794351	-0.174563	-0.763368
C	-2.741488	-0.898333	-0.147615
H	-0.253567	-0.486266	-2.236269
H	-1.964018	0.881661	-0.960740
H	-2.610453	-1.957632	0.060707
H	-0.460264	-1.826952	-1.114495
C	1.012058	-0.804504	2.006562
H	-0.002999	-0.667093	2.393137
H	1.230972	-1.877504	2.001235
H	1.709515	-0.319824	2.697793
C	3.068820	-0.529913	-0.851929
H	3.164484	-0.117594	-1.862017
H	3.903405	-0.151453	-0.251869
H	3.167891	-1.618481	-0.919789
C	1.045595	2.174570	0.125298
H	1.845121	2.586683	0.750146
H	1.133241	2.620028	-0.871489
H	0.087620	2.486664	0.554102
O	-3.961912	-0.491008	0.305959
C	-4.297526	0.870001	0.108814
H	-3.586593	1.534810	0.619734
H	-5.294221	1.006688	0.533265
H	-4.315587	1.126512	-0.959636



N,N–dimethyl–4–(trimethylstannyl)aniline (*2*)

E(RB+HF-LYP/6-311+G(d,p) -488.7222701 Hartree
Electronic state: 1-A
Cartesian Coordinates (Angstroms):

C	0.051253	-0.001565	0.016672
C	0.795065	1.190796	0.024485
C	0.796058	-1.193543	0.025573
C	2.187610	1.204603	0.049347
H	0.284152	2.152379	0.001502
C	2.188363	-1.206338	0.050630
H	0.286569	-2.156048	0.003122
C	2.925294	-0.000509	0.076795
H	2.698754	2.160454	0.044029
H	2.700269	-2.161780	0.046168
Sn	-2.089616	-0.000395	-0.005792
C	-2.783454	-1.682005	-1.157579
C	-2.885797	-0.142448	1.991622
C	-2.776986	1.831398	-0.904687
H	-2.443321	-1.606936	-2.195533
H	-2.411919	-2.627133	-0.747368
H	-3.877891	-1.724709	-1.159757
H	-3.981013	-0.125871	1.972936

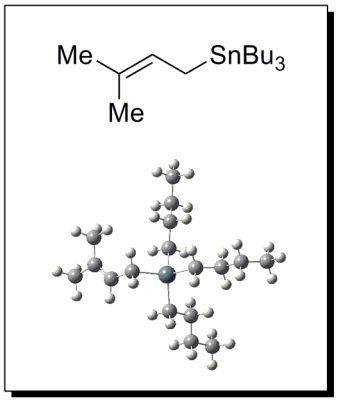


H	-2.567385	-1.071839	2.475289
H	-2.542444	0.694106	2.609066
H	-3.871318	1.853152	-0.944823
H	-2.446009	2.705352	-0.333583
H	-2.397495	1.930616	-1.926883
N	4.315654	-0.000154	0.135327
C	5.035403	-1.245235	-0.068884
C	5.034584	1.244875	-0.072100
H	6.105986	1.059753	0.030713
H	4.854650	1.686037	-1.066322
H	4.755689	1.989574	0.682801
H	6.106587	-1.059462	0.035187
H	4.755851	-1.988592	0.687063
H	4.857131	-1.688405	-1.062521

Tributyl(3-methylbut-2-enyl)stannane (*3*)

E(RB+HF-LYP/6-311+G(d,p) -672.8569395 Hartree
Electronic state: 1-A
Cartesian Coordinates (Angstroms):

1	6	0	1.755562	-0.389305	-1.823036
2	6	0	2.790756	-1.303925	-1.246001
3	6	0	3.959475	-0.997942	-0.652600
4	1	0	2.536338	-2.364507	-1.302094
5	1	0	1.398609	-0.776970	-2.786159
6	1	0	2.139354	0.618754	-2.010456
7	6	0	-1.510450	0.928464	-1.607023
8	6	0	-0.705169	-2.214486	-0.076900
9	6	0	0.541771	0.813346	1.297655
10	1	0	-0.288731	0.707397	2.008949
11	1	0	1.389292	0.271591	1.738612
12	1	0	-1.035632	1.855358	-1.957844
13	1	0	-1.772327	0.365563	-2.513786
14	1	0	-1.063328	-2.668480	-1.011366
15	1	0	0.172250	-2.802863	0.225598
16	50	0	-0.004093	-0.211491	-0.533603
17	6	0	-2.784883	1.265476	-0.814157
18	6	0	-3.803346	2.091867	-1.615840
19	1	0	-2.523258	1.817907	0.100567
20	1	0	-3.272040	0.339450	-0.474988
21	6	0	-5.074253	2.421489	-0.825044
22	1	0	-3.324843	3.023370	-1.950395
23	1	0	-4.070278	1.542131	-2.529709
24	1	0	-5.779448	3.007971	-1.425340
25	1	0	-5.589987	1.507581	-0.504631
26	1	0	-4.841795	3.002172	0.076425
27	6	0	-1.794408	-2.317270	1.005027
28	6	0	-2.211879	-3.764289	1.313226
29	1	0	-2.686598	-1.751471	0.698347
30	1	0	-1.446078	-1.845328	1.935584
31	6	0	-3.296958	-3.866251	2.390891
32	1	0	-2.565581	-4.240580	0.387640
33	1	0	-1.324901	-4.332655	1.627539
34	1	0	-3.570576	-4.909368	2.587530
35	1	0	-2.958455	-3.427034	3.337615

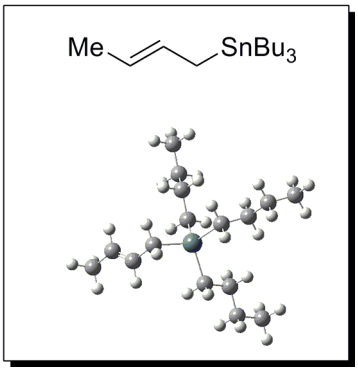


36	1	0	-4.207911	-3.334885	2.088019
37	6	0	0.898522	2.299937	1.128353
38	6	0	1.275615	2.994711	2.446564
39	1	0	0.054328	2.840402	0.674544
40	1	0	1.736284	2.406653	0.423183
41	6	0	1.631742	4.475092	2.270962
42	1	0	0.439957	2.898041	3.154346
43	1	0	2.122910	2.462936	2.902399
44	1	0	1.894074	4.941082	3.227858
45	1	0	2.486824	4.599913	1.594834
46	1	0	0.790790	5.037755	1.846455
47	6	0	4.856608	-2.082405	-0.103849
48	6	0	4.490002	0.404383	-0.480115
49	1	0	5.491643	0.499445	-0.923441
50	1	0	3.851238	1.165376	-0.936047
51	1	0	4.599941	0.655706	0.584855
52	1	0	5.846652	-2.061350	-0.582471
53	1	0	5.033060	-1.949956	0.973824
54	1	0	4.430607	-3.079900	-0.254537

But-2enyltributylstannane (*4*)

E(RB+HF-LYP/6-311+G(d,p) -633.5408622 Hartree
Electronic state: 1-A
Cartesian Coordinates (Angstroms):

1	6	0	1.927498	-0.344595	-1.880113
2	6	0	3.003321	-1.205996	-1.297513
3	6	0	4.142947	-0.779802	-0.735968
4	1	0	2.813071	-2.282114	-1.315048
5	1	0	4.349389	0.292611	-0.716041
6	1	0	1.584589	-0.738550	-2.845556
7	1	0	2.290323	0.675189	-2.056591
8	6	0	-1.396939	0.854473	-1.604605
9	6	0	-0.439765	-2.238472	-0.077089
10	6	0	0.754149	0.844024	1.235192
11	1	0	-0.049536	0.726351	1.974704
12	1	0	1.629866	0.329198	1.652436
13	1	0	-0.951286	1.752817	-2.053621
14	1	0	-1.727860	0.231461	-2.447079
15	1	0	-0.771045	-2.722607	-1.006425
16	1	0	0.456528	-2.787058	0.244275
17	50	0	0.182346	-0.217181	-0.566410
18	6	0	-2.605575	1.250990	-0.739065
19	6	0	-3.688394	2.018272	-1.514697
20	1	0	-2.272796	1.868317	0.108467
21	1	0	-3.060563	0.353765	-0.293948
22	6	0	-4.891331	2.410360	-0.649537
23	1	0	-3.241633	2.920773	-1.955809
24	1	0	-4.027333	1.402718	-2.360113
25	1	0	-5.644173	2.953786	-1.232215
26	1	0	-5.377517	1.524777	-0.221499
27	1	0	-4.587072	3.055056	0.184446
28	6	0	-1.535595	-2.363954	0.995651
29	6	0	-1.907833	-3.819930	1.318967

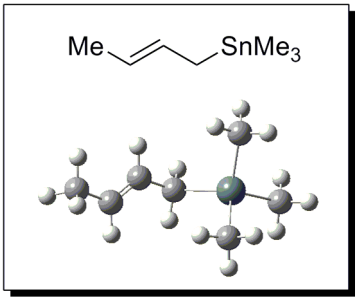


30	1	0	-2.442979	-1.832535	0.672425
31	1	0	-1.212709	-1.868137	1.922979
32	6	0	-3.000578	-3.944131	2.386484
33	1	0	-2.235496	-4.319655	0.396142
34	1	0	-1.005980	-4.354378	1.650033
35	1	0	-3.241455	-4.993191	2.594007
36	1	0	-2.687132	-3.481669	3.330749
37	1	0	-3.925347	-3.447490	2.067054
38	6	0	1.069179	2.336562	1.036841
39	6	0	1.460892	3.057699	2.336463
40	1	0	0.201081	2.850339	0.597147
41	1	0	1.886320	2.453507	0.309412
42	6	0	1.777108	4.543706	2.134042
43	1	0	0.644492	2.950604	3.064936
44	1	0	2.331061	2.552205	2.778802
45	1	0	2.049626	5.028222	3.078827
46	1	0	2.613513	4.680162	1.437116
47	1	0	0.913478	5.080626	1.721897
48	6	0	5.190429	-1.668060	-0.125167
49	1	0	6.162749	-1.545322	-0.622606
50	1	0	5.352168	-1.432614	0.936305
51	1	0	4.909257	-2.725012	-0.194442

But-2enyltrimethylstannane (*5*)

E(RB+HF-LYP/6-311+G(d,p) -279.7372214 Hartree
Electronic state: 1-A
Cartesian Coordinates (Angstroms):

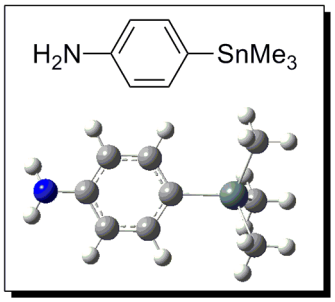
1	6	0	-0.820174	0.162641	-1.336940
2	50	0	0.875053	-0.012915	0.027729
3	6	0	-2.090073	0.497413	-0.618879
4	6	0	-3.103022	-0.343232	-0.369260
5	1	0	-0.568684	0.934749	-2.075530
6	1	0	-2.171546	1.522212	-0.247688
7	1	0	-3.036955	-1.369019	-0.738453
8	6	0	-4.354499	0.011019	0.384015
9	1	0	-0.911862	-0.786876	-1.878309
10	1	0	-5.251482	-0.137776	-0.233405
11	1	0	-4.482215	-0.619189	1.275474
12	1	0	-4.342469	1.056678	0.711741
13	6	0	0.549893	-1.714256	1.304683
14	1	0	-0.453547	-1.674078	1.740434
15	1	0	0.639153	-2.650100	0.743036
16	1	0	1.277876	-1.738363	2.122359
17	6	0	2.690196	-0.268583	-1.107054
18	1	0	2.854210	0.581628	-1.777581
19	1	0	3.556623	-0.346395	-0.441430
20	1	0	2.649071	-1.177682	-1.716189
21	6	0	1.019293	1.778580	1.215607
22	1	0	1.857861	1.712822	1.917077
23	1	0	1.176982	2.658432	0.582775
24	1	0	0.104673	1.937211	1.796204



4-(trimethylstannyl) aniline (*6*)

E(RB+HF-LYP/6-311+G(d,p) -410.1100404 Hartree
Electronic state: 1-A
Cartesian Coordinates (Angstroms):

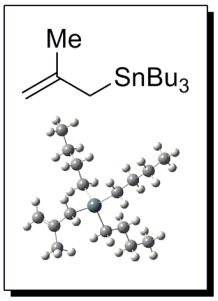
1	6	0	0.707780	-0.001398	-0.007315
2	6	0	1.447306	1.195163	-0.008999
3	6	0	1.448094	-1.197706	-0.006382
4	6	0	2.840477	1.205215	-0.004163
5	1	0	0.932607	2.154745	-0.016383
6	6	0	2.841047	-1.206956	-0.001456
7	1	0	0.934588	-2.158072	-0.011939
8	6	0	3.561481	-0.000588	0.000007
9	1	0	3.379521	2.150947	-0.011308
10	1	0	3.380705	-2.152358	-0.006388
11	50	0	-1.435036	-0.000278	0.002214
12	6	0	-2.141900	-1.695003	-1.120976
13	6	0	-2.198412	-0.121743	2.013701
14	6	0	-2.133145	1.822812	-0.904681
15	1	0	-1.811115	-1.634090	-2.162828
16	1	0	-1.768668	-2.635512	-0.701814
17	1	0	-3.236381	-1.735369	-1.112531
18	1	0	-3.293772	-0.105792	2.011930
19	1	0	-1.872126	-1.046114	2.501722
20	1	0	-1.846131	0.721313	2.617136
21	1	0	-3.227910	1.845596	-0.928392
22	1	0	-1.792537	2.702098	-0.347594
23	1	0	-1.768963	1.910869	-1.933407
24	7	0	4.958244	-0.000485	-0.054666
25	1	0	5.399052	-0.836477	0.309013
26	1	0	5.398851	0.836753	0.306352



Tributyl(2-methylallyl)stannane (*7*)

E = -633.5403619 Hartree
Electronic state: 1-A
Cartesian Coordinates (Angstroms):

1	6	0	1.945581	-1.009040	-1.622975
2	6	0	2.772463	-2.084089	-0.974246
3	6	0	3.852853	-1.814853	-0.225358
4	1	0	4.427969	-2.604847	0.250160
5	1	0	4.202810	-0.796784	-0.068616
6	1	0	1.558866	-1.339986	-2.594942
7	1	0	2.547194	-0.110606	-1.805541
8	6	0	-0.940199	0.985373	-1.660053
9	6	0	-0.942042	-2.025237	0.251646
10	6	0	1.052529	0.710570	1.305173
11	1	0	0.231920	0.889443	2.012725
12	1	0	1.741102	0.018030	1.807757
13	1	0	-0.245194	1.603616	-2.245240
14	1	0	-1.468144	0.357340	-2.391407
15	1	0	-1.252398	-2.591163	-0.637706
16	1	0	-0.285718	-2.695173	0.823565
17	50	0	0.250598	-0.337091	-0.413600

