

Organotin carboxylate catalyst in urethane formation in polar solvent: An experimental and computational study

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Supplementary Information

Scheme 1S. Mechanisms for the catalysis in urethane formation with organotin compounds used as catalysts

Figure 1S. IRC for the transition states TS1, TS2 and TS3 for the interaction between DMTDA, methanol and methyl isocyanate.

Figure S2. IRC for TS1 and TS2 for the interaction between DMTMA, methanol and methyl isocyanate (O-coordinated interaction).

Figure S3. IRC TS1 for TS2 for the interaction between DMTMA, methanol and methyl isocyanate (N-coordinated interaction).

Tables S1 a)-f). Coordinates of the structures shown in Figure 10.

Tables S2 a)-b). Coordinates of the structures shown in Figure 11.

Tables S3 a)-d). Coordinates of the structures shown in Figure 14.

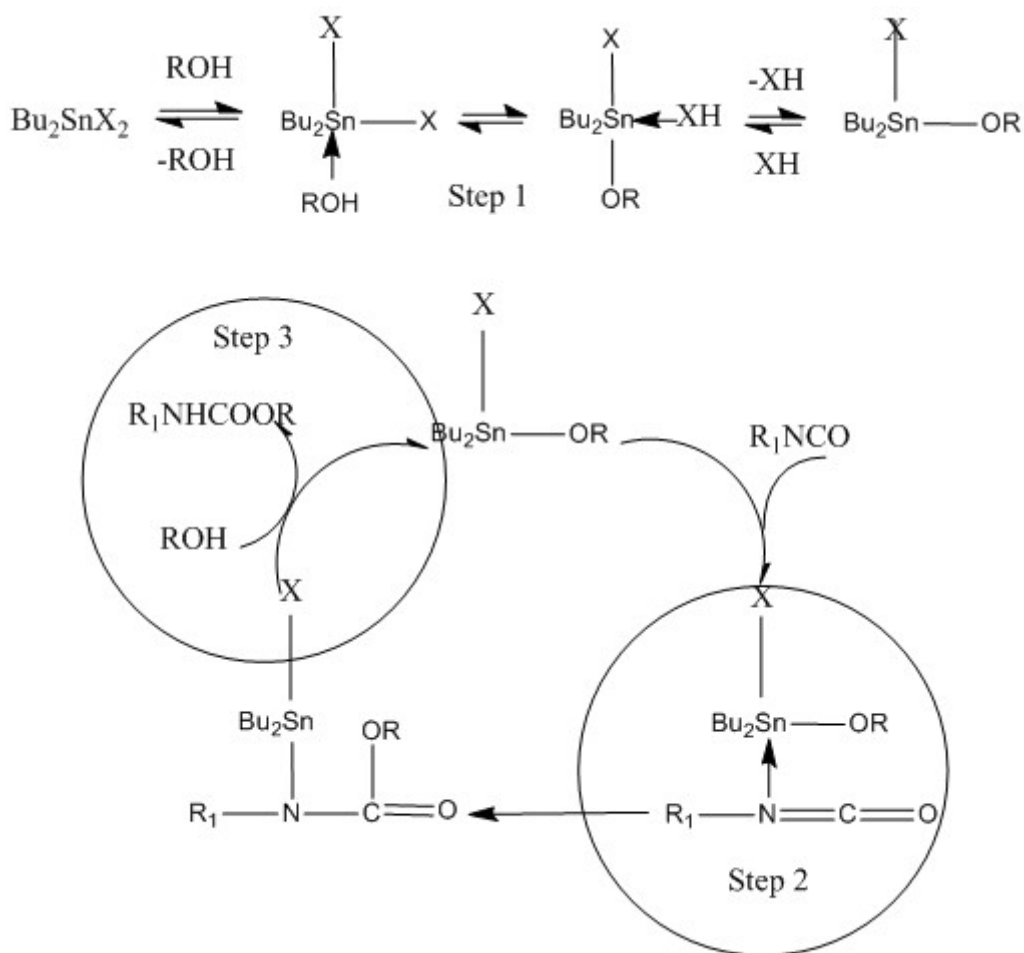
Tables S4 a)-d). Coordinates of the structures shown in Figure 15.

Scheme 1S. Mechanisms for the catalysis in urethane formation with organotin compounds used as catalysts

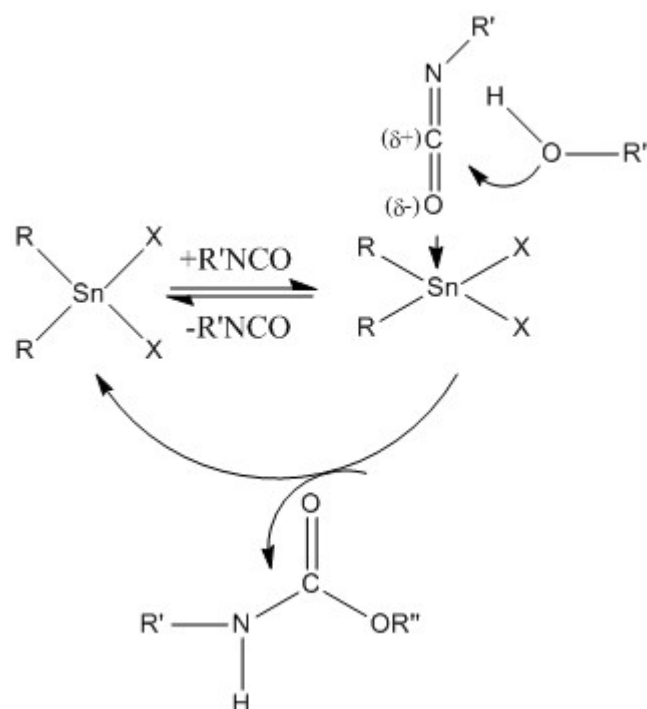
Scheme 1S a). Insertion mechanism: Mechanism of alkoxide formation and urethane catalysis.

In the insertion mechanism, the organotin catalyst will undergo a series of reactions to form the alkoxide intermediate. Three steps are involved in the reaction:

- 1) Association exchange of alcohol into the tin compound to form the alkoxide
- 2) Coordination of the isocyanate with the alkoxide to form the stanyl carbamate
- 3) Exchange of the stanyl carbamate with an alcohol molecule to regenerate the alkoxide intermediate



Scheme 1S b). Lewis interaction between isocyanate oxygen and tin atom of the organotin compound in urethane formation.



Scheme 1S c). Ionic mechanism for tin catalyzed urethane formation.

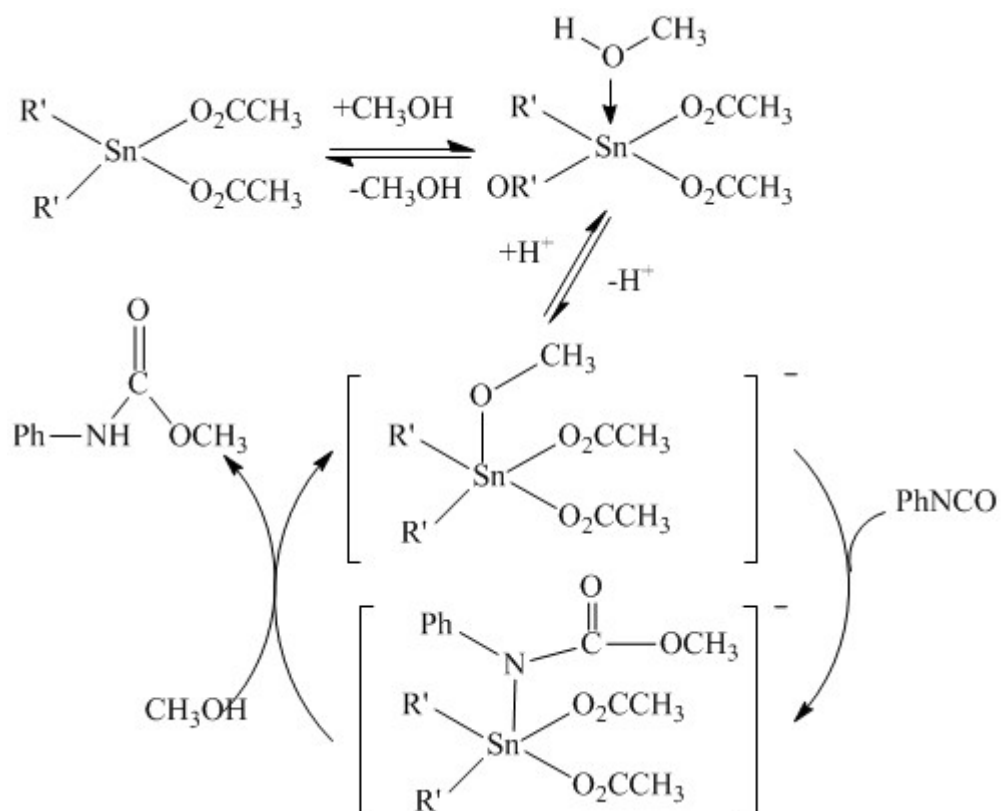


Figure 1S. IRC for the transition states TS1 ,TS2 and TS3 for the interaction between DMTDA, methanol and methyl isocyanate.

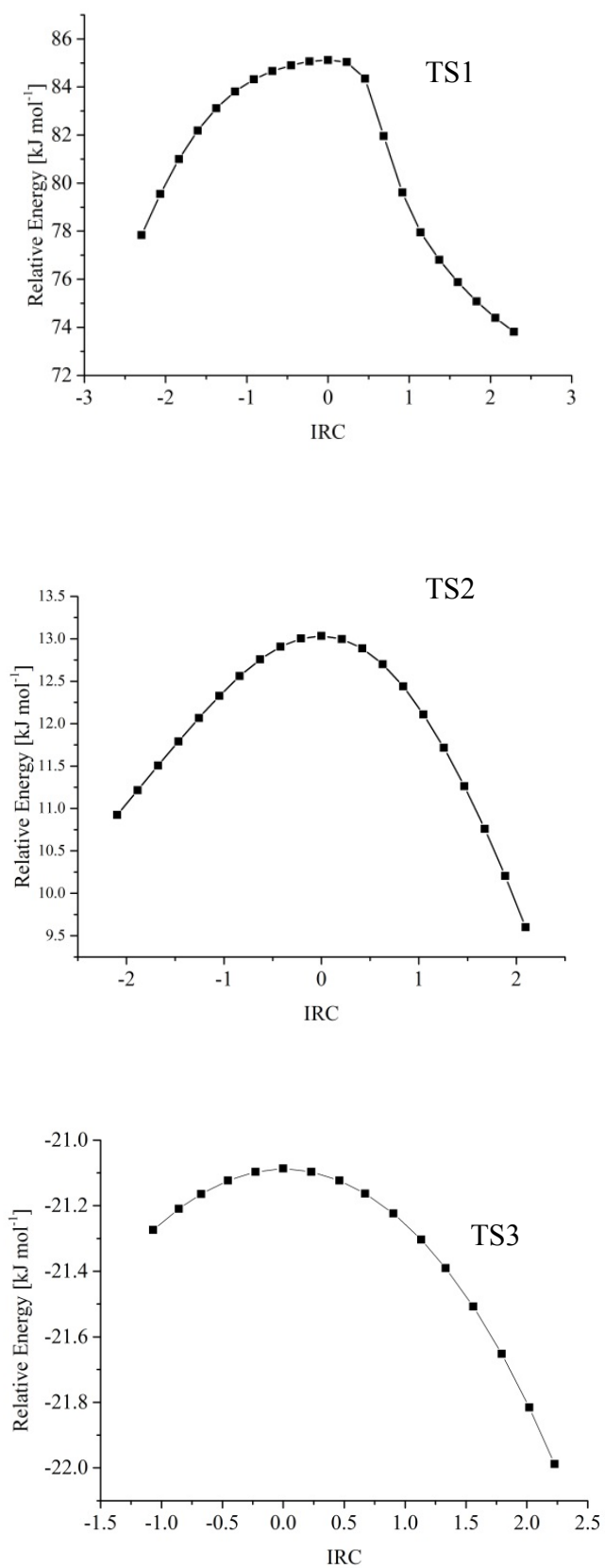


Figure S2. IRC for TS1 and TS2 for the interaction between DMTMA, methanol and methyl isocyanate (O-coordinated interaction).