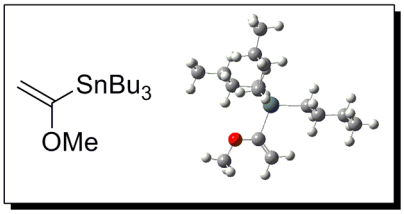


18	6	0	-1.944925	1.891019	-0.928089
19	6	0	-2.743139	2.802078	-1.875064
20	1	0	-1.418147	2.518646	-0.194350
21	1	0	-2.651296	1.281288	-0.346425
22	6	0	-3.740569	3.709987	-1.147075
23	1	0	-2.041069	3.417142	-2.455655
24	1	0	-3.277120	2.178628	-2.606240
25	1	0	-4.294174	4.342997	-1.850178
26	1	0	-4.473193	3.120975	-0.581155
27	1	0	-3.228738	4.370748	-0.436236
28	6	0	-2.179091	-1.663729	1.092857
29	6	0	-2.981956	-2.889224	1.558481
30	1	0	-2.845661	-1.006319	0.515035
31	1	0	-1.878371	-1.083734	1.977944
32	6	0	-4.215530	-2.523407	2.391075
33	1	0	-3.290731	-3.471219	0.678383
34	1	0	-2.323758	-3.547743	2.142993
35	1	0	-4.765472	-3.417324	2.707275
36	1	0	-3.934096	-1.968726	3.294981
37	1	0	-4.906888	-1.892449	1.818627
38	6	0	1.775824	2.031798	0.994719
39	6	0	2.345625	2.725514	2.242620
40	1	0	1.092320	2.728083	0.486092
41	1	0	2.599827	1.851771	0.288159
42	6	0	3.074248	4.036480	1.927439
43	1	0	1.527113	2.920158	2.950313
44	1	0	3.032019	2.035690	2.753730
45	1	0	3.467163	4.505773	2.836831
46	1	0	3.919650	3.867265	1.248756
47	1	0	2.402960	4.757674	1.444522
48	6	0	2.320479	-3.507503	-1.212195
49	1	0	2.945005	-4.227564	-0.674145
50	1	0	1.277951	-3.658983	-0.900905
51	1	0	2.363469	-3.752521	-2.282838

Tributyl(1-methoxyvinyl)stannane (*8*)

E = -669.429763 Hartree
Electronic state: 1-A
Cartesian Coordinates (Angstroms):

1	6	0	-0.262469	-2.121696	0.900417
2	6	0	0.476219	-3.236784	0.770227
3	1	0	1.299319	-3.254337	0.063298
4	6	0	0.222211	1.325585	1.194282
5	6	0	1.880451	-0.520177	-1.362128
6	6	0	-1.639394	-0.016910	-1.537070
7	1	0	-1.448760	0.867612	-2.160444
8	1	0	-1.666193	-0.872367	-2.225878
9	1	0	-0.644433	1.268976	1.865592
10	1	0	1.102831	1.132094	1.821501
11	1	0	1.820388	-1.461686	-1.924952
12	1	0	1.902607	0.278506	-2.116208
13	50	0	0.054888	-0.301350	-0.221347
14	6	0	0.320203	2.726452	0.567036

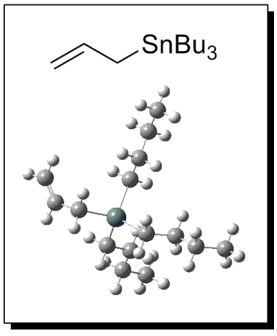


15	6	0	0.452263	3.851565	1.605991
16	1	0	-0.565587	2.923055	-0.055139
17	1	0	1.182103	2.774843	-0.115681
18	6	0	0.550152	5.247221	0.980151
19	1	0	-0.409585	3.812021	2.287167
20	1	0	1.339364	3.662561	2.227017
21	1	0	0.638426	6.025588	1.746952
22	1	0	1.425234	5.327054	0.323048
23	1	0	-0.337444	5.474241	0.376347
24	6	0	3.170053	-0.486645	-0.523721
25	6	0	4.449312	-0.643927	-1.360852
26	1	0	3.143288	-1.281213	0.236066
27	1	0	3.226788	0.459320	0.035045
28	6	0	5.730047	-0.615778	-0.519188
29	1	0	4.397366	-1.588326	-1.921253
30	1	0	4.485741	0.155197	-2.114975
31	1	0	6.623588	-0.728785	-1.144026
32	1	0	5.824150	0.330473	0.028181
33	1	0	5.735893	-1.426353	0.220152
34	6	0	-2.993697	0.122073	-0.820065
35	6	0	-4.181804	0.255439	-1.785994
36	1	0	-2.977126	1.000095	-0.157254
37	1	0	-3.159214	-0.743418	-0.163580
38	6	0	-5.529571	0.399679	-1.070438
39	1	0	-4.017754	1.122960	-2.441305
40	1	0	-4.207205	-0.623388	-2.446013
41	1	0	-6.356157	0.490975	-1.784732
42	1	0	-5.734319	-0.469572	-0.433063
43	1	0	-5.544257	1.289492	-0.428601
44	1	0	0.309439	-4.152319	1.332017
45	8	0	-1.328432	-1.978029	1.757425
46	6	0	-1.674134	-3.087318	2.577034
47	1	0	-1.952352	-3.958795	1.969505
48	1	0	-2.529601	-2.770253	3.176941
49	1	0	-0.842526	-3.365204	3.238114

Allyltributylstannane (*9*)

E = -594.2228542 Hartree
Electronic state: 1-A
Cartesian Coordinates (Angstroms):

1	6	0	1.452902	-1.581404	-1.935226
2	6	0	1.766099	-2.951924	-1.429280
3	6	0	2.915397	-3.345757	-0.867562
4	1	0	0.956809	-3.680878	-1.508909
5	1	0	3.051794	-4.358197	-0.497703
6	1	0	3.763362	-2.670912	-0.764341
7	1	0	0.945347	-1.624638	-2.907321
8	1	0	2.367111	-0.990347	-2.068318
9	6	0	-0.453708	1.352436	-1.573187
10	6	0	-1.560107	-1.726861	-0.084507
11	6	0	1.259870	-0.030595	1.235030
12	1	0	0.560928	0.373495	1.980262
13	1	0	1.617021	-0.986727	1.640650
14	1	0	0.454618	1.805426	-1.994352

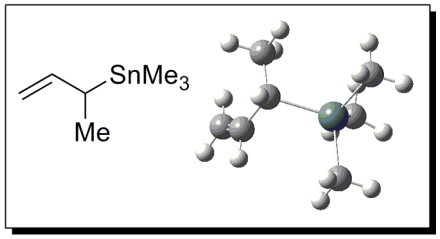


15	1	0	-1.075191	1.073606	-2.435508
16	1	0	-2.120233	-1.921129	-1.009645
17	1	0	-1.165811	-2.699863	0.239393
18	50	0	0.145929	-0.477294	-0.569658
19	6	0	-1.193787	2.385866	-0.706275
20	6	0	-1.546890	3.676846	-1.462437
21	1	0	-0.583777	2.647353	0.170985
22	1	0	-2.120598	1.948892	-0.306316
23	6	0	-2.284008	4.703893	-0.595881
24	1	0	-0.623804	4.123246	-1.858950
25	1	0	-2.162101	3.423193	-2.337549
26	1	0	-2.523181	5.610372	-1.163913
27	1	0	-3.226280	4.294574	-0.210467
28	1	0	-1.676964	5.003158	0.267784
29	6	0	-2.505430	-1.166932	0.992246
30	6	0	-3.671157	-2.110000	1.331605
31	1	0	-2.918282	-0.200950	0.666108
32	1	0	-1.942008	-0.956461	1.913178
33	6	0	-4.611443	-1.549344	2.404255
34	1	0	-4.240830	-2.320200	0.415147
35	1	0	-3.264717	-3.075337	1.665300
36	1	0	-5.428699	-2.245787	2.624660
37	1	0	-4.074322	-1.358810	3.341782
38	1	0	-5.059984	-0.601157	2.082315
39	6	0	2.444929	0.933018	1.052806
40	6	0	3.215708	1.203133	2.355096
41	1	0	2.092165	1.892254	0.645558
42	1	0	3.146062	0.530119	0.306732
43	6	0	4.396450	2.163374	2.174225
44	1	0	2.521240	1.609326	3.104313
45	1	0	3.576362	0.247653	2.761591
46	1	0	4.923876	2.333281	3.120052
47	1	0	5.123651	1.766697	1.454604
48	1	0	4.061062	3.138951	1.800345

But-3-en-2-yltrimethylstannane (*10*)

E = -279.7285755 Hartree
Electronic state: 1-A
Cartesian Coordinates (Angstroms):

1	6	0	1.325776	0.491689	-0.770078
2	50	0	-0.654268	-0.055073	0.022604
3	6	0	2.250009	-0.669459	-0.571210
4	6	0	3.263714	-0.761139	0.299981
5	1	0	1.165149	0.625055	-1.849479
6	1	0	2.046284	-1.534937	-1.205630
7	1	0	3.540284	0.054511	0.962598
8	6	0	-0.479251	-0.266915	2.156589
9	1	0	0.392712	-0.882044	2.400657
10	1	0	-0.356848	0.706527	2.642528
11	1	0	-1.368135	-0.747074	2.578917
12	6	0	-2.073186	1.493010	-0.466958
13	1	0	-2.148664	1.625701	-1.551443
14	1	0	-3.068637	1.238085	-0.087443

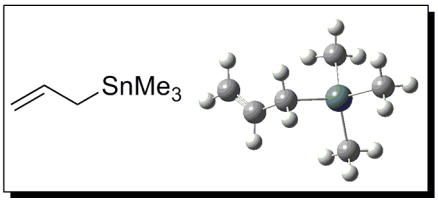


15	1	0	-1.780047	2.451857	-0.027017
16	6	0	-1.294519	-1.912598	-0.860527
17	1	0	-2.287049	-2.194084	-0.492542
18	1	0	-1.350690	-1.830987	-1.951286
19	1	0	-0.600906	-2.723335	-0.615411
20	6	0	1.813560	1.815855	-0.166796
21	1	0	3.860607	-1.665925	0.374113
22	1	0	1.143439	2.642485	-0.429113
23	1	0	2.817741	2.069729	-0.533523
24	1	0	1.871564	1.775445	0.927891

Allyltrimethylstannane (*11*)

E = -240.4191441 Hartree
Electronic state: 1-A
Cartesian Coordinates (Angstroms):

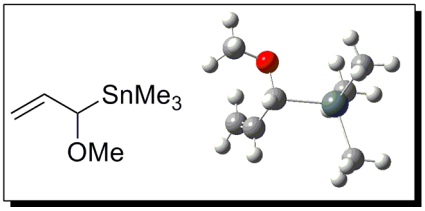
1	6	0	-1.306158	-0.252315	1.163713
2	6	0	-2.485026	-0.551983	0.294938
3	6	0	-3.455464	0.304432	-0.045480
4	1	0	-2.524350	-1.563412	-0.114735
5	1	0	-4.265455	0.013670	-0.708657
6	1	0	-3.477600	1.324866	0.332943
7	1	0	-1.122715	-1.065192	1.877582
8	1	0	-1.464129	0.665642	1.742486
9	6	0	2.194478	0.224105	1.325392
10	6	0	0.805004	-1.706036	-1.273395
11	6	0	0.283086	1.784698	-1.211142
12	1	0	1.059811	1.847618	-1.980326
13	1	0	-0.692428	1.774164	-1.707648
14	1	0	0.341513	2.687630	-0.594374
15	1	0	3.122771	0.378369	0.764940
16	1	0	2.057728	1.079524	1.995281
17	1	0	2.316294	-0.672960	1.941588
18	1	0	0.907435	-2.618852	-0.676988
19	1	0	-0.042900	-1.837327	-1.953440
20	1	0	1.710536	-1.595632	-1.879474
21	50	0	0.517159	0.015290	-0.011267



(1-Methoxyallyl)trimethylstannane (*12*)

E = -354.9264979 Hartree
Electronic state: 1-A
Cartesian Coordinates (Angstroms):

1	6	0	1.229562	0.066230	-0.631684
2	50	0	-0.877435	0.024647	0.014497
3	6	0	1.832047	-1.303355	-0.628639
4	6	0	2.615912	-1.816494	0.326299
5	1	0	1.261583	0.480412	-1.654106
6	1	0	1.555854	-1.921857	-1.485313
7	1	0	2.903955	-1.229158	1.193556
8	6	0	-0.887658	-0.535132	2.086401
9	1	0	-0.388973	-1.499730	2.222235

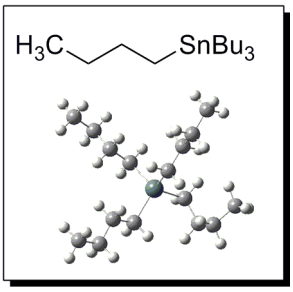


10	1	0	-0.352834	0.211651	2.680749
11	1	0	-1.910287	-0.617207	2.468935
12	6	0	-1.686802	1.997300	-0.264489
13	1	0	-1.744170	2.251968	-1.327922
14	1	0	-2.694224	2.072143	0.158418
15	1	0	-1.049675	2.736259	0.230945
16	6	0	-1.985482	-1.400774	-1.160578
17	1	0	-3.033839	-1.423915	-0.843796
18	1	0	-1.960719	-1.142444	-2.224517
19	1	0	-1.574653	-2.408775	-1.043511
20	1	0	2.993287	-2.832957	0.264849
21	8	0	1.836018	0.977576	0.285533
22	6	0	3.056614	1.528022	-0.186190
23	1	0	3.797746	0.748626	-0.406309
24	1	0	3.440806	2.178174	0.604992
25	1	0	2.894590	2.129062	-1.095033

Tetrabutylstannane (*13*)

E = -634.765664 Hartree
Electronic state: 1-A
Cartesian Coordinates (Angstroms):

1	6	0	1.743407	-0.824710	-1.904400
2	6	0	2.485949	-2.148421	-1.642119
3	6	0	3.276533	-2.218293	-0.324344
4	1	0	1.766511	-2.978676	-1.660957
5	1	0	3.672266	-3.236729	-0.210041
6	1	0	1.283773	-0.862768	-2.901374
7	1	0	2.450542	0.013710	-1.941014
8	6	0	-1.160328	1.072945	-1.606333
9	6	0	-0.944063	-2.110763	0.008551
10	6	0	0.863752	0.652827	1.274344
11	1	0	-0.001085	0.843875	1.924825
12	1	0	1.489515	-0.071493	1.813469
13	1	0	-0.514548	1.808705	-2.106292
14	1	0	-1.645758	0.508079	-2.414876
15	1	0	-1.355745	-2.549468	-0.911142
16	1	0	-0.210577	-2.838009	0.383818
17	50	0	0.134068	-0.303992	-0.533737
18	6	0	-2.226137	1.805577	-0.772963
19	6	0	-3.083442	2.779264	-1.597663
20	1	0	-1.747800	2.365718	0.044142
21	1	0	-2.891539	1.077443	-0.286020
22	6	0	-4.141661	3.510671	-0.764171
23	1	0	-2.424210	3.513394	-2.082669
24	1	0	-3.572816	2.226042	-2.411918
25	1	0	-4.732378	4.199312	-1.379386
26	1	0	-4.837192	2.802786	-0.296127
27	1	0	-3.677755	4.096645	0.039220
28	6	0	-2.065727	-1.928684	1.046039
29	6	0	-2.780661	-3.239867	1.410719
30	1	0	-2.812677	-1.213295	0.671437
31	1	0	-1.658539	-1.482244	1.965300
32	6	0	-3.891680	-3.054992	2.450340