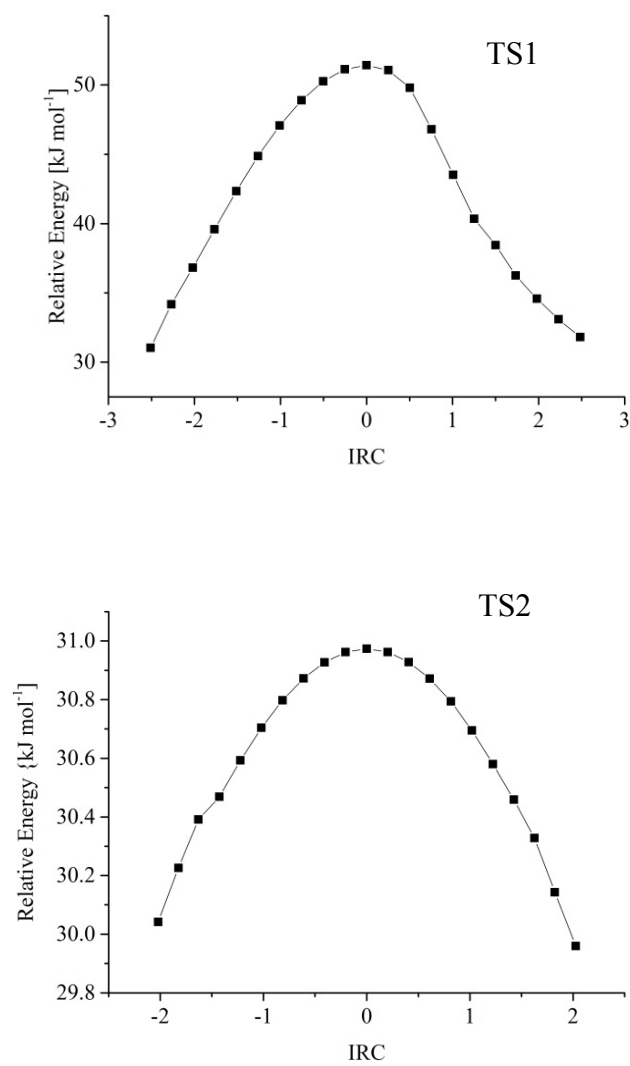
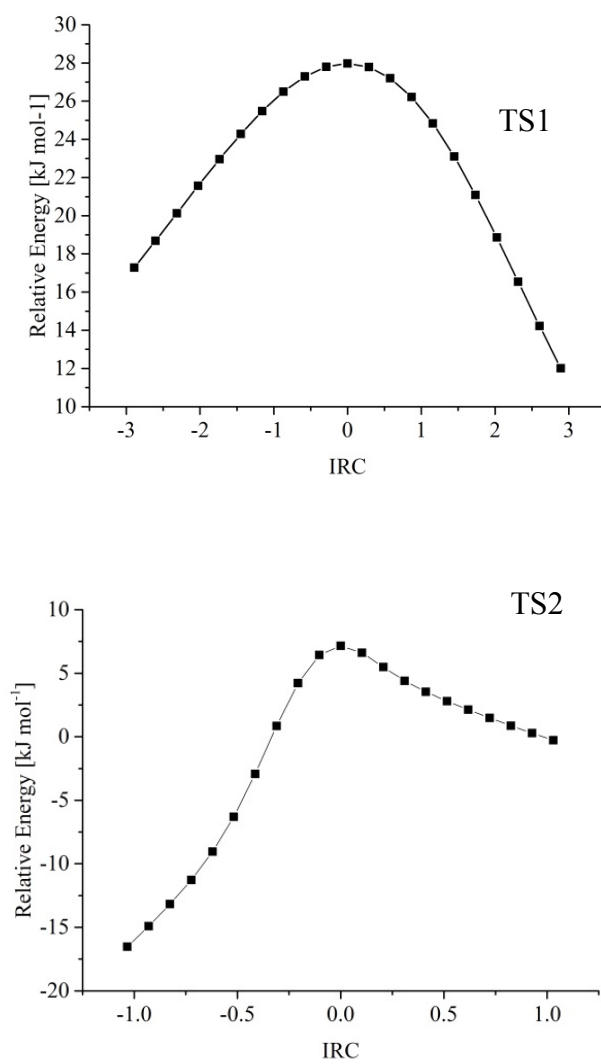


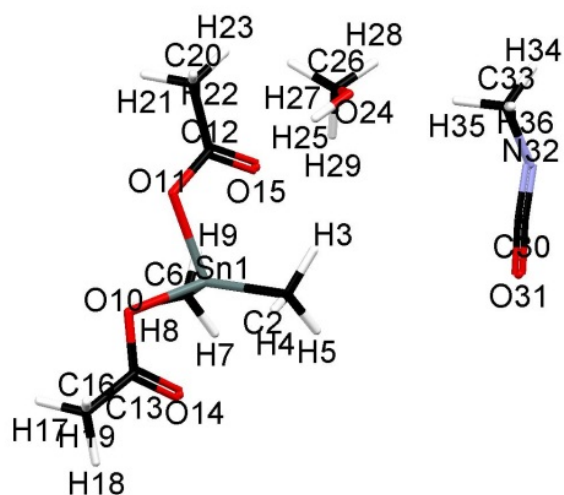
Figure S3. IRC TS1 for TS2 for the interaction between DMTMA, methanol and methyl isocyanate (N-coordinated interaction).



Tables S1. Coordinates of the structures shown in Figure 10.

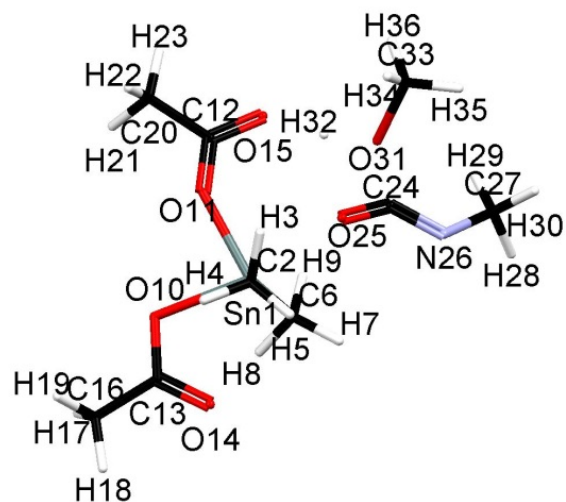
a) Coordinate for Structure (1)

Number	Label	X	Y	Z
1	Sn1	-0.5029	-0.4885	0
2	C2	-1.4641	-1.765	-1.3858
3	H3	-2.3624	-1.2823	-1.7741
4	H4	-0.7785	-1.9832	-2.2085
5	H5	-1.7362	-2.6999	-0.8908
6	C6	-0.6715	-0.3064	2.1005
7	H7	-0.8791	-1.2863	2.5362
8	H8	0.2716	0.071	2.5036
9	H9	-1.4791	0.3839	2.3489
10	O10	1.4887	-0.258	-0.549
11	O11	-0.7234	1.4302	-0.754
12	C12	-1.9666	1.8172	-0.6379
13	C13	2.0007	-1.405	-0.1858
14	O14	1.2428	-2.2507	0.3401
15	O15	-2.811	1.0555	-0.1242
16	C16	3.4645	-1.6304	-0.4258
17	H17	4.0419	-0.8536	0.0844
18	H18	3.765	-2.6141	-0.0664
19	H19	3.6745	-1.5451	-1.4964
20	C20	-2.2919	3.1931	-1.153
21	H21	-1.6562	3.9306	-0.6542
22	H22	-2.0701	3.2406	-2.2236
23	H23	-3.3416	3.4326	-0.9839
24	O24	-5.5742	1.4074	0.2401
25	H25	-4.6085	1.3223	0.1065
26	C26	-5.8164	1.7895	1.5925
27	H27	-5.3738	2.7673	1.8266
28	H28	-6.8993	1.86	1.7258
29	H29	-5.4267	1.048	2.3031
30	C30	-7.2071	-2.8381	-0.1237
31	O31	-6.635	-3.7723	0.3462
32	N32	-7.8936	-1.9577	-0.5518
33	C33	-7.9111	-0.6974	-1.2625
34	H34	-8.9122	-0.2688	-1.192
35	H35	-7.1852	-0.0045	-0.8262
36	H36	-7.675	-0.8634	-2.3177



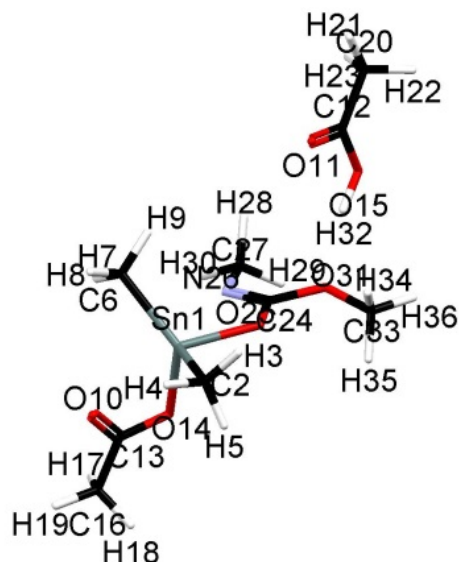
b) Coordinates for Structure (2)

Number	Label	X	Y	Z
1	Sn1	-0.6178	-0.0287	0
2	C2	-0.9932	-0.3436	2.0555
3	H3	-0.2691	0.2301	2.6379
4	H4	-2.0088	-0.0271	2.3003
5	H5	-0.878	-1.4046	2.2894
6	C6	-0.1681	-0.9562	-1.8525
7	H7	0.1829	-1.9761	-1.6806
8	H8	-1.0695	-0.9805	-2.4669
9	H9	0.6129	-0.397	-2.3735
10	O10	-2.5294	0.7416	-0.5449
11	O11	-0.1309	1.9779	-0.1126
12	C12	0.7978	2.7878	-0.4751
13	C13	-3.3463	-0.2747	-0.55
14	O14	-2.9359	-1.4202	-0.269
15	O15	1.9718	2.4652	-0.7972
16	C16	-4.784	0.0112	-0.9095
17	H17	-4.8322	0.4382	-1.9162
18	H18	-5.3807	-0.9005	-0.8685
19	H19	-5.1957	0.7545	-0.2198
20	C20	0.4097	4.2451	-0.5094
21	H21	-0.4287	4.3799	-1.1994
22	H22	0.0661	4.5496	0.4839
23	H23	1.2504	4.8657	-0.8183
24	C24	2.5808	-0.7594	-0.0148
25	O25	1.5513	-0.3839	0.618
26	N26	3.0557	-1.8916	-0.3002
27	C27	4.2587	-2.1001	-1.091
28	H28	4.0763	-2.9179	-1.7953
29	H29	4.5744	-1.2184	-1.6592
30	H30	5.0848	-2.4151	-0.4417
31	O31	3.3581	0.4991	-0.5153
32	C33	4.4663	0.9179	0.3397
33	H34	4.0973	1.1334	1.3447
34	H35	5.2019	0.1158	0.3594
35	H36	4.8922	1.8109	-0.1171
36	H32	2.6358	1.3324	-0.6246