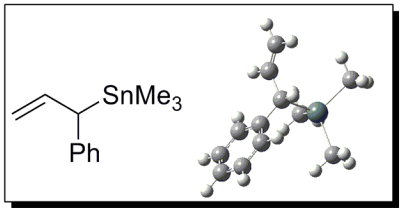


33	1	0	-3.200239	-3.685670	0.497604
34	1	0	-2.039051	-3.958996	1.786916
35	1	0	-4.380851	-4.006475	2.689143
36	1	0	-3.494256	-2.640972	3.385521
37	1	0	-4.664063	-2.365770	2.086705
38	6	0	1.647394	1.958393	1.057449
39	6	0	2.151979	2.593686	2.363204
40	1	0	1.019277	2.690572	0.528310
41	1	0	2.510785	1.774992	0.400357
42	6	0	2.932151	3.894591	2.143600
43	1	0	1.294040	2.784831	3.023375
44	1	0	2.786465	1.868022	2.891673
45	1	0	3.278992	4.319898	3.092516
46	1	0	3.813828	3.726219	1.512499
47	1	0	2.311025	4.650797	1.647317
48	6	0	4.437975	-1.221934	-0.230638
49	1	0	5.139854	-1.357840	-1.063307
50	1	0	4.089598	-0.183225	-0.258015
51	1	0	4.998388	-1.355408	0.701890
52	1	0	2.594555	-2.064115	0.525113
53	1	0	3.185609	-2.342011	-2.470871

Trimethyl (1-phenylallyl)stannane (*14*)

E = -471.4627176 Hartree
Electronic state: 1-A
Cartesian Coordinates (Angstroms):

1	6	0	0.205600	1.052401	-0.509528
2	50	0	-1.311264	-0.472041	0.025824
3	6	0	-0.141296	2.333527	0.187013
4	6	0	-0.809964	3.359735	-0.352635
5	1	0	0.161290	2.411759	1.231586
6	1	0	-1.134957	3.351727	-1.391399
7	1	0	0.069461	1.186717	-1.589967
8	6	0	-1.404239	-0.651292	2.168504
9	6	0	-0.741754	-2.349297	-0.858517
10	6	0	-3.199810	0.199749	-0.754851
11	1	0	-0.796754	-2.299875	-1.951004
12	1	0	-1.403627	-3.153982	-0.520974
13	1	0	0.284642	-2.607022	-0.580507
14	1	0	-1.695239	0.298577	2.628471
15	1	0	-0.433676	-0.949939	2.577030
16	1	0	-2.141486	-1.407910	2.457617
17	1	0	-3.366488	1.247218	-0.484962
18	1	0	-4.025704	-0.395819	-0.351893
19	1	0	-3.223381	0.119013	-1.846629
20	1	0	-1.051411	4.247095	0.225663
21	6	0	1.594387	0.513486	-0.250875
22	6	0	2.369462	0.026328	-1.316791
23	6	0	2.147956	0.444845	1.040307
24	6	0	3.641186	-0.507886	-1.106318
25	1	0	1.969109	0.073680	-2.327410
26	6	0	3.421936	-0.083262	1.252786
27	1	0	1.580165	0.807684	1.893365

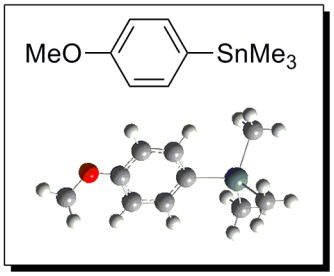


28	6	0	4.176806	-0.564668	0.181411
29	1	0	4.216532	-0.873384	-1.953307
30	1	0	3.824693	-0.119110	2.262038
31	1	0	5.168392	-0.976393	0.348058

(4-Methoxyphenyl) trimethylstannane (*15*)

E = -469.2787401 Hartree
Electronic state: 1-A
Cartesian Coordinates (Angstroms):

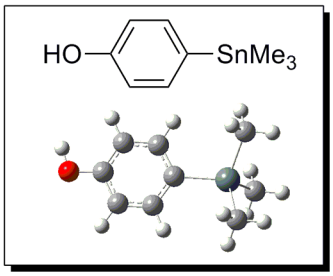
1	6	0	0.363614	-0.099356	-0.003557
2	6	0	1.175247	1.044402	-0.006395
3	6	0	1.022955	-1.345617	0.000277
4	6	0	2.572813	0.971010	-0.000904
5	1	0	0.724032	2.035243	-0.017826
6	6	0	2.409714	-1.443801	0.005685
7	1	0	0.446985	-2.269613	-0.005829
8	6	0	3.195564	-0.281913	0.005998
9	1	0	3.155894	1.885502	-0.004770
10	1	0	2.910440	-2.407588	0.006888
11	50	0	-1.777418	0.042830	0.001367
12	6	0	-2.583517	-1.577205	-1.163299
13	6	0	-2.544960	-0.073407	2.010270
14	6	0	-2.341580	1.929381	-0.867302
15	1	0	-2.236924	-1.518631	-2.200129
16	1	0	-2.279401	-2.548632	-0.758994
17	1	0	-3.678200	-1.543176	-1.167390
18	1	0	-3.637601	0.004068	2.010317
19	1	0	-2.270776	-1.023467	2.480503
20	1	0	-2.145236	0.737403	2.628043
21	1	0	-3.432006	2.023535	-0.907695
22	1	0	-1.955034	2.770252	-0.281584
23	1	0	-1.955003	2.019754	-1.887606
24	8	0	4.546766	-0.479429	0.010622
25	6	0	5.390843	0.659478	0.007782
26	1	0	6.412918	0.275778	0.011376
27	1	0	5.238080	1.274292	-0.889375
28	1	0	5.234461	1.281388	0.899420



4-(Trimethylstannyl) phenol (*16*)

E = -429.9729334 Hartree
Electronic state: 1-A
Cartesian Coordinates (Angstroms):

1	6	0	0.717658	-0.004526	-0.004998
2	6	0	1.455730	1.190821	-0.004570
3	6	0	1.451771	-1.206228	-0.002658
4	6	0	2.851958	1.195664	0.002753
5	1	0	0.943889	2.151560	-0.014975
6	6	0	2.844774	-1.223637	0.004768
7	1	0	0.931759	-2.162673	-0.011437
8	6	0	3.550241	-0.015697	0.008457

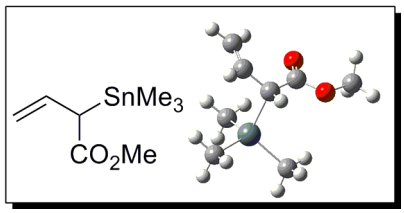


9	1	0	3.398007	2.138383	0.001184
10	1	0	3.400776	-2.156448	0.005052
11	50	0	-1.429194	0.001794	0.000944
12	6	0	-2.129791	-1.730357	-1.065699
13	6	0	-2.184136	-0.048853	2.017431
14	6	0	-2.115560	1.795491	-0.969798
15	1	0	-1.771560	-1.720771	-2.100156
16	1	0	-1.782506	-2.656197	-0.594960
17	1	0	-3.224567	-1.754661	-1.084612
18	1	0	-3.279500	-0.042591	2.018778
19	1	0	-1.847723	-0.951111	2.538625
20	1	0	-1.837397	0.819605	2.587029
21	1	0	-3.210124	1.825132	-0.993112
22	1	0	-1.768306	2.691712	-0.444758
23	1	0	-1.752218	1.843852	-2.001427
24	8	0	4.916191	-0.081472	0.014808
25	1	0	5.273789	0.820242	0.014999

Methyl 2-(trimethylstannyl)but-3-enoate (*17*)

E = -468.2905367 Hartree
Electronic state: 1-A
Cartesian Coordinates (Angstroms):

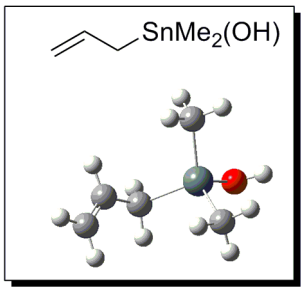
1	6	0	-0.699835	0.708069	-0.841909
2	50	0	1.067475	-0.304793	0.055008
3	6	0	-0.432589	2.185636	-0.828138
4	6	0	-0.822083	3.096338	0.071900
5	1	0	-0.735136	0.330030	-1.867875
6	1	0	0.182086	2.518221	-1.666007
7	1	0	-1.432640	2.833553	0.927981
8	6	0	1.232769	0.383637	2.077367
9	1	0	1.439406	1.457495	2.096127
10	1	0	0.292480	0.210160	2.609181
11	1	0	2.037337	-0.137427	2.606354
12	6	0	0.748924	-2.429049	-0.041597
13	1	0	0.548981	-2.743105	-1.070797
14	1	0	1.631294	-2.969337	0.317760
15	1	0	-0.106619	-2.722230	0.574361
16	6	0	2.767188	0.256677	-1.135038
17	1	0	3.678606	-0.208403	-0.744520
18	1	0	2.641132	-0.064931	-2.173988
19	1	0	2.908241	1.341746	-1.125053
20	1	0	-0.544481	4.139803	-0.050891
21	6	0	-1.902654	0.219138	-0.104397
22	8	0	-2.350770	0.656826	0.939873
23	8	0	-2.441120	-0.867032	-0.726718
24	6	0	-3.565244	-1.457724	-0.060589
25	1	0	-3.290940	-1.794832	0.943409
26	1	0	-3.860953	-2.305352	-0.680359
27	1	0	-4.386293	-0.740405	0.023064



Allyldimethylstannanol (*18*)

E = -276.34729 Hartree
Electronic state: 1-A
Cartesian Coordinates (Angstroms):

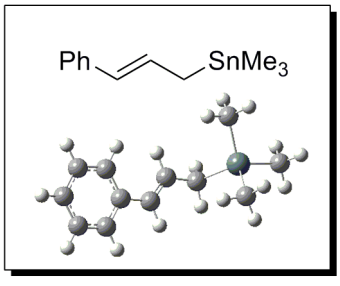
1	6	0	1.337844	-0.251612	-1.094006
2	6	0	2.479193	-0.541689	-0.170637
3	6	0	3.436202	0.319195	0.193224
4	1	0	2.499362	-1.546992	0.254786
5	1	0	4.220984	0.037612	0.889741
6	1	0	3.474275	1.333296	-0.200606
7	1	0	1.178129	-1.070122	-1.806121
8	1	0	1.515369	0.661135	-1.673953
9	6	0	-0.839999	-1.559698	1.407619
10	6	0	-0.576144	1.925076	0.948086
11	1	0	-1.466192	2.033151	1.576403
12	1	0	0.307229	2.041528	1.585018
13	1	0	-0.574809	2.732960	0.209837
14	1	0	-0.849458	-2.536968	0.915097
15	1	0	-0.040997	-1.559171	2.156946
16	1	0	-1.793521	-1.431430	1.930491
17	50	0	-0.518196	0.011291	-0.017972
18	8	0	-1.851977	-0.085290	-1.434931
19	1	0	-2.767321	0.075142	-1.165327



Cinnamyltrimethylstannane (*19*)

E = -471.4752397 Hartree
Electronic state: 1-A
Cartesian Coordinates (Angstroms):

1	6	0	0.792811	-0.471487	-1.468009
2	50	0	2.239988	0.023179	0.099922
3	6	0	-0.575250	0.017324	-1.133763
4	6	0	-1.590279	-0.745328	-0.684299
5	1	0	1.160250	-0.021878	-2.399088
6	1	0	-0.730087	1.091099	-1.246626
7	1	0	-1.419232	-1.819722	-0.597461
8	6	0	-2.939191	-0.305443	-0.301788
9	6	0	-3.899052	-1.276593	0.039492
10	6	0	-3.334390	1.046328	-0.254375
11	6	0	-5.196514	-0.920126	0.404800
12	1	0	-3.617390	-2.327067	0.013453
13	6	0	-4.629785	1.403764	0.108304
14	1	0	-2.619536	1.827365	-0.497696
15	6	0	-5.570765	0.423718	0.440168
16	1	0	-5.915280	-1.694077	0.662004
17	1	0	-4.907292	2.454582	0.136540
18	1	0	-6.580461	0.706525	0.725173
19	1	0	0.807617	-1.560357	-1.596745
20	6	0	2.085630	2.122044	0.555530
21	6	0	4.225423	-0.426806	-0.606827
22	6	0	1.771336	-1.152054	1.839023

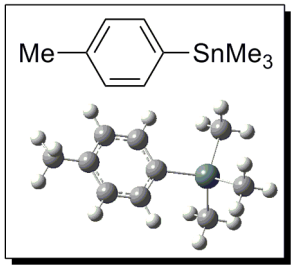


23	1	0	4.318808	-1.485900	-0.868939
24	1	0	4.971331	-0.201664	0.162983
25	1	0	4.466472	0.165662	-1.495663
26	1	0	1.086709	2.365062	0.931710
27	1	0	2.273466	2.732764	-0.333912
28	1	0	2.814341	2.408091	1.321372
29	1	0	0.708444	-1.058807	2.083835
30	1	0	2.352591	-0.821468	2.706127
31	1	0	1.990026	-2.211186	1.667290

Trimethyl(p-tolyl)stannane (*20*)

E = -394.0746097 Hartree
Electronic state: 1-A
Cartesian Coordinates (Angstroms):

1	6	0	-0.700103	-0.002946	-0.001923
2	6	0	-1.434728	-1.202166	-0.005181
3	6	0	-1.433200	1.195284	-0.005199
4	6	0	-2.829833	-1.203346	-0.010291
5	1	0	-0.918855	-2.161526	-0.008010
6	6	0	-2.830107	1.196435	-0.010392
7	1	0	-0.914583	2.152411	-0.007929
8	6	0	-3.552677	-0.002562	-0.009702
9	1	0	-3.367216	-2.150036	-0.016847
10	1	0	-3.367145	2.143233	-0.016962
11	50	0	1.449847	-0.000256	0.001170
12	6	0	2.129041	2.040982	-0.005726
13	6	0	2.174566	-1.003707	1.762648
14	6	0	2.180344	-1.017830	-1.749723
15	1	0	1.777942	2.572781	-0.896239
16	1	0	1.771381	2.581088	0.877146
17	1	0	3.223558	2.077769	-0.001785
18	1	0	3.269272	-1.039820	1.765314
19	1	0	1.847869	-0.480697	2.667275
20	1	0	1.801457	-2.032025	1.813187
21	1	0	3.274994	-1.055591	-1.747609
22	1	0	1.805971	-2.045964	-1.794192
23	1	0	1.858147	-0.501083	-2.659543
24	6	0	-5.063797	-0.004833	0.015888
25	1	0	-5.474116	-0.846636	-0.552992
26	1	0	-5.473679	0.919811	-0.404318
27	1	0	-5.444369	-0.092766	1.042636

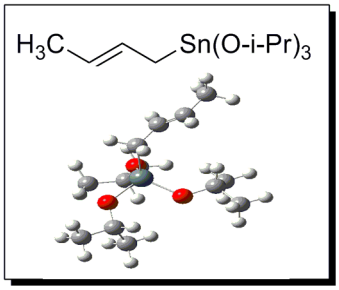


But-2-enyltriisopropoxystannane (*21*)

E = -741.3388885 Hartree
Electronic state: 1-A
Cartesian Coordinates (Angstroms):

1	6	0	-1.342399	-0.142737	-2.005998
2	50	0	0.132523	-0.046465	-0.452722
3	8	0	1.908472	-0.414694	-1.081640
4	8	0	-0.107285	-1.326760	0.969117

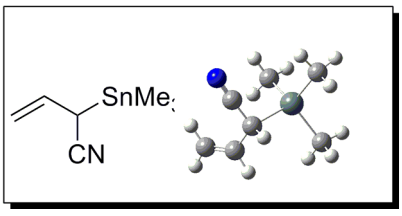
5	8	0	0.043171	1.758648	0.200508
6	6	0	-2.664400	0.420105	-1.575121
7	6	0	-3.796564	-0.281224	-1.438213
8	1	0	-0.918185	0.426643	-2.842876
9	1	0	-2.676844	1.487926	-1.351732
10	1	0	-3.784471	-1.349574	-1.664609
11	6	0	-5.114935	0.289344	-0.998679
12	1	0	-1.430975	-1.186177	-2.327794
13	1	0	-5.889430	0.138607	-1.763133
14	1	0	-5.478452	-0.200005	-0.084544
15	1	0	-5.040902	1.363872	-0.799454
16	6	0	1.077788	2.450995	0.910680
17	6	0	-1.300189	-1.504592	1.741978
18	6	0	2.744113	-1.488720	-0.626360
19	1	0	1.576771	1.761728	1.611174
20	1	0	2.154817	-2.416588	-0.564324
21	1	0	-2.178049	-1.503037	1.075447
22	6	0	3.841013	-1.673208	-1.672972
23	6	0	3.309377	-1.188077	0.762852
24	6	0	-1.204115	-2.873486	2.412397
25	6	0	-1.459235	-0.371058	2.757925
26	6	0	0.410082	3.560860	1.720404
27	6	0	2.121360	2.992969	-0.068601
28	1	0	-0.320840	3.141695	2.419583
29	1	0	-0.114499	4.251465	1.050021
30	1	0	1.153273	4.128737	2.292802
31	1	0	2.577471	2.173531	-0.633910
32	1	0	2.915474	3.532884	0.461768
33	1	0	1.648070	3.682988	-0.777159
34	1	0	4.503781	-2.503528	-1.401862
35	1	0	4.441961	-0.760292	-1.755395
36	1	0	3.403032	-1.882752	-2.654305
37	1	0	2.498053	-1.099503	1.493092
38	1	0	3.879560	-0.251668	0.746238
39	1	0	3.976762	-1.992419	1.095826
40	1	0	-0.601645	-0.356519	3.440802
41	1	0	-1.508720	0.599908	2.252537
42	1	0	-2.373246	-0.497977	3.350582
43	1	0	-2.103480	-3.084798	3.002950
44	1	0	-0.334290	-2.905928	3.078471
45	1	0	-1.087416	-3.660555	1.660293



2-(trimethylstannyl)but-3-enenitrile (*22*)

E = -332.6587185 Hartree
Electronic state: 1-A
Cartesian Coordinates (Angstroms):

1	6	0	1.263282	0.046715	-0.875482
2	50	0	-0.769543	-0.029826	0.044396
3	6	0	2.011041	-1.223455	-0.569015
4	6	0	3.005492	-1.372933	0.310354
5	1	0	1.093723	0.141768	-1.955267
6	1	0	1.655104	-2.090470	-1.125310
7	1	0	3.401342	-0.535441	0.879131

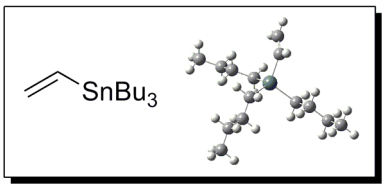


8	6	0	-0.464024	-0.096675	2.162581
9	1	0	0.198527	-0.927555	2.422641
10	1	0	-0.001429	0.832744	2.507844
11	1	0	-1.412538	-0.229859	2.692640
12	6	0	-1.805070	1.740314	-0.585751
13	1	0	-2.001537	1.717992	-1.662368
14	1	0	-2.763760	1.835410	-0.065369
15	1	0	-1.203691	2.626961	-0.362965
16	6	0	-1.714480	-1.810919	-0.699086
17	1	0	-2.728668	-1.900696	-0.295687
18	1	0	-1.786196	-1.791712	-1.791427
19	1	0	-1.153229	-2.703461	-0.405766
20	1	0	3.462935	-2.343582	0.476683
21	6	0	1.898684	1.257053	-0.388525
22	7	0	2.363856	2.231230	0.047852

Tributyl(vinyl)stannane (*23*)

E = -554.906023 Hartree
Electronic state: 1-A
Cartesian Coordinates (Angstroms):

1	6	0	-0.101261	-2.084823	1.728120
2	6	0	0.752948	-3.112964	1.811127
3	1	0	1.555364	-3.267626	1.089857
4	1	0	-0.871261	-2.013828	2.500080
5	6	0	0.010143	1.358763	1.145106
6	6	0	1.731609	-0.913265	-1.013726
7	6	0	-1.796774	-0.752786	-1.059639
8	1	0	-1.715100	0.001456	-1.854784
9	1	0	-1.755237	-1.727704	-1.564078
10	1	0	-0.835990	1.412652	1.844049
11	1	0	0.914102	1.404504	1.767239
12	1	0	1.785972	-1.985247	-1.249483
13	1	0	1.570821	-0.406056	-1.974992
14	50	0	-0.037028	-0.589059	0.195301
15	6	0	-0.028766	2.559146	0.184717
16	6	0	-0.007460	3.916796	0.904947
17	1	0	-0.929185	2.507961	-0.445318
18	1	0	0.824340	2.514338	-0.508862
19	6	0	-0.054412	5.113057	-0.051788
20	1	0	-0.858144	3.966276	1.599510
21	1	0	0.896484	3.977409	1.527552
22	1	0	-0.038247	6.063780	0.493499
23	1	0	0.803125	5.107534	-0.736177
24	1	0	-0.964807	5.096107	-0.663934
25	6	0	3.058126	-0.445415	-0.391604
26	6	0	4.275272	-0.694485	-1.296493
27	1	0	3.222134	-0.951847	0.570977
28	1	0	3.005351	0.628404	-0.159102
29	6	0	5.594592	-0.207073	-0.687952
30	1	0	4.344888	-1.769276	-1.517028
31	1	0	4.109635	-0.196742	-2.262685
32	1	0	6.440895	-0.400884	-1.357087
33	1	0	5.565844	0.872098	-0.492132

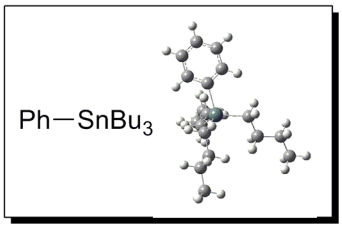


34	1	0	5.802243	-0.709346	0.265143
35	6	0	-3.140649	-0.598242	-0.328008
36	6	0	-4.358969	-0.708106	-1.258867
37	1	0	-3.178486	0.373015	0.187679
38	1	0	-3.228874	-1.360994	0.459677
39	6	0	-5.696761	-0.545096	-0.529167
40	1	0	-4.274878	0.051820	-2.048785
41	1	0	-4.332790	-1.681316	-1.769284
42	1	0	-6.543825	-0.633073	-1.219275
43	1	0	-5.820286	-1.309435	0.248214
44	1	0	-5.765850	0.435259	-0.041306
45	1	0	0.697309	-3.859339	2.605137

Tributyl(phenyl)stannane (*24*)

E = -708.561046 Hartree
Electronic state: 1-A
Cartesian Coordinates (Angstroms):

1	6	0	0.788772	0.568599	1.783472
2	6	0	1.066009	-2.098570	-0.576120
3	6	0	-0.110806	1.059730	-1.641693
4	1	0	0.926225	1.308977	-1.905302
5	1	0	-0.522401	0.537570	-2.516704
6	1	0	0.009998	1.190506	2.245686
7	1	0	1.000927	-0.233203	2.504461
8	1	0	1.044092	-2.806449	0.263692
9	1	0	0.517391	-2.586725	-1.393418
10	50	0	-0.063033	-0.341512	0.009667
11	6	0	2.056888	1.410026	1.554948
12	6	0	2.615011	2.032299	2.844661
13	1	0	1.847497	2.215961	0.836186
14	1	0	2.842418	0.794122	1.092911
15	6	0	3.874401	2.875244	2.615742
16	1	0	1.835231	2.652338	3.309394
17	1	0	2.834398	1.230292	3.563952
18	1	0	4.247378	3.302037	3.553962
19	1	0	4.681378	2.272589	2.180383
20	1	0	3.675942	3.706730	1.927867
21	6	0	2.519344	-1.834130	-1.005087
22	6	0	3.274106	-3.106601	-1.421427
23	1	0	3.070868	-1.351049	-0.184840
24	1	0	2.540325	-1.120086	-1.841709
25	6	0	4.723790	-2.841889	-1.842997
26	1	0	3.257643	-3.821408	-0.586433
27	1	0	2.732337	-3.590731	-2.246422
28	1	0	5.232651	-3.768587	-2.132610
29	1	0	4.769925	-2.155994	-2.698136
30	1	0	5.298202	-2.388664	-1.025303
31	6	0	-0.911742	2.346263	-1.376828
32	6	0	-0.932308	3.310146	-2.573684
33	1	0	-0.495747	2.873805	-0.505428
34	1	0	-1.947023	2.092524	-1.106937
35	6	0	-1.726717	4.592972	-2.303568
36	1	0	0.101397	3.566797	-2.846328

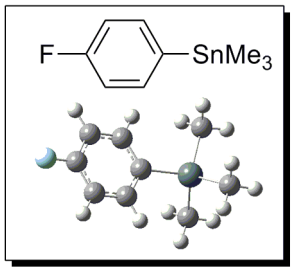


37	1	0	-1.356183	2.790418	-3.444828
38	1	0	-1.724409	5.257952	-3.175073
39	1	0	-2.772229	4.367534	-2.059242
40	1	0	-1.303387	5.150272	-1.458552
41	6	0	-2.085985	-0.917227	0.478105
42	6	0	-3.024789	-1.176205	-0.537299
43	6	0	-2.515680	-1.055907	1.810100
44	6	0	-4.334253	-1.560768	-0.238310
45	1	0	-2.740481	-1.076380	-1.583999
46	6	0	-3.823590	-1.440724	2.117529
47	1	0	-1.825743	-0.859751	2.629204
48	6	0	-4.736139	-1.694563	1.092184
49	1	0	-5.040365	-1.754325	-1.042426
50	1	0	-4.130050	-1.540430	3.156185
51	1	0	-5.754457	-1.993217	1.328107

(4-fluorophenyl)trimethylstannane (*25*)

E = -453.9905587Hartree
Electronic state: 1-A
Cartesian Coordinates (Angstroms):

1	6	0	-0.726852	-0.003784	-0.000208
2	6	0	-1.458359	-1.205720	-0.000037
3	6	0	-1.457578	1.197506	-0.000275
4	6	0	-2.854466	-1.219229	0.000160
5	1	0	-0.940847	-2.163524	-0.000136
6	6	0	-2.854766	1.210896	-0.000083
7	1	0	-0.937162	2.153035	-0.000563
8	6	0	-3.529153	-0.003725	0.000157
9	1	0	-3.419530	-2.146084	0.000277
10	1	0	-3.419562	2.137922	-0.000151
11	50	0	1.425342	-0.000196	0.000002
12	6	0	2.094774	2.043294	-0.012102
13	6	0	2.146275	-1.000218	1.763734
14	6	0	2.145629	-1.021485	-1.751710
15	1	0	1.739723	2.572564	-0.902525
16	1	0	1.738819	2.583532	0.871348
17	1	0	3.189134	2.083457	-0.011707
18	1	0	3.241009	-1.033464	1.768474
19	1	0	1.816568	-0.477110	2.667138
20	1	0	1.776080	-2.029544	1.814416
21	1	0	3.240347	-1.055098	-1.756438
22	1	0	1.775254	-2.051281	-1.789831
23	1	0	1.815731	-0.509273	-2.661261
24	9	0	-4.879521	-0.004508	0.000336

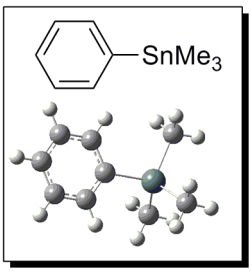


Trimethyl(phenyl)stannane (26*)*

E = -354.7571045 Hartree
Electronic state: 1-A
Cartesian Coordinates (Angstroms):

1	6	0	-1.060715	-0.003687	-0.000128

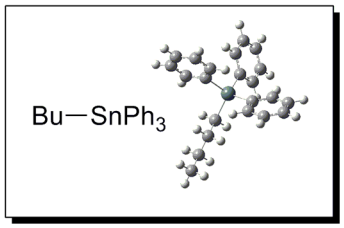
2	6	0	-1.788740	-1.207233	0.000088
3	6	0	-1.789853	1.198081	-0.000168
4	6	0	-3.185437	-1.212750	0.000321
5	1	0	-1.266486	-2.163057	-0.000012
6	6	0	-3.187642	1.201098	0.000058
7	1	0	-1.266336	2.152449	-0.000462
8	6	0	-3.888267	-0.005956	0.000325
9	1	0	-3.724961	-2.156958	0.000472
10	1	0	-3.728488	2.144557	-0.000001
11	1	0	-4.975394	-0.007093	0.000533
12	50	0	1.091818	0.000247	-0.000010
13	6	0	1.768437	2.041995	-0.012077
14	6	0	1.816285	-1.000271	1.762810
15	6	0	1.815290	-1.021398	-1.751025
16	1	0	1.413990	2.572058	-0.902285
17	1	0	1.413235	2.582984	0.871229
18	1	0	2.862915	2.079753	-0.011772
19	1	0	2.911022	-1.034832	1.765877
20	1	0	1.488509	-0.476764	2.666728
21	1	0	1.444582	-2.029033	1.814066
22	1	0	2.910007	-1.056254	-1.754508
23	1	0	1.443426	-2.050649	-1.789635
24	1	0	1.486929	-0.508770	-2.660945



Butyltriphenylstannane (27*)*

E = -856.1475506 Hartree
Electronic state: 1-A
Cartesian Coordinates (Angstroms):

1	50	0	-0.112230	0.002492	0.258265
2	6	0	-2.209347	-0.010227	0.715000
3	6	0	-2.762073	-0.962788	1.590412
4	6	0	-3.076415	0.936644	0.142234
5	6	0	-4.129562	-0.975277	1.877276
6	1	0	-2.125070	-1.708596	2.063804
7	6	0	-4.444337	0.930190	0.427611
8	1	0	-2.683468	1.693303	-0.533828
9	6	0	-4.973392	-0.027471	1.294800
10	1	0	-4.534945	-1.721669	2.556261
11	1	0	-5.096212	1.672731	-0.026375
12	1	0	-6.037413	-0.034280	1.517528
13	6	0	0.384379	1.811375	-0.784779
14	6	0	0.508099	1.833722	-2.185257
15	6	0	0.592890	3.015188	-0.087746
16	6	0	0.823768	3.013538	-2.864777
17	1	0	0.364403	0.919633	-2.757705
18	6	0	0.908376	4.197519	-0.761657
19	1	0	0.511610	3.040245	0.997758
20	6	0	1.023946	4.197822	-2.153316
21	1	0	0.914710	3.007331	-3.948341
22	1	0	1.065462	5.116346	-0.201760
23	1	0	1.270292	5.116385	-2.679992
24	6	0	0.327927	-1.656584	-1.032991
25	6	0	-0.608149	-2.685304	-1.237589