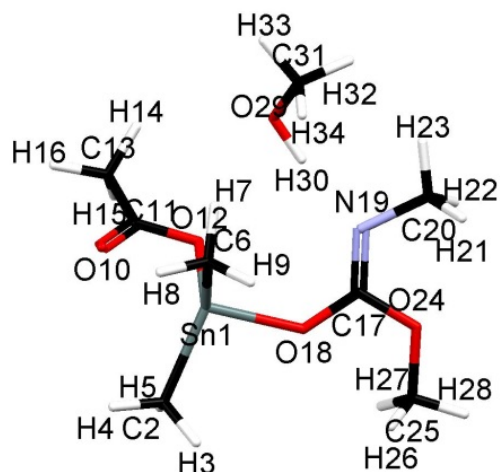
c) Coordinate for Structure (3)

Number	Label	X	Y	Z
1	Sn1	0.0718	-0.5747	0
2	C2	0.7363	-1.9894	1.4262
3	H3	-0.1109	-2.5868	1.7726
4	H4	1.4868	-2.6473	0.983
5	H5	1.177	-1.4689	2.2807
6	C6	-0.4244	-1.0176	-2.0081
7	H7	-0.225	-0.1467	-2.6352
8	H8	0.1824	-1.86	-2.349
9	H9	-1.4837	-1.2741	-2.0751
10	O10	2.4202	-0.1015	-0.6588
11	C13	2.1902	1.025	-0.1645
12	O14	0.9984	1.2494	0.3243
13	C16	3.1988	2.1331	-0.1003
14	H17	2.8217	2.999	-0.653
15	H18	3.3355	2.4424	0.9401
16	H19	4.1503	1.8101	-0.5215
17	C24	-2.4105	0.9181	0.506
18	O25	-1.6039	-0.0077	0.9917
19	N26	-2.1967	1.5433	-0.587
20	C27	-3.1258	2.5797	-1.0237
21	H28	-3.9867	2.1511	-1.555
22	H29	-3.5133	3.1878	-0.1958
23	H30	-2.6103	3.2423	-1.725
24	O31	-3.5236	1.1553	1.2777
25	C33	-3.5545	0.6172	2.6228
26	H34	-3.5627	-0.4736	2.6013
27	H35	-2.6944	0.9751	3.1911
28	H36	-4.4777	0.9971	3.0606
29	O11	-5.5009	-1.205	-0.4913
30	C12	-6.356	-0.3393	-0.374
31	O15	-6.1083	0.8496	0.2026
32	C20	-7.7812	-0.4625	-0.8434
33	H21	-7.9397	-1.4368	-1.3044
34	H22	-8.4628	-0.3366	0.0035
35	H23	-8.0043	0.3303	-1.5641
36	H32	-5.1682	0.8922	0.4994



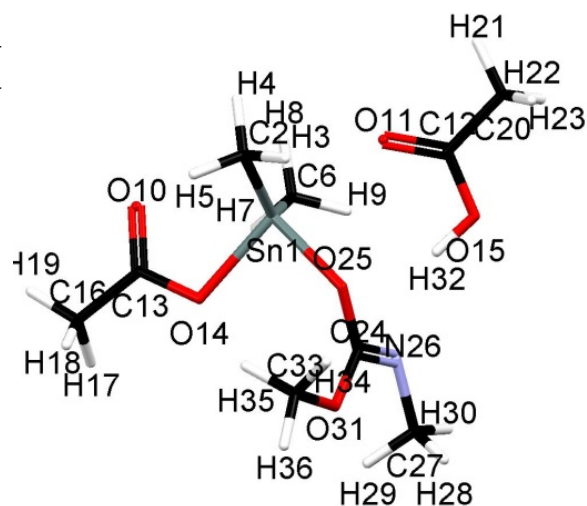
d) Coordinate for Structure (4)

Number	Label	X	Y	Z
1	Sn1	-0.7206	0.3235	0
2	C2	0.0364	-1.648	0.0605
3	H3	-0.6947	-2.3348	-0.3729
4	H4	0.9701	-1.7083	-0.5026
5	H5	0.2245	-1.9349	1.0985
6	C6	-0.9215	1.5329	-1.7218
7	H7	-0.9616	2.5815	-1.4225
8	H8	-0.0615	1.3674	-2.3748
9	H9	-1.84	1.2659	-2.2497
10	O10	1.4581	1.2894	0.5024
11	C11	0.9349	1.625	1.5923
12	O12	-0.3153	1.3049	1.7861
13	C13	1.6596	2.3688	2.6724
14	H14	1.1593	3.3258	2.8491
15	H15	1.6131	1.7972	3.604
16	H16	2.6978	2.5401	2.3901
17	C17	-3.644	0.6676	0.8285
18	O18	-2.5999	-0.1027	0.6185
19	N19	-3.6451	1.9551	0.7687
20	C20	-4.9153	2.6328	1.0413
21	H21	-5.6853	2.3826	0.2994
22	H22	-5.3173	2.3817	2.0315
23	H23	-4.753	3.713	1.0071
24	O24	-4.7865	0.0004	1.1328
25	C25	-4.7566	-1.439	1.2005
26	H26	-4.4687	-1.8671	0.238
27	H27	-4.0659	-1.777	1.9762
28	H28	-5.7763	-1.7315	1.4522
29	O29	-1.8347	4.1023	0.4598
30	H30	-2.4174	3.3067	0.5484
31	C31	-2.4129	5.0112	-0.4699
32	H32	-3.3483	5.4491	-0.0929
33	H33	-1.6974	5.8225	-0.6336
34	H34	-2.6198	4.535	-1.4388



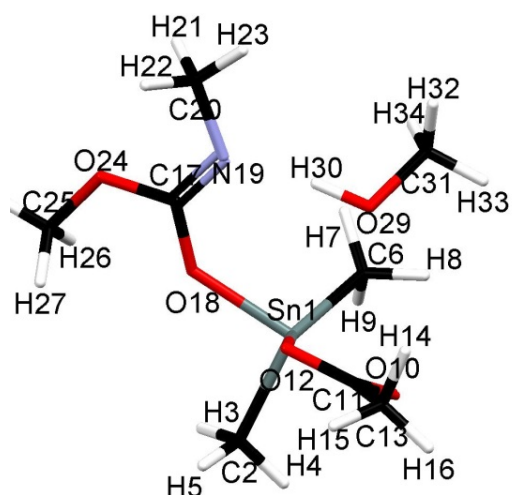
e) Coordinate for Structure (5)