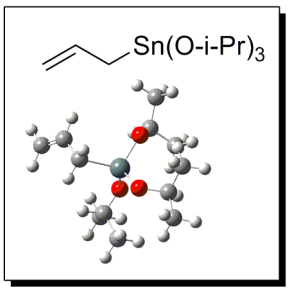


26	6	0	1.570504	-1.759210	-1.685345
27	6	0	-0.314668	-3.777373	-2.058782
28	1	0	-1.583181	-2.637005	-0.756826
29	6	0	1.868354	-2.848432	-2.508316
30	1	0	2.319751	-0.979393	-1.561377
31	6	0	0.925115	-3.860931	-2.695094
32	1	0	-1.054752	-4.560778	-2.203837
33	1	0	2.834690	-2.905757	-3.003650
34	1	0	1.154488	-4.709237	-3.335102
35	6	0	1.036417	-0.117888	2.085183
36	6	0	2.553890	-0.249022	1.875224
37	1	0	0.659234	-0.970799	2.665194
38	1	0	0.810298	0.776735	2.681244
39	6	0	3.346109	-0.322807	3.190238
40	1	0	2.770137	-1.146707	1.278308
41	1	0	2.924119	0.602725	1.285862
42	6	0	4.858216	-0.454538	2.977584
43	1	0	3.134807	0.575624	3.787531
44	1	0	2.981285	-1.174451	3.781930
45	1	0	5.394463	-0.501864	3.932440
46	1	0	5.101509	-1.363528	2.413565
47	1	0	5.255018	0.399517	2.414632

Allyltriisopropoxystannane (28*)*

E = -702.0196833 Hartree
Electronic state: 1-A
Cartesian Coordinates (Angstroms):

1	8	0	-1.532419	-0.893114	-0.965779
2	8	0	-0.294932	1.830176	0.025191
3	8	0	0.840726	-0.734649	1.140818
4	6	0	0.043705	2.429017	1.285581
5	6	0	-2.800834	-0.770659	-0.308296
6	6	0	1.466317	-2.018044	1.225904
7	1	0	1.070644	2.147567	1.564106
8	1	0	-2.652938	-0.718924	0.782746
9	1	0	2.095266	-2.187707	0.334477
10	6	0	1.364082	-0.096025	-2.187813
11	6	0	2.572577	0.777239	-2.043761
12	1	0	2.384321	1.851233	-2.060568
13	1	0	1.636179	-1.146224	-2.338537
14	6	0	3.825814	0.344069	-1.878975
15	1	0	4.067862	-0.716806	-1.854399
16	1	0	4.655329	1.036137	-1.766467
17	1	0	0.738587	0.209940	-3.034523
18	50	0	0.086229	0.016416	-0.466515
19	6	0	-0.015960	3.942112	1.087715
20	6	0	-3.513880	0.502749	-0.767924
21	6	0	2.373791	-2.001356	2.454078
22	1	0	3.114454	-1.199652	2.370341
23	1	0	2.901508	-2.955924	2.566050
24	1	0	1.777987	-1.824108	3.356718
25	1	0	0.263614	4.467922	2.008274
26	1	0	0.666543	4.250901	0.289229

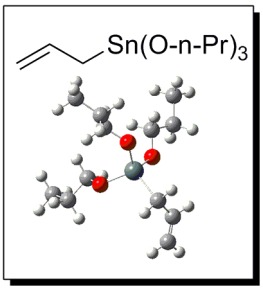


27	1	0	-1.030510	4.246825	0.806312
28	1	0	-2.905882	1.384790	-0.540913
29	1	0	-4.485039	0.611718	-0.269563
30	1	0	-3.682761	0.467649	-1.850692
31	6	0	0.411764	-3.125443	1.295219
32	6	0	-3.601203	-2.032189	-0.626334
33	6	0	-0.900973	1.948507	2.388596
34	1	0	-1.939346	2.188286	2.130626
35	1	0	-0.807943	0.865862	2.526745
36	1	0	-0.662670	2.431673	3.344007
37	1	0	-4.585456	-2.002589	-0.143903
38	1	0	-3.746290	-2.121888	-1.708991
39	1	0	-3.069753	-2.923711	-0.277557
40	1	0	-0.213273	-2.991309	2.185650
41	1	0	-0.240899	-3.096163	0.415207
42	1	0	0.880809	-4.115450	1.345589

Allyltripropoxystannane (29*)*

E = -702.0039612 Hartree
Electronic state: 1-A
Cartesian Coordinates (Angstroms):

1	50	0	-0.210855	-0.031255	-0.704153
2	8	0	-0.537955	-1.615309	0.333551
3	6	0	-1.296888	-0.068788	-2.542281
4	8	0	-0.741415	1.508925	0.320149
5	6	0	0.166806	2.274739	1.107192
6	6	0	-0.735929	-1.619637	1.745656
7	1	0	0.238560	-1.613013	2.261451
8	1	0	-1.281153	-0.721167	2.073668
9	1	0	0.434632	1.725923	2.025634
10	1	0	1.103843	2.461633	0.559374
11	6	0	-0.486392	3.602119	1.480930
12	6	0	-1.513916	-2.870274	2.144793
13	1	0	-2.478462	-2.861671	1.621516
14	1	0	-0.966733	-3.748799	1.780144
15	1	0	-0.755153	4.128405	0.556101
16	1	0	-1.426795	3.389158	2.004766
17	6	0	0.420583	4.480617	2.349053
18	6	0	-1.729714	-2.967810	3.658895
19	1	0	0.682434	3.979378	3.289224
20	1	0	-0.071869	5.425312	2.603871
21	1	0	1.356774	4.723913	1.831295
22	1	0	-0.774358	-3.000159	4.197536
23	1	0	-2.288015	-3.873129	3.920838
24	1	0	-2.295298	-2.107868	4.038801
25	8	0	1.677339	0.077987	-1.054201
26	6	0	2.671192	-0.532439	-0.234804
27	1	0	2.902136	0.119146	0.624162
28	1	0	2.314256	-1.490823	0.173355
29	6	0	3.936030	-0.761106	-1.057369
30	1	0	3.682722	-1.402309	-1.911392
31	6	0	-2.701417	0.428170	-2.371001

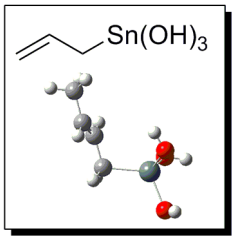


32	1	0	-2.805996	1.490138	-2.148681
33	6	0	-3.798966	-0.329350	-2.448160
34	1	0	-4.789560	0.091587	-2.301602
35	1	0	-3.747005	-1.395303	-2.660928
36	1	0	-1.276847	-1.098017	-2.916286
37	1	0	-0.728133	0.554221	-3.243293
38	6	0	5.066672	-1.390579	-0.236678
39	1	0	5.353414	-0.750695	0.607235
40	1	0	5.959935	-1.547451	-0.851004
41	1	0	4.770151	-2.364626	0.172026
42	1	0	4.257124	0.202154	-1.473518

But-2-enylstannanetriol (30*)*

E = -387.5229021 Hartree
Electronic state: 1-A
Cartesian Coordinates (Angstroms):

1	6	0	0.794727	-0.777940	-1.111112
2	50	0	-0.865187	-0.005717	-0.003614
3	8	0	-2.468959	0.356634	-0.994067
4	8	0	-0.472861	1.717424	0.763985
5	8	0	-1.245944	-1.315415	1.344584
6	1	0	0.452989	1.828378	1.025826
7	1	0	-2.044760	-1.151907	1.866754
8	1	0	-2.691923	1.300269	-0.993171
9	6	0	2.043377	-0.704788	-0.281969
10	6	0	3.024633	0.195204	-0.429416
11	1	0	0.550987	-1.809116	-1.389292
12	1	0	2.124619	-1.441796	0.518958
13	1	0	2.947568	0.930979	-1.232989
14	6	0	4.262574	0.266736	0.419140
15	1	0	0.882191	-0.189867	-2.030839
16	1	0	5.168159	0.131655	-0.187800
17	1	0	4.359274	1.245564	0.908807
18	1	0	4.260470	-0.502754	1.198554

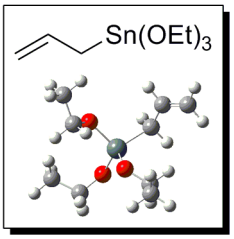


Allyltriethoxystannane (31*)*

E = -584.0642206 Hartree
Electronic state: 1-A
Cartesian Coordinates (Angstroms):

1	8	0	-1.354993	-1.162127	-1.291798
2	8	0	-0.801403	1.566611	0.264333
3	8	0	0.557157	-0.959500	1.186430
4	6	0	-1.170917	1.775533	1.628214
5	6	0	-2.523838	-1.701847	-0.680937
6	6	0	1.555288	-1.975159	1.191057
7	1	0	-2.176897	1.364890	1.808522
8	1	0	-0.481879	1.253731	2.306137
9	1	0	-2.314445	-2.041985	0.345224
10	1	0	-2.800106	-2.592030	-1.261299
11	1	0	1.186307	-2.882624	0.687360

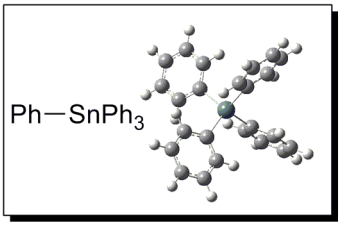
12	1	0	2.454832	-1.643253	0.647382
13	6	0	1.430655	0.401790	-1.879458
14	6	0	2.456564	1.358747	-1.352579
15	1	0	2.091579	2.358798	-1.117187
16	1	0	1.883875	-0.534702	-2.221186
17	6	0	3.743275	1.070859	-1.136677
18	1	0	4.156965	0.088049	-1.355292
19	1	0	4.431418	1.810985	-0.738567
20	1	0	0.876490	0.828432	-2.724637
21	50	0	-0.050647	-0.063993	-0.408088
22	6	0	-1.167785	3.270169	1.917150
23	6	0	-3.677597	-0.703310	-0.678638
24	6	0	1.920225	-2.300760	2.632616
25	1	0	2.308976	-1.410251	3.137550
26	1	0	2.683852	-3.086961	2.671185
27	1	0	1.036332	-2.645802	3.179289
28	1	0	-1.479148	3.463657	2.950968
29	1	0	-0.165644	3.687864	1.771602
30	1	0	-1.856139	3.790957	1.243089
31	1	0	-3.416713	0.192467	-0.102994
32	1	0	-4.577792	-1.148846	-0.237260
33	1	0	-3.910824	-0.389722	-1.701681



Tetraphenylstannane (32*)*

E = -929.940112 Hartree
Electronic state: 1-A
Cartesian Coordinates (Angstroms):

1	50	0	0.001016	-0.004099	-0.003494
2	6	0	1.177261	1.213759	1.309915
3	6	0	0.812057	2.544672	1.577223
4	6	0	2.325634	0.703853	1.941582
5	6	0	1.561514	3.337069	2.450279
6	1	0	-0.063261	2.975778	1.095355
7	6	0	3.077701	1.492523	2.816579
8	1	0	2.650776	-0.316221	1.745416
9	6	0	2.695080	2.810593	3.072939
10	1	0	1.262854	4.364816	2.641997
11	1	0	3.962825	1.079491	3.294348
12	1	0	3.279861	3.425850	3.752102
13	6	0	1.325654	-1.263441	-1.120831
14	6	0	2.558747	-0.780327	-1.593890
15	6	0	0.978766	-2.592839	-1.417547
16	6	0	3.411302	-1.593439	-2.345619
17	1	0	2.870171	0.238009	-1.368098
18	6	0	1.828788	-3.409856	-2.167158
19	1	0	0.038098	-3.003098	-1.055580
20	6	0	3.046020	-2.909782	-2.634290
21	1	0	4.360481	-1.200681	-2.702119
22	1	0	1.542527	-4.436123	-2.383961
23	1	0	3.708673	-3.544111	-3.217594
24	6	0	-1.367865	-1.199230	1.132674
25	6	0	-2.501226	-1.775543	0.531630
26	6	0	-1.148554	-1.443641	2.499527

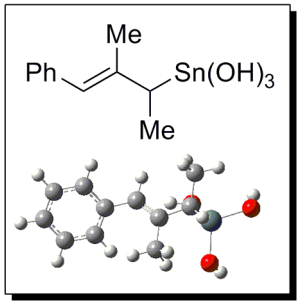


27	6	0	-3.379910	-2.575247	1.267439
28	1	0	-2.714057	-1.594317	-0.520301
29	6	0	-2.024918	-2.241658	3.239267
30	1	0	-0.287977	-1.003552	2.999418
31	6	0	-3.141323	-2.810441	2.622875
32	1	0	-4.250941	-3.010984	0.784004
33	1	0	-1.837783	-2.417322	4.295830
34	1	0	-3.824529	-3.431147	3.197079
35	6	0	-1.133630	1.241105	-1.327470
36	6	0	-0.646066	1.575723	-2.602726
37	6	0	-2.378761	1.765302	-0.937162
38	6	0	-1.371938	2.410128	-3.456253
39	1	0	0.308034	1.177435	-2.942676
40	6	0	-3.107773	2.601504	-1.787271
41	1	0	-2.796273	1.514543	0.036177
42	6	0	-2.603815	2.925959	-3.048245
43	1	0	-0.977874	2.655058	-4.439580
44	1	0	-4.068851	2.996057	-1.466454
45	1	0	-3.170032	3.575015	-3.711462

(3-methyl-4-phenylbut-3-en-2-yl)stannanetriol (33*)*

E = -657.8840274 Hartree
Electronic state: 1-A
Cartesian Coordinates (Angstroms):

1	6	0	0.876749	1.072025	0.999810
2	50	0	2.149610	-0.203787	-0.180943
3	8	0	3.961102	0.398916	-0.393498
4	8	0	1.538031	-0.297364	-2.007141
5	8	0	2.165802	-1.937275	0.648768
6	1	0	0.574871	-0.342614	-2.100718
7	1	0	2.807383	-2.563221	0.281300
8	1	0	4.177322	0.609816	-1.314879
9	6	0	-0.500059	0.439500	1.011138
10	6	0	-1.464242	0.844590	0.152500
11	1	0	1.287752	1.039498	2.015978
12	1	0	-1.245176	1.708446	-0.473554
13	6	0	-2.828585	0.312848	-0.036089
14	6	0	-3.872071	1.214680	-0.321079
15	6	0	-3.138909	-1.059816	-0.008393
16	6	0	-5.176037	0.770874	-0.529222
17	1	0	-3.651276	2.278732	-0.367506
18	6	0	-4.444056	-1.505748	-0.219092
19	1	0	-2.347485	-1.785962	0.148467
20	6	0	-5.469974	-0.593933	-0.473597
21	1	0	-5.963588	1.490328	-0.738093
22	1	0	-4.656030	-2.571626	-0.196464
23	1	0	-6.485355	-0.943388	-0.639666
24	6	0	0.986180	2.508804	0.462644
25	1	0	0.302711	3.174810	1.003930
26	1	0	2.006310	2.886872	0.588983
27	1	0	0.742673	2.580661	-0.603366
28	6	0	-0.675099	-0.652939	2.042291
29	1	0	-1.716902	-0.958993	2.148866



30	1	0	-0.071525	-1.539187	1.803961
31	1	0	-0.325044	-0.294355	3.019417

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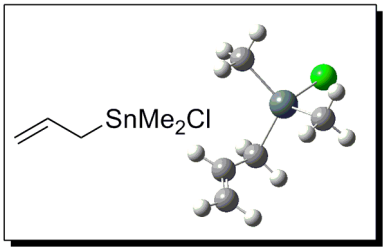
allylchlorodimethylstannane (34*)*

E = -660.7526183 Hartree
Electronic state: 1-A
Cartesian Coordinates (Angstroms):

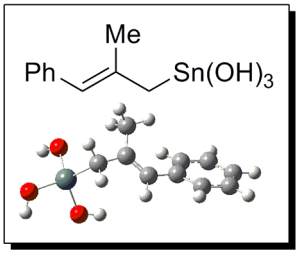
1	6	0	-1.324850	-1.254538	-0.234488
2	6	0	-2.607583	-0.547129	-0.543647
3	6	0	-3.590578	-0.290268	0.327160
4	1	0	-2.718000	-0.193441	-1.570282
5	1	0	-4.485742	0.249327	0.031463
6	1	0	-3.541296	-0.623957	1.362031
7	1	0	-1.032871	-1.942146	-1.035523
8	1	0	-1.392223	-1.828662	0.695778
9	6	0	0.433293	1.527016	-1.649263
10	6	0	0.172441	1.177616	1.898781
11	1	0	0.976843	1.913282	1.987567
12	1	0	-0.788299	1.692527	2.001424
13	1	0	0.271309	0.454522	2.713192
14	1	0	0.565962	0.969855	-2.580986
15	1	0	-0.470589	2.139652	-1.732024
16	1	0	1.293140	2.190010	-1.517462
17	50	0	0.272415	0.188009	0.008488
18	17	0	2.306158	-1.064566	0.025244



(2-methyl-3-phenylallyl)stannanetriol (35*)*

E = -618.574524 Hartree
Electronic state: 1-A
Cartesian Coordinates (Angstroms):

1	6	0	-0.867197	-0.302627	1.512261
2	50	0	-2.231679	-0.093178	-0.124681
3	8	0	-3.993503	-0.803716	0.143838
4	8	0	-1.637560	-1.056921	-1.682582
5	8	0	-2.364260	1.790470	-0.471955
6	1	0	-0.678080	-1.055137	-1.815063
7	1	0	-3.027818	2.046701	-1.129177
8	1	0	-4.193605	-1.538206	-0.456564
9	6	0	0.490185	0.236236	1.134134
10	6	0	1.451344	-0.612766	0.704486
11	1	0	-1.293313	0.222030	2.374410
12	1	0	1.218374	-1.678318	0.753282
13	6	0	2.813552	-0.320410	0.221030
14	6	0	3.849377	-1.222204	0.533196
15	6	0	3.131211	0.787354	-0.587354
16	6	0	5.153294	-1.007691	0.092618
17	1	0	3.622705	-2.096197	1.139677
18	6	0	4.436525	1.002260	-1.030430
19	1	0	2.345542	1.468892	-0.897823
20	6	0	5.455036	0.111013	-0.688174

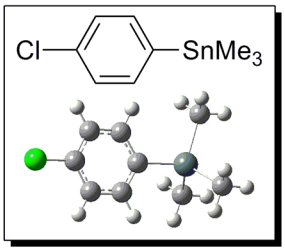


21	1	0	5.934671	-1.715739	0.356370
22	1	0	4.654440	1.863537	-1.656725
23	1	0	6.470461	0.278772	-1.036611
24	6	0	0.642537	1.732221	1.271025
25	1	0	1.679946	2.055813	1.172387
26	1	0	0.032006	2.269738	0.532438
27	1	0	0.278700	2.049325	2.257376
28	1	0	-0.832649	-1.371314	1.748920

(4-chlorophenyl)trimethylstannane (36*)*

E = -814.3505244 Hartree
Electronic state: 1-A
Cartesian Coordinates (Angstroms):

1	6	0	-0.381938	-0.003076	-0.000258
2	6	0	-1.114067	-1.203442	-0.000119
3	6	0	-1.112804	1.196939	-0.000330
4	6	0	-2.510284	-1.216655	0.000045
5	1	0	-0.598400	-2.162304	-0.000218
6	6	0	-2.510115	1.210506	-0.000168
7	1	0	-0.593903	2.153367	-0.000597
8	6	0	-3.195399	-0.002499	0.000042
9	1	0	-3.060478	-2.152171	0.000141
10	1	0	-3.059695	2.146394	-0.000235
11	50	0	1.773418	-0.000187	0.000013
12	6	0	2.438292	2.044157	-0.012100
13	6	0	2.485564	-1.002205	1.765405
14	6	0	2.485147	-1.023530	-1.753217
15	1	0	2.082062	2.572428	-0.902608
16	1	0	2.081148	2.583396	0.871444
17	1	0	3.532525	2.086809	-0.011713
18	1	0	3.580185	-1.036586	1.774510
19	1	0	2.152706	-0.479551	2.667854
20	1	0	2.114021	-2.031126	1.813174
21	1	0	3.579755	-1.058228	-1.762172
22	1	0	2.113529	-2.052923	-1.788409
23	1	0	2.152156	-0.511845	-2.661874
24	17	0	-4.956053	-0.002911	0.000251

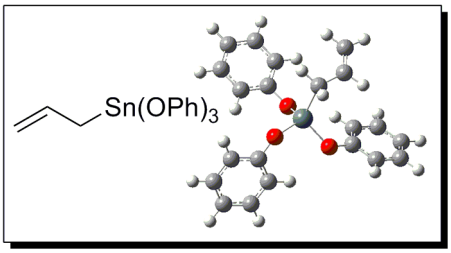


Allyltriphenoxystannane (37*)*

E = -1041.345339 Hartree
Electronic state: 1-A
Cartesian Coordinates (Angstroms):

1	8	0	1.385528	-1.411514	0.093912
2	8	0	-0.232710	0.990532	-0.894563
3	8	0	-1.432348	-1.044516	1.226971
4	6	0	0.755850	1.081934	2.374899
5	6	0	2.103643	1.709366	2.179892
6	1	0	2.955674	1.030008	2.201150
7	1	0	-0.022535	1.834556	2.539544
8	6	0	2.315534	3.011939	1.973224

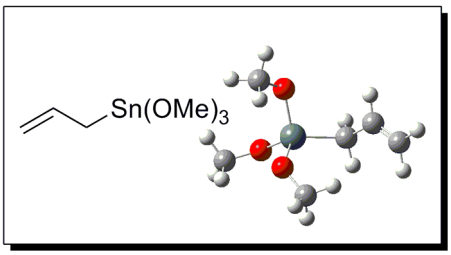
9	1	0	1.497284	3.728326	1.937383
10	1	0	3.317787	3.405983	1.833033
11	1	0	0.740281	0.388399	3.223577
12	50	0	0.132041	-0.071916	0.682799
13	6	0	-2.212158	-1.923411	0.517335
14	6	0	-1.670499	-2.845054	-0.387849
15	6	0	-3.592661	-1.906143	0.754198
16	6	0	-2.514003	-3.733376	-1.056898
17	1	0	-0.596767	-2.866809	-0.554056
18	6	0	-4.423897	-2.803096	0.082946
19	1	0	-3.992253	-1.191996	1.467933
20	6	0	-3.891314	-3.719358	-0.827087
21	1	0	-2.085754	-4.443403	-1.759654
22	1	0	-5.493994	-2.783011	0.273157
23	1	0	-4.541757	-4.414481	-1.350097
24	6	0	-1.084953	2.069624	-0.922618
25	6	0	-0.558769	3.342630	-1.176243
26	6	0	-2.465233	1.907773	-0.744755
27	6	0	-1.410670	4.444921	-1.249087
28	1	0	0.513194	3.448459	-1.313984
29	6	0	-3.307385	3.019162	-0.815870
30	1	0	-2.870549	0.914490	-0.571545
31	6	0	-2.787389	4.290550	-1.066745
32	1	0	-0.994550	5.429126	-1.448692
33	1	0	-4.377362	2.885079	-0.679564
34	1	0	-3.447555	5.151281	-1.123316
35	6	0	2.641688	-1.225239	-0.426707
36	6	0	3.638590	-2.142200	-0.069104
37	6	0	2.937348	-0.185450	-1.317929
38	6	0	4.923142	-2.011712	-0.595654
39	1	0	3.387736	-2.946136	0.616183
40	6	0	4.229220	-0.062648	-1.833418
41	1	0	2.152607	0.505914	-1.613607
42	6	0	5.227679	-0.970740	-1.477032
43	1	0	5.690374	-2.727980	-0.312864
44	1	0	4.449661	0.746890	-2.524501
45	1	0	6.230059	-0.871756	-1.883560



Allyltrimethoxystannane (38*)*

E = -466.1068898 Hartree
Electronic state: 1-A
Cartesian Coordinates (Angstroms):

1	8	0	-1.637979	-0.815453	-1.216874
2	8	0	-0.497311	1.882312	0.022625
3	8	0	-0.300526	-0.735839	1.571297
4	6	0	-1.240425	2.456497	1.087886
5	6	0	-2.917893	-1.127414	-0.686877
6	6	0	0.654018	-1.648433	2.086312
7	1	0	-0.952907	3.511126	1.173806
8	1	0	-2.322612	2.415071	0.894224
9	1	0	-1.042897	1.963357	2.049273
10	1	0	-2.858070	-1.590123	0.308288
11	1	0	-3.404556	-1.836089	-1.367269

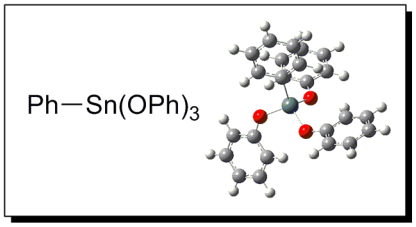


12	1	0	-3.555134	-0.233702	-0.614400
13	1	0	0.590143	-2.635581	1.602876
14	1	0	0.451353	-1.787499	3.154747
15	1	0	1.685920	-1.281683	1.982122
16	6	0	1.592204	-0.255262	-1.303432
17	6	0	2.730585	0.492645	-0.677192
18	1	0	2.634983	1.578519	-0.670425
19	1	0	1.802777	-1.327041	-1.382500
20	6	0	3.811860	-0.067491	-0.126759
21	1	0	3.954862	-1.146429	-0.110695
22	1	0	4.597843	0.534831	0.319686
23	1	0	1.375126	0.114973	-2.313248
24	50	0	-0.225048	-0.000623	-0.206450

Triphenoxy(phenyl)stannane (39*)*

E = -1155.684085 Hartree
Electronic state: 1-A
Cartesian Coordinates (Angstroms):

1	8	0	1.071910	-1.693485	-0.273325
2	8	0	-0.310855	0.707820	-1.450538
3	8	0	-1.502709	-0.723018	1.131074
4	50	0	0.092971	-0.117979	0.253055
5	6	0	-2.420324	-1.683900	0.786225
6	6	0	-2.091929	-2.795435	0.000678
7	6	0	-3.722220	-1.538285	1.281205
8	6	0	-3.072128	-3.744868	-0.294800
9	1	0	-1.075674	-2.918645	-0.364239
10	6	0	-4.690060	-2.496509	0.983120
11	1	0	-3.955561	-0.673658	1.895281
12	6	0	-4.372721	-3.603436	0.191844
13	1	0	-2.809592	-4.603068	-0.907969
14	1	0	-5.698394	-2.374142	1.370336
15	1	0	-5.129767	-4.346629	-0.041305
16	6	0	-1.083252	1.816915	-1.679848
17	6	0	-0.761604	2.617507	-2.783659
18	6	0	-2.182823	2.151291	-0.878505
19	6	0	-1.529062	3.744289	-3.073839
20	1	0	0.088123	2.340553	-3.400080
21	6	0	-2.940448	3.285923	-1.175243
22	1	0	-2.455213	1.514591	-0.040137
23	6	0	-2.619863	4.088501	-2.270887
24	1	0	-1.270318	4.357995	-3.932956
25	1	0	-3.790689	3.535399	-0.545766
26	1	0	-3.213885	4.968692	-2.499071
27	6	0	2.335205	-1.713353	-0.809185
28	6	0	3.222681	-2.702074	-0.365589
29	6	0	2.740222	-0.805831	-1.797785
30	6	0	4.507911	-2.771855	-0.901156
31	1	0	2.888522	-3.400378	0.395514
32	6	0	4.033391	-0.881925	-2.320911
33	1	0	2.032045	-0.070085	-2.171465
34	6	0	4.923181	-1.861226	-1.876985
35	1	0	5.190328	-3.541571	-0.549830

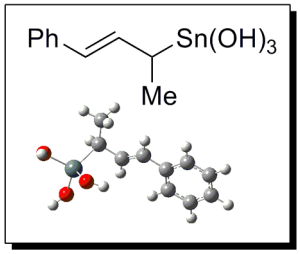


36	1	0	4.338329	-0.175161	-3.088484
37	1	0	5.926511	-1.918433	-2.289067
38	6	0	1.039300	1.115038	1.668839
39	6	0	0.438018	1.275465	2.927964
40	6	0	2.251830	1.767646	1.393418
41	6	0	1.042964	2.079655	3.895920
42	1	0	-0.498292	0.772656	3.154314
43	6	0	2.852636	2.568818	2.365830
44	1	0	2.739850	1.651584	0.428916
45	6	0	2.248347	2.725678	3.615051
46	1	0	0.573095	2.200075	4.868328
47	1	0	3.791867	3.069537	2.147265
48	1	0	2.717908	3.350928	4.369749

(4-phenylbut-3-en-2-yl)stannanetriol (40*)*

E = -618.571006 Hartree
Electronic state: 1-A
Cartesian Coordinates (Angstroms):

1	6	0	-0.814455	0.968935	-1.082982
2	50	0	-2.143684	-0.249035	0.098860
3	8	0	-3.935111	0.426381	0.248020
4	8	0	-1.610785	-0.366507	1.947241
5	8	0	-2.173651	-1.969791	-0.750073
6	1	0	-0.659412	-0.485062	2.084931
7	1	0	-2.850963	-2.579839	-0.422898
8	1	0	-4.178143	0.628029	1.164781
9	6	0	0.556530	0.375431	-0.954460
10	6	0	1.588914	0.897396	-0.264809
11	1	0	-1.166248	0.824856	-2.112802
12	1	0	0.684134	-0.579427	-1.464591
13	1	0	1.452362	1.858657	0.228897
14	6	0	2.932263	0.319825	-0.104397
15	6	0	3.904383	1.057252	0.596019
16	6	0	3.304403	-0.940077	-0.612610
17	6	0	5.195839	0.564627	0.779448
18	1	0	3.638535	2.032313	0.998622
19	6	0	4.593414	-1.432635	-0.430787
20	1	0	2.579857	-1.543146	-1.152172
21	6	0	5.547677	-0.684033	0.265755
22	1	0	5.926347	1.157139	1.324055
23	1	0	4.855756	-2.407845	-0.832725
24	1	0	6.552464	-1.072694	0.406720
25	6	0	-0.959734	2.443977	-0.685795
26	1	0	-0.281034	3.070928	-1.277833
27	1	0	-1.984024	2.792211	-0.853643
28	1	0	-0.724443	2.610777	0.371844