Number	Label	X	Y	Z
1	Sn1	-1.0774	-0.7182	-0.0235
2	C2	-1.0171	-1.883	1.7345
3	H3	-1.7853	-1.5243	2.4227
4	H4	-1.212	-2.9302	1.4929
5	H5	-0.0328	-1.7973	2.1992
6	C6	-1.4197	-1.0741	-2.0819
7	H7	-0.5432	-0.7625	-2.6537
8	H8	-1.588	-2.1428	-2.2347
9	H9	-2.2968	-0.5203	-2.4204
10	O10	1.3477	-1.7337	-0.5255
11	C13	1.6598	-0.5418	-0.3373
12	O14	0.7332	0.3354	-0.0428
13	C16	3.0735	-0.0313	-0.4274
14	H17	3.1308	0.7597	-1.1814
15	H18	3.3653	0.4092	0.531
16	H19	3.7579	-0.8394	-0.6857
17	C24	-1.8239	2.2251	0.07
18	O25	-1.9462	1.009	0.603
19	N26	-2.3965	2.5334	-1.0336
20	C27	-2.2727	3.9082	-1.5115
21	H28	-2.6784	4.6355	-0.7947
22	H29	-1.2279	4.1878	-1.7051
23	H30	-2.8281	4.0079	-2.4479
24	O31	-1.1248	3.1332	0.7929
25	C33	-0.5568	2.737	2.0589
26	H34	-1.3391	2.4081	2.7466
27	H35	0.1791	1.9435	1.9183
28	H36	-0.0733	3.6349	2.4445
29	O11	-3.5276	-1.4161	0.1066
30	C12	-4.6109	-0.829	0.0463
31	O15	-4.7107	0.4894	-0.0935
32	C20	-5.938	-1.5245	0.1226
33	H21	-5.7935	-2.603	0.1686
34	H22	-6.4754	-1.1835	1.0131
35	H23	-6.545	-1.2616	-0.7485
36	H32	-3.8144	0.8986	-0.1067



f) Coordinate for Structure (6)

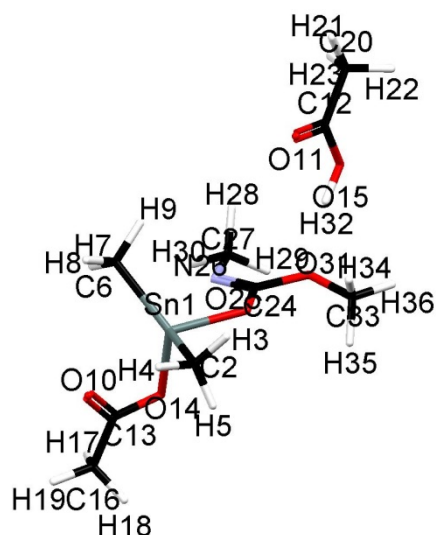
Number	Label	X	Y	Z
1	Sn1	-0.2794	0.0588	0
2	C2	-0.702	-1.9942	-0.3262
3	H3	0.051	-2.6088	0.1748
4	H4	-1.688	-2.2472	0.0722
5	H5	-0.6843	-2.2148	-1.3969
6	C6	-0.2073	0.7676	1.9978
7	H7	0.7316	1.2947	2.1752
8	H8	-1.045	1.4404	2.1853
9	H9	-0.2717	-0.0941	2.6687
10	O10	-2.3991	0.8487	-0.488
11	C11	-1.9691	1.1633	-1.6357
12	O12	-0.7294	0.902	-1.888
13	C13	-2.8202	1.8304	-2.6705
14	H14	-2.5928	2.9022	-2.66
15	H15	-2.5815	1.4469	-3.6646
16	H16	-3.878	1.6914	-2.4474
17	C17	2.609	0.8958	-0.7547
18	O18	1.6878	-0.0135	-0.5502
19	N19	2.4137	2.1708	-0.7177
20	C20	3.5479	3.0558	-0.9757
21	H21	4.3535	2.9249	-0.2409
22	H22	3.9813	2.8973	-1.9722
23	H23	3.2018	4.0913	-0.9176
24	O24	3.847	0.4111	-1.0277
25	C25	4.0406	-1.0165	-1.0721
26	H26	3.808	-1.4702	-0.1062
27	H27	3.4217	-1.468	-1.8505
28	H28	5.0967	-1.152	-1.3061
29	O29	-0.0607	3.0854	-0.175
30	H30	0.8868	2.8399	-0.4058
31	C31	-0.0547	4.0607	0.8608
32	H32	0.2684	5.043	0.4874
33	H33	-1.0742	4.1589	1.2461
34	H34	0.6019	3.774	1.6935



Tables S2. Coordinates of the structures shown in Figure 11.

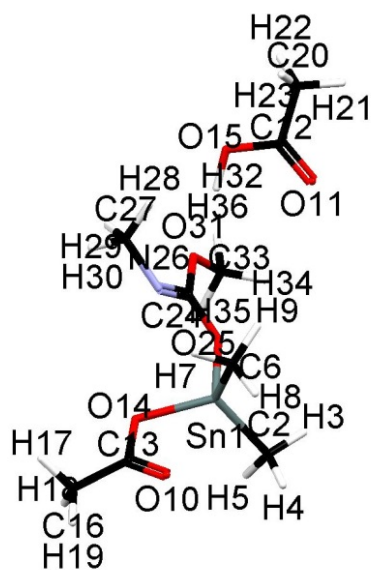
a) Coordinates for Structure Figure 11 (left)

Number	Label	X	Y	Z
1	Sn1	0.4741	0.5747	0
2	C2	-0.1839	2.2641	1.0976
3	H3	0.6603	2.9316	1.2897
4	H4	-0.9535	2.8033	0.5409
5	H5	-0.6007	1.9414	2.0556
6	C6	0.907	0.6456	-2.0701
7	H7	0.7566	-0.3432	-2.5061
8	H8	0.2433	1.3662	-2.5543
9	H9	1.9484	0.9419	-2.2147
10	O10	-1.8852	-0.0358	-0.5229
11	C13	-1.6482	-1.0095	0.2239
12	O14	-0.456	-1.1126	0.7499
13	C16	-2.6538	-2.0744	0.5537
14	H17	-2.2714	-3.0469	0.2289
15	H18	-2.7917	-2.1233	1.638
16	H19	-3.6048	-1.8655	0.0645
17	C24	2.9323	-0.7709	0.6997
18	O25	2.1812	0.2606	1.047
19	N26	2.619	-1.5677	-0.2468
20	C27	3.4657	-2.713	-0.5539
21	H28	4.3011	-2.4317	-1.2096
22	H29	3.8888	-3.1868	0.3418
23	H30	2.8686	-3.4582	-1.0874
24	O31	4.0812	-0.9132	1.4371
25	C33	4.2363	-0.0998	2.6251
26	H34	4.3135	0.9549	2.3583
27	H35	3.396	-0.2603	3.3028
28	H36	5.1629	-0.4435	3.0856
29	O11	6.4947	1.268	0.1979
30	C12	7.0691	0.2466	-0.1413
31	O15	6.5572	-0.9812	0.0661
32	C20	8.4091	0.1947	-0.8295
33	H21	8.7971	1.2043	-0.9617
34	H22	9.1099	-0.4008	-0.2365
35	H23	8.3065	-0.295	-1.8031
36	H32	5.6802	-0.9049	0.5099



**b) Coordinate for Structure Figure 11
(right)**

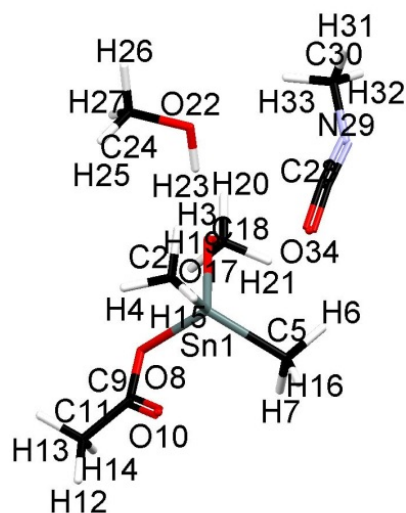
Number	Label	X	Y	Z
1	Sn1	0.0718	-0.5747	0
2	C2	0.7363	-1.9894	1.4262
3	H3	-0.1109	-2.5868	1.7726
4	H4	1.4868	-2.6473	0.983
5	H5	1.177	-1.4689	2.2807
6	C6	-0.4244	-1.0176	-2.0081
7	H7	-0.225	-0.1467	-2.6352
8	H8	0.1824	-1.86	-2.349
9	H9	-1.4837	-1.2741	-2.0751
10	O10	2.4202	-0.1015	-0.6588
11	C13	2.1902	1.025	-0.1645
12	O14	0.9984	1.2494	0.3243
13	C16	3.1988	2.1331	-0.1003
14	H17	2.8217	2.999	-0.653
15	H18	3.3355	2.4424	0.9401
16	H19	4.1503	1.8101	-0.5215
17	C24	-2.4105	0.9181	0.506
18	O25	-1.6039	-0.0077	0.9917
19	N26	-2.1967	1.5433	-0.587
20	C27	-3.1258	2.5797	-1.0237
21	H28	-3.9867	2.1511	-1.555
22	H29	-3.5133	3.1878	-0.1958
23	H30	-2.6103	3.2423	-1.725
24	O31	-3.5236	1.1553	1.2777
25	C33	-3.5545	0.6172	2.6228
26	H34	-3.5627	-0.4736	2.6013
27	H35	-2.6944	0.9751	3.1911
28	H36	-4.4777	0.9971	3.0606
29	O11	-5.5009	-1.205	-0.4913
30	C12	-6.356	-0.3393	-0.374
31	O15	-6.1083	0.8496	0.2026
32	C20	-7.7812	-0.4625	-0.8434
33	H21	-7.9397	-1.4368	-1.3044
34	H22	-8.4628	-0.3366	0.0035
35	H23	-8.0043	0.3303	-1.5641
36	H32	-5.1682	0.8922	0.4994



Tables S3. Coordinates of the structures shown in Figure 14.

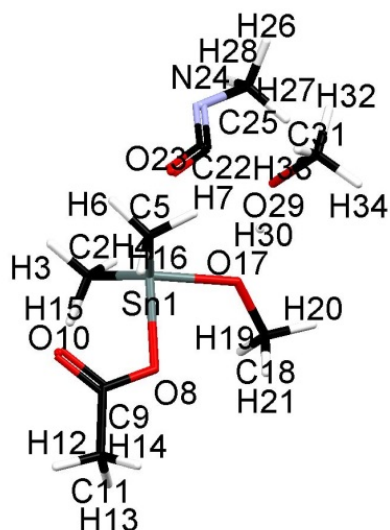
a) Coordinate for Structure (1)

Number	Label	X	Y	Z
1	Sn1	0.3305	0.0575	0
2	C2	-0.0707	0.4988	-2.0284
3	H3	-1.0965	0.861	-2.1218
4	H4	0.6221	1.268	-2.378
5	C5	0.4855	-1.8221	0.969
6	H6	-0.4774	-2.0988	1.4031
7	H7	1.2396	-1.7667	1.7581
8	O8	1.905	1.2366	0.6655
9	C9	2.9696	0.7346	0.0886
10	O10	2.8462	-0.2496	-0.6664
11	C11	4.2851	1.4013	0.3817
12	H12	5.1006	0.8761	-0.1151
13	H13	4.2501	2.4396	0.0371
14	H14	4.4559	1.4208	1.4621
15	H15	0.0535	-0.3981	-2.6391
16	H16	0.7855	-2.5812	0.2432
17	O17	-1.0152	1.1437	0.9617
18	C18	-1.0396	1.2628	2.3839
19	H19	-0.1421	1.7718	2.7586
20	H20	-1.9164	1.8553	2.668
21	H21	-1.1169	0.2825	2.8736
22	O22	-3.1343	2.3612	-0.2428
23	H23	-2.3486	1.9339	0.1727
24	C24	-2.7928	3.6936	-0.6119
25	H25	-1.9741	3.7193	-1.3446
26	H26	-3.6762	4.1499	-1.0679
27	H27	-2.5016	4.2991	0.2578
28	C28	-3.474	-1.1212	-0.2467
29	N29	-4.5296	-0.9088	0.2707
30	C30	-5.5498	0.0866	0.5181
31	H31	-6.3765	-0.0593	-0.1825
32	H32	-5.9297	-0.0396	1.5339
33	H33	-5.1307	1.0887	0.3972
34	O34	-2.4316	-1.4596	-0.718