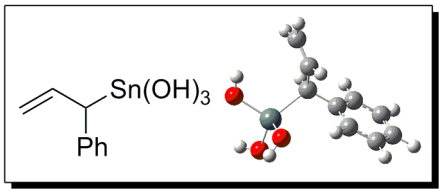


Trimethyl(1-phenylallyl)stannane (41*)*

E = -579.2480199 Hartree
Electronic state: 1-A

Cartesian Coordinates (Angstroms):

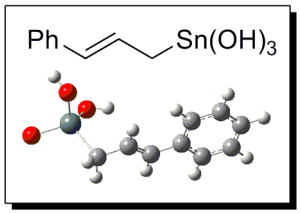
1	6	0	0.277134	1.004153	-0.325768
2	50	0	-1.349814	-0.393919	-0.077418
3	8	0	-1.422388	-1.918774	-1.237948
4	8	0	-3.026963	0.482211	-0.432633
5	8	0	-1.237501	-1.019987	1.736147
6	1	0	-3.080559	1.380245	-0.072612
7	1	0	-1.753534	-1.817129	1.927083
8	1	0	-2.164400	-1.879645	-1.860687
9	6	0	-0.001494	2.127349	0.641497
10	6	0	-0.601985	3.281834	0.330395
11	1	0	0.294250	1.941601	1.673817
12	1	0	-0.904139	3.517830	-0.688610
13	1	0	0.157176	1.379389	-1.349367
14	1	0	-0.793118	4.040960	1.083423
15	6	0	1.650735	0.377816	-0.172926
16	6	0	2.627259	0.595547	-1.155172
17	6	0	1.991021	-0.394448	0.949537
18	6	0	3.909517	0.060422	-1.022886
19	1	0	2.381614	1.193578	-2.029860
20	6	0	3.275298	-0.922726	1.085551
21	1	0	1.239664	-0.601961	1.708227
22	6	0	4.239677	-0.698283	0.100899
23	1	0	4.649947	0.239510	-1.798164
24	1	0	3.518225	-1.520469	1.960175
25	1	0	5.237435	-1.115556	0.206198



Cinnamylstannanetriol (42*)*

E = -579.2602477 Hartree
Electronic state: 1-A
Cartesian Coordinates (Angstroms):

1	6	0	-0.834178	-0.389992	1.520223
2	50	0	-2.210084	0.018728	-0.072019
3	8	0	-3.940544	-0.797161	0.070429
4	8	0	-1.587114	-0.656028	-1.763794
5	8	0	-2.404190	1.926374	-0.089374
6	1	0	-0.631322	-0.578836	-1.900178
7	1	0	-3.080606	2.269642	-0.691197
8	1	0	-4.111464	-1.422876	-0.650313
9	6	0	0.531003	0.094122	1.146161
10	6	0	1.534954	-0.695761	0.721919
11	1	0	-1.217650	0.113986	2.414058
12	1	0	0.677197	1.172277	1.202258
13	1	0	1.357990	-1.772496	0.692801
14	6	0	2.881944	-0.283540	0.301646
15	6	0	3.830295	-1.277956	0.000244
16	6	0	3.278538	1.062406	0.177666
17	6	0	5.123970	-0.947580	-0.401347
18	1	0	3.544499	-2.323994	0.086687
19	6	0	4.569922	1.393229	-0.222185
20	1	0	2.570247	1.858294	0.389575
21	6	0	5.501076	0.391100	-0.513760
22	1	0	5.836441	-1.736814	-0.626523

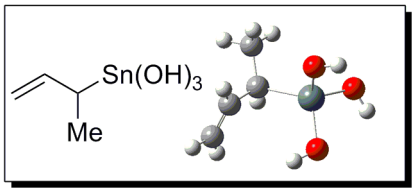


23	1	0	4.851894	2.439171	-0.310884
24	1	0	6.507606	0.653558	-0.827595
25	1	0	-0.850995	-1.469965	1.700756

But-3-en-2-yltrimethylstannane (43*)*

E = -387.5154995 Hartree
Electronic state: 1-A
Cartesian Coordinates (Angstroms):

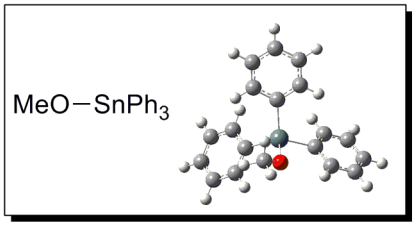
1	6	0	-1.367304	0.612310	-0.500103
2	50	0	0.612303	-0.064561	0.001486
3	8	0	2.041897	0.515723	-1.141752
4	8	0	0.752654	-1.983038	-0.091264
5	8	0	0.935352	0.603091	1.771459
6	1	0	-0.073075	-2.438036	0.133179
7	1	0	1.844207	0.509745	2.091929
8	1	0	2.453867	-0.219679	-1.620703
9	6	0	-2.323420	-0.207290	0.317589
10	6	0	-3.031365	-1.254658	-0.122140
11	1	0	-2.409720	0.084337	1.366198
12	1	0	-2.990349	-1.580570	-1.160043
13	1	0	-1.497308	0.373223	-1.563114
14	1	0	-3.690182	-1.812314	0.537500
15	6	0	-1.514891	2.128930	-0.278218
16	1	0	-2.529691	2.456182	-0.537231
17	1	0	-1.329449	2.399661	0.767041
18	1	0	-0.810792	2.693546	-0.899402



Methoxytriphenylstannane (44*)*

E = -813.4428143 Hartree
Electronic state: 1-A
Cartesian Coordinates (Angstroms):

1	50	0	0.038303	-0.083011	0.406692
2	6	0	1.942562	-0.804380	-0.209877
3	6	0	2.827516	-1.306954	0.759402
4	6	0	2.354020	-0.796590	-1.553323
5	6	0	4.087197	-1.788394	0.394212
6	1	0	2.527143	-1.318980	1.804048
7	6	0	3.613563	-1.276608	-1.919873
8	1	0	1.695251	-0.412568	-2.330551
9	6	0	4.481465	-1.773520	-0.945145
10	1	0	4.761004	-2.174295	1.155352
11	1	0	3.916720	-1.263038	-2.963911
12	1	0	5.461735	-2.147977	-1.229238
13	6	0	-1.659718	-1.193871	-0.258181
14	6	0	-2.361809	-0.857470	-1.428023
15	6	0	-2.089575	-2.309622	0.480581
16	6	0	-3.456014	-1.616394	-1.851637
17	1	0	-2.063098	0.007388	-2.017730
18	6	0	-3.184270	-3.068960	0.060986
19	1	0	-1.568515	-2.586742	1.394600

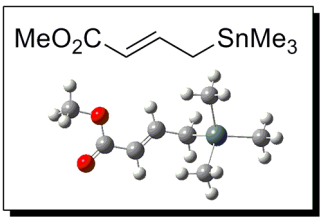


20	6	0	-3.867395	-2.723770	-1.107218
21	1	0	-3.987341	-1.342610	-2.759909
22	1	0	-3.504391	-3.928635	0.644593
23	1	0	-4.718570	-3.314771	-1.435755
24	6	0	-0.211076	1.981730	-0.080930
25	6	0	0.909348	2.791514	-0.336064
26	6	0	-1.485086	2.574506	-0.129092
27	6	0	0.763022	4.149400	-0.629138
28	1	0	1.908376	2.360997	-0.311951
29	6	0	-1.635358	3.932480	-0.421238
30	1	0	-2.374575	1.974913	0.054622
31	6	0	-0.510385	4.721111	-0.670843
32	1	0	1.640896	4.760137	-0.824934
33	1	0	-2.628333	4.374033	-0.454829
34	1	0	-0.625832	5.777792	-0.898487
35	8	0	0.166632	-0.376691	2.322902
36	6	0	-0.679253	0.233618	3.276239
37	1	0	-0.289263	0.011838	4.277788
38	1	0	-0.720500	1.328808	3.166592
39	1	0	-1.711434	-0.149163	3.226846

(E)-methyl 4-(trimethylstannyl)but-2-enoate (45*)*

E = -468.298483 Hartree
Electronic state: 1-A
Cartesian Coordinates (Angstroms):

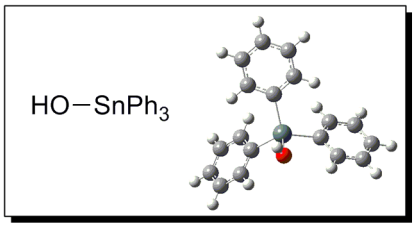
1	6	0	0.254022	-0.563621	-1.421609
2	50	0	1.745130	0.054942	0.070135
3	6	0	-1.114504	-0.173001	-1.009479
4	6	0	-2.035402	-0.986302	-0.456947
5	1	0	0.540049	-0.081278	-2.363819
6	1	0	-1.380371	0.875661	-1.136394
7	1	0	-1.842425	-2.045864	-0.309816
8	1	0	0.351050	-1.648035	-1.545822
9	6	0	1.404628	-1.093160	1.853764
10	1	0	0.352027	-1.033262	2.147947
11	1	0	1.654968	-2.147337	1.696428
12	1	0	2.013789	-0.719139	2.683165
13	6	0	3.696985	-0.336875	-0.748073
14	1	0	3.855123	0.232579	-1.669802
15	1	0	4.479046	-0.053351	-0.035773
16	1	0	3.818500	-1.400108	-0.979252
17	6	0	1.503172	2.156532	0.459209
18	1	0	2.244289	2.502517	1.187420
19	1	0	1.629526	2.743728	-0.456358
20	1	0	0.507638	2.364693	0.863974
21	6	0	-3.373045	-0.560962	-0.013431
22	8	0	-4.202256	-1.311571	0.468066
23	8	0	-3.603105	0.768722	-0.193984
24	6	0	-4.899006	1.219484	0.215818
25	1	0	-5.054142	1.038203	1.283371
26	1	0	-5.684989	0.704481	-0.344099
27	1	0	-4.918792	2.289639	0.003900



Triphenylstannanol (46)

E = -774.1414721 Hartree
Electronic state: 1-A
Cartesian Coordinates (Angstroms):

1	50	0	-0.012928	-0.088698	-0.566194
2	6	0	-1.860368	-0.905706	0.109178
3	6	0	-2.642092	-1.665176	-0.778062
4	6	0	-2.329238	-0.716769	1.420201
5	6	0	-3.854192	-2.223266	-0.364153
6	1	0	-2.304197	-1.814337	-1.800778
7	6	0	-3.541677	-1.272453	1.835659
8	1	0	-1.753912	-0.126294	2.131402
9	6	0	-4.304521	-2.028536	0.943142
10	1	0	-4.447721	-2.808426	-1.062395
11	1	0	-3.890410	-1.115191	2.853414
12	1	0	-5.247696	-2.462608	1.265370
13	6	0	1.761506	-1.067297	0.100261
14	6	0	2.289625	-0.870350	1.387481
15	6	0	2.431552	-1.943646	-0.770305
16	6	0	3.450240	-1.532050	1.795883
17	1	0	1.802307	-0.190209	2.084201
18	6	0	3.592180	-2.606948	-0.364274
19	1	0	2.046660	-2.102336	-1.775078
20	6	0	4.101730	-2.402747	0.919683
21	1	0	3.845971	-1.367506	2.795150
22	1	0	4.099231	-3.281688	-1.049760
23	1	0	5.004684	-2.918704	1.236361
24	6	0	0.099668	1.994722	-0.114724
25	6	0	-1.067322	2.764733	0.033324
26	6	0	1.342916	2.636929	0.021196
27	6	0	-0.995281	4.133346	0.303664
28	1	0	-2.044643	2.294082	-0.054037
29	6	0	1.418831	4.005578	0.290816
30	1	0	2.264485	2.065853	-0.074055
31	6	0	0.248824	4.755032	0.430794
32	1	0	-1.907910	4.713334	0.416642
33	1	0	2.388763	4.485908	0.393874
34	1	0	0.306319	5.819963	0.641391
35	8	0	-0.064439	-0.428238	-2.481831
36	1	0	0.145659	0.336570	-3.035937

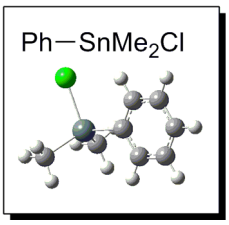


Chlorodimethyl(phenyl)stannane (47)

E = -775.0898941 Hartree
Electronic state: 1-A
Cartesian Coordinates (Angstroms):

1	50	0	-0.939638	-0.278665	0.000218
2	17	0	-1.809293	1.939819	-0.001606
3	6	0	1.182609	-0.048032	0.000069
4	6	0	1.790491	1.217807	0.000605
5	6	0	2.007878	-1.186489	-0.000539

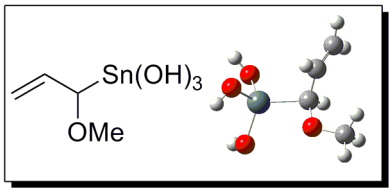
6	6	0	3.182265	1.341246	0.000553
7	1	0	1.177360	2.115659	0.001015
8	6	0	3.399112	-1.065031	-0.000585
9	1	0	1.574639	-2.186181	-0.001021
10	6	0	3.987757	0.201126	-0.000034
11	1	0	3.636680	2.328762	0.000957
12	1	0	4.021491	-1.956353	-0.001067
13	1	0	5.070350	0.298090	-0.000079
14	6	0	-1.681224	-1.189568	1.784134
15	1	0	-2.772799	-1.251435	1.754710
16	1	0	-1.276280	-2.201283	1.894423
17	1	0	-1.386468	-0.599758	2.656360
18	6	0	-1.680759	-1.192471	-1.782404
19	1	0	-2.772317	-1.254664	-1.753048
20	1	0	-1.386079	-0.603827	-2.655445
21	1	0	-1.275465	-2.204211	-1.891181



But-3-en-2-ylstannanetriol (48*)*

E = -462.7082789 Hartree
Electronic state: 1-A
Cartesian Coordinates (Angstroms):

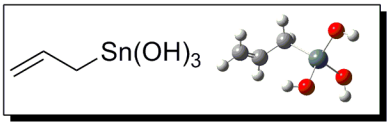
1	6	0	1.308513	-0.017621	-0.314553
2	50	0	-0.832398	-0.030411	-0.018736
3	8	0	-1.664613	-1.662982	-0.593103
4	8	0	-1.688088	1.374617	-1.016813
5	8	0	-1.271826	0.268329	1.828943
6	1	0	-2.137377	2.020066	-0.450482
7	1	0	-1.751658	-0.469539	2.234029
8	1	0	-2.427418	-1.494258	-1.167647
9	6	0	1.934414	1.147308	0.392094
10	6	0	2.419267	2.235248	-0.213481
11	1	0	1.936700	1.077957	1.480122
12	1	0	2.426456	2.332256	-1.297461
13	1	0	1.495530	0.047819	-1.399155
14	1	0	2.811951	3.075252	0.352521
15	8	0	1.714684	-1.282730	0.198692
16	6	0	3.058121	-1.614310	-0.122325
17	1	0	3.205598	-1.659696	-1.212481
18	1	0	3.768704	-0.889837	0.298508
19	1	0	3.248270	-2.601074	0.306660



Allylstannanetriol (49*)*

E = -348.2040773 Hartree
Electronic state: 1-A
Cartesian Coordinates (Angstroms):

1	8	0	1.755954	-0.960349	-1.092648
2	8	0	0.148562	-1.181807	1.445562
3	8	0	1.354402	1.635567	0.594119
4	6	0	-1.298547	0.631046	-0.981576
5	6	0	-2.438332	-0.236926	-0.540767

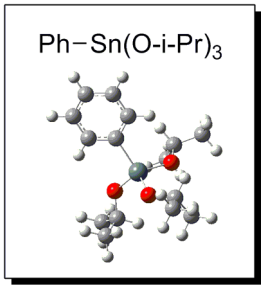


6	1	0	-2.495214	-1.220012	-1.010339
7	1	0	-1.455797	1.681190	-0.713985
8	6	0	-3.349096	0.084163	0.384990
9	1	0	-3.346236	1.052851	0.881387
10	1	0	-4.141405	-0.604497	0.663937
11	1	0	-1.133072	0.571849	-2.062531
12	50	0	0.512930	0.023907	-0.009338
13	1	0	2.234515	1.527601	0.983288
14	1	0	1.914524	-1.854282	-0.752518
15	1	0	-0.779317	-1.167019	1.725523

Triisopropoxy(phenyl)stannane (50)

E = -816.3587235 Hartree
Electronic state: 1-A
Cartesian Coordinates (Angstroms):

1	8	0	0.605098	1.782120	0.478064
2	8	0	1.121184	-0.411335	-1.660354
3	8	0	0.566130	-1.373289	1.132734
4	6	0	1.754132	-1.677417	-1.900676
5	6	0	1.932914	2.324641	0.442035
6	6	0	0.019428	-1.495179	2.450947
7	1	0	1.101978	-2.493839	-1.552780
8	1	0	2.660634	1.548331	0.729767
9	1	0	-1.059033	-1.262658	2.431504
10	50	0	0.090962	0.027542	-0.103373
11	6	0	1.937561	-1.806295	-3.411120
12	6	0	2.269826	2.812622	-0.967880
13	6	0	0.191737	-2.949229	2.884063
14	1	0	-0.313635	-3.620575	2.181979
15	1	0	-0.225298	-3.112746	3.884839
16	1	0	1.255570	-3.212339	2.901930
17	1	0	2.400595	-2.766526	-3.668216
18	1	0	0.972085	-1.736213	-3.922758
19	1	0	2.579796	-0.999529	-3.782722
20	1	0	2.210400	1.985932	-1.683112
21	1	0	3.282299	3.233388	-1.005328
22	1	0	1.561152	3.591173	-1.274905
23	6	0	0.710423	-0.516318	3.402894
24	6	0	1.991570	3.447045	1.476111
25	6	0	3.077800	-1.764209	-1.139725
26	1	0	3.744644	-0.950181	-1.448125
27	1	0	2.900406	-1.689175	-0.061860
28	1	0	3.582496	-2.718090	-1.337222
29	1	0	2.989746	3.900039	1.504657
30	1	0	1.262890	4.227104	1.226791
31	1	0	1.754442	3.065194	2.474610
32	1	0	1.783090	-0.736788	3.454543
33	1	0	0.590612	0.514659	3.050296
34	1	0	0.292098	-0.584482	4.414430
35	6	0	-1.999406	0.169733	-0.357481
36	6	0	-2.810215	-0.972988	-0.450918
37	6	0	-2.597928	1.437721	-0.443820
38	6	0	-4.189539	-0.851614	-0.631879

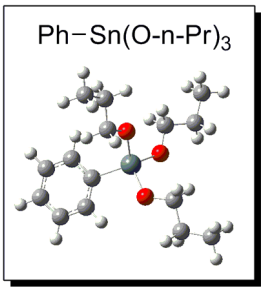


39	1	0	-2.372180	-1.966446	-0.378376
40	6	0	-3.977474	1.558123	-0.625026
41	1	0	-1.985460	2.331966	-0.362310
42	6	0	-4.772751	0.414243	-0.720492
43	1	0	-4.807714	-1.742923	-0.702272
44	1	0	-4.431170	2.543752	-0.690344
45	1	0	-5.846329	0.508637	-0.862104

Phenyltripropoxystannane (51*)*

E = -816.3423324 Hartree
Electronic state: 1-A
Cartesian Coordinates (Angstroms):

1	6	0	-1.799791	-0.807278	-0.720676
2	6	0	-2.062321	-2.186775	-0.697327
3	6	0	-2.789137	0.066364	-1.200184
4	6	0	-3.288231	-2.681083	-1.148230
5	1	0	-1.309989	-2.874454	-0.319884
6	6	0	-4.014416	-0.429060	-1.651085
7	1	0	-2.613761	1.140038	-1.222197
8	6	0	-4.263238	-1.803039	-1.626061
9	1	0	-3.482363	-3.750314	-1.125496
10	1	0	-4.773639	0.255764	-2.019966
11	1	0	-5.216805	-2.188548	-1.977554
12	50	0	0.069396	-0.099948	-0.041887
13	8	0	0.818958	-1.577139	0.915593
14	6	0	2.196675	-1.691810	1.269001
15	1	0	2.379024	-1.169664	2.221951
16	1	0	2.840152	-1.222167	0.510283
17	8	0	-0.097387	1.516850	0.989487
18	8	0	1.380998	0.373911	-1.353935
19	6	0	1.568113	1.696497	-1.854082
20	1	0	0.795290	1.927597	-2.606157
21	1	0	1.472425	2.440865	-1.050338
22	6	0	-0.938527	1.651951	2.129935
23	1	0	-1.939852	1.229879	1.940195
24	1	0	-0.515154	1.100769	2.985116
25	6	0	2.559479	-3.166896	1.414157
26	6	0	-1.067547	3.130018	2.487178
27	6	0	2.948259	1.797364	-2.496605
28	1	0	-1.483827	3.661523	1.621730
29	1	0	-0.060097	3.534178	2.647489
30	1	0	3.026145	1.026314	-3.273504
31	1	0	3.703001	1.555342	-1.737422
32	1	0	1.882191	-3.619704	2.149530
33	1	0	2.365165	-3.668085	0.457145
34	6	0	3.218415	3.183252	-3.092240
35	6	0	-1.939180	3.363651	3.725563
36	6	0	4.018079	-3.374598	1.835448
37	1	0	4.711219	-2.946688	1.100613
38	1	0	4.253495	-4.440138	1.931513
39	1	0	4.226463	-2.900490	2.802680
40	1	0	-2.013512	4.431097	3.959898
41	1	0	-2.958169	2.985414	3.575905



42	1	0	-1.524994	2.858868	4.607095
43	1	0	4.213271	3.229720	-3.548441
44	1	0	2.485613	3.434515	-3.869187
45	1	0	3.168564	3.965440	-2.324535

Phenyltriethoxystannane (52)

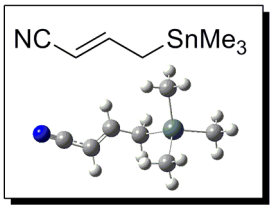
E = -698.402907 Hartree
Electronic state: 1-A
Cartesian Coordinates (Angstroms):

1	6	0	-1.779855	0.125439	0.243472
2	6	0	-2.438278	1.355402	0.081715
3	6	0	-2.536156	-1.016977	0.551252
4	6	0	-3.824164	1.440613	0.231306
5	1	0	-1.867695	2.246083	-0.168319
6	6	0	-3.921873	-0.930623	0.700410
7	1	0	-2.051115	-1.983371	0.672878
8	6	0	-4.565408	0.298704	0.542051
9	1	0	-4.324828	2.396949	0.103993
10	1	0	-4.498214	-1.820873	0.938594
11	1	0	-5.643964	0.365854	0.658915
12	50	0	0.315814	0.035492	0.024576
13	8	0	0.765987	1.658376	-0.888139
14	6	0	2.090067	2.182509	-0.982058
15	1	0	2.663410	1.618984	-1.734685
16	1	0	2.619548	2.079475	-0.023974
17	8	0	0.896827	-1.556293	-0.889417
18	8	0	1.364675	0.008239	1.625424
19	6	0	2.025850	-1.149308	2.136543
20	1	0	1.308881	-1.771491	2.695136
21	1	0	2.425577	-1.767915	1.321622
22	6	0	0.466147	-1.924539	-2.196416
23	1	0	-0.631374	-1.869491	-2.281815
24	1	0	0.881740	-1.232639	-2.945358
25	6	0	2.013109	3.649026	-1.382787
26	6	0	0.933727	-3.343642	-2.488062
27	6	0	3.149429	-0.703654	3.061889
28	1	0	0.505874	-4.044272	-1.762963
29	1	0	2.024912	-3.406013	-2.419766
30	1	0	0.628373	-3.653103	-3.494975
31	1	0	2.751855	-0.090486	3.877539
32	1	0	3.884613	-0.105859	2.512272
33	1	0	3.660081	-1.572426	3.495172
34	1	0	1.486880	3.756838	-2.337260
35	1	0	3.018743	4.073796	-1.489134
36	1	0	1.470529	4.225096	-0.625505

4-(trimethylstannyl)but-2-enenitrile (53)

E = -332.6657166 Hartree
Electronic state: 1-A
Cartesian Coordinates (Angstroms):

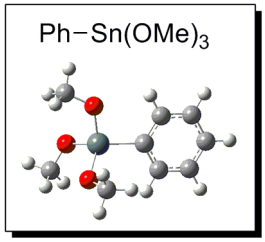
1	6	0	-0.530678	-1.187165	-0.832516
2	50	0	1.069786	0.052863	0.036146
3	6	0	-1.837115	-0.494542	-0.792252
4	6	0	-2.820611	-0.716869	0.106571
5	1	0	-0.228896	-1.403839	-1.863774
6	1	0	-1.997906	0.287145	-1.534739
7	1	0	-2.722045	-1.489780	0.866259
8	1	0	-0.549623	-2.129450	-0.273559
9	6	0	0.705286	0.180288	2.149006
10	1	0	-0.320408	0.511324	2.340081
11	1	0	0.846821	-0.792668	2.630697
12	1	0	1.387290	0.895211	2.620660
13	6	0	2.940945	-0.922095	-0.380848
14	1	0	3.092430	-1.030665	-1.459672
15	1	0	3.776604	-0.340366	0.022233
16	1	0	2.973128	-1.919023	0.070502
17	6	0	0.999036	1.997055	-0.878033
18	1	0	1.803516	2.632816	-0.493788
19	1	0	1.113914	1.927009	-1.964686
20	1	0	0.046355	2.492456	-0.665565
21	6	0	-4.035595	0.028873	0.116307
22	7	0	-5.034010	0.629058	0.138380



Trimethoxy(phenyl)stannane (54)

E = -580.4452848 Hartree
Electronic state: 1-A
Cartesian Coordinates (Angstroms):

1	6	0	1.424889	0.033509	-0.099714
2	6	0	2.105150	1.261436	-0.148060
3	6	0	2.168262	-1.157636	-0.090608
4	6	0	3.500639	1.295014	-0.190796
5	1	0	1.542821	2.191495	-0.147152
6	6	0	3.563560	-1.122645	-0.133740
7	1	0	1.665375	-2.121490	-0.046048
8	6	0	4.229444	0.103938	-0.184784
9	1	0	4.018311	2.250049	-0.227691
10	1	0	4.129818	-2.050375	-0.126325
11	1	0	5.315510	0.131018	-0.218451
12	50	0	-0.684333	0.030991	-0.039220
13	8	0	-1.135176	1.849977	0.344248
14	6	0	-2.435070	2.400331	0.186632
15	1	0	-3.093379	2.125068	1.023736
16	1	0	-2.913708	2.081491	-0.748968
17	1	0	-2.342551	3.492666	0.171977
18	8	0	-1.379855	-1.236971	1.230960
19	8	0	-1.637802	-0.410411	-1.636637
20	6	0	-2.171035	-1.694607	-1.924588
21	1	0	-1.403878	-2.362622	-2.344666
22	1	0	-2.959868	-1.572953	-2.676325
23	1	0	-2.605317	-2.180111	-1.041102
24	6	0	-0.950521	-1.307707	2.580031
25	1	0	0.146006	-1.294589	2.678748
26	1	0	-1.316007	-2.249084	3.007153

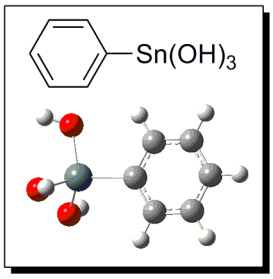


27	1	0	-1.355758	-0.480686	3.181322

Phenylstannanetriol (55)

E = -462.5407686 Hartree
Electronic state: 1-A
Cartesian Coordinates (Angstroms):

1	6	0	1.028932	-0.045343	-0.004020
2	6	0	1.721028	1.177453	0.001651
3	6	0	1.762158	-1.243192	-0.010355
4	6	0	3.117521	1.200066	0.005665
5	1	0	1.166308	2.112419	-0.005886
6	6	0	3.158253	-1.219024	-0.004466
7	1	0	1.250047	-2.202968	-0.026682
8	6	0	3.835627	0.002560	0.004617
9	1	0	3.644233	2.150884	0.007816
10	1	0	3.716592	-2.151556	-0.009980
11	1	0	4.922410	0.020389	0.008267
12	50	0	-1.081486	-0.010764	-0.000552
13	8	0	-1.524131	1.812759	-0.421391
14	8	0	-1.908974	-0.507703	1.655788
15	8	0	-1.913378	-1.215501	-1.236542
16	1	0	-1.319897	-0.486485	2.423326
17	1	0	-1.864392	-0.945527	-2.164875
18	1	0	-2.410258	2.089480	-0.145763



Methyl 2-(trihydroxystannyl)but-3-enoate (56)

E = -576.0730293 Hartree
Electronic state: 1-A
Cartesian Coordinates (Angstroms):

1	6	0	0.692208	0.681791	0.837289
2	50	0	-1.048504	-0.297306	-0.015235
3	8	0	-0.645411	-1.844995	-1.069756
4	8	0	-1.981816	0.910654	-1.174391
5	8	0	-2.097301	-0.837782	1.487145
6	1	0	-1.630912	1.813867	-1.112442
7	1	0	-2.883928	-1.364288	1.282023
8	1	0	-0.668952	-1.667915	-2.022667
9	6	0	0.420376	2.163139	0.794629
10	6	0	0.734165	3.029540	-0.176845
11	1	0	0.743854	0.320443	1.867157
12	1	0	-0.123482	2.528267	1.666221
13	1	0	1.278701	2.725487	-1.064042
14	1	0	0.478726	4.080567	-0.074086
15	6	0	1.877724	0.177586	0.059654
16	8	0	2.221504	0.560240	-1.042443
17	8	0	2.495885	-0.818718	0.727299
18	6	0	3.572211	-1.460221	0.021597
19	1	0	3.203341	-1.912513	-0.902679
20	1	0	3.947802	-2.226124	0.700336
21	1	0	4.357031	-0.738706	-0.218835