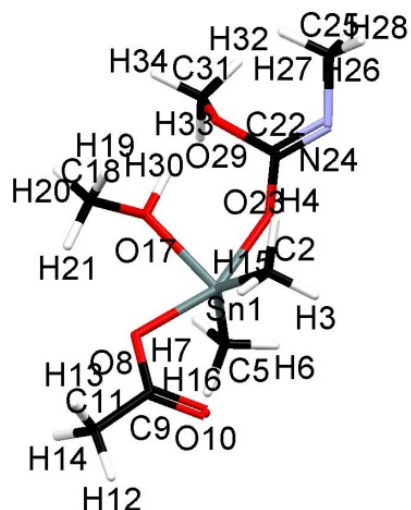
b) Coordinate for Structure (2)

Number	Label	X	Y	Z
1	Sn1	-0.4741	-0.1437	0
2	C2	-0.5598	-1.3339	-1.7514
3	H3	-0.6524	-2.3871	-1.4751
4	H4	-1.4324	-1.0448	-2.3422
5	C5	-0.3282	-0.5333	2.0732
6	H6	-0.5345	-1.5888	2.2651
7	H7	-1.0701	0.0731	2.598
8	O8	1.2718	0.9707	-0.3337
9	C9	2.3308	0.2044	-0.2383
10	O10	2.2282	-1.0091	0.0096
11	C11	3.6593	0.8902	-0.4497
12	H12	4.4807	0.1844	-0.3237
13	H13	3.6942	1.3199	-1.4559
14	H14	3.7669	1.7154	0.261
15	H15	0.3476	-1.1957	-2.3425
16	H16	0.6732	-0.2884	2.4315
17	O17	-1.5167	1.5707	-0.2816
18	C18	-1.1014	2.6704	-1.1086
19	H19	-0.964	2.3535	-2.1488
20	H20	-1.882	3.436	-1.0716
21	H21	-0.1659	3.0918	-0.7345
22	C22	-3.853	-0.5244	-0.1003
23	O23	-2.7477	-0.8685	0.3574
24	N24	-4.8815	-1.071	-0.5594
25	C25	-6.0747	-0.3917	-1.0335
26	H26	-6.8893	-0.5174	-0.3102
27	H27	-5.9202	0.6772	-1.2095
28	H28	-6.3985	-0.8578	-1.9693
29	O29	-3.9027	1.1728	-0.0754
30	C31	-4.4508	1.7192	1.1489
31	H32	-5.5063	1.4507	1.2035
32	H33	-3.9151	1.3264	2.018
33	H34	-4.3478	2.8051	1.1032
34	H30	-2.8378	1.4213	-0.1672



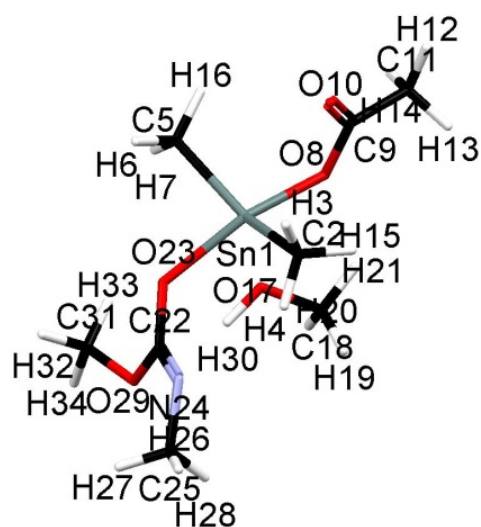
c) Coordinate for Structure (3)

Number	Label	X	Y	Z
1	Sn1	-0.6111	-0.5278	0
2	C2	-0.7126	-1.4929	-1.8837
3	H3	-0.6617	-2.575	-1.7373
4	H4	-1.66	-1.2468	-2.3691
5	C5	-0.247	-1.0089	2.0273
6	H6	-0.7069	-1.9716	2.2616
7	H7	-0.7069	-0.239	2.6529
8	O8	1.12	0.6558	-0.3012
9	C9	2.1959	-0.0878	-0.3683
10	O10	2.1399	-1.3257	-0.2703
11	C11	3.4945	0.6581	-0.5718
12	H12	4.3356	-0.0352	-0.6028
13	H13	3.4501	1.2253	-1.507
14	H14	3.6388	1.3783	0.2396
15	H15	0.1215	-1.1766	-2.5126
16	H16	0.8252	-1.0515	2.2218
17	O17	-1.4833	1.4321	-0.1963
18	C18	-1.0559	2.5769	-0.9846
19	H19	-1.3363	2.434	-2.0309
20	H20	-1.5388	3.4672	-0.578
21	H21	0.0238	2.6489	-0.8869
22	C22	-3.8272	-0.5805	-0.1372
23	O23	-2.6984	-0.9214	0.4122
24	N24	-4.6871	-1.3839	-0.6304
25	C25	-5.9309	-0.8881	-1.2051
26	H26	-6.7689	-1.0834	-0.5229
27	H27	-5.9195	0.1829	-1.4404
28	H28	-6.1389	-1.4418	-2.1271
29	O29	-4.0159	0.8398	-0.1601
30	H30	-2.485	1.3549	-0.1801
31	C31	-4.7689	1.3611	0.9621
32	H32	-5.7793	0.9452	0.9639
33	H33	-4.2621	1.1239	1.9028
34	H34	-4.8149	2.4419	0.8251



d) Coordinate for Structure (4)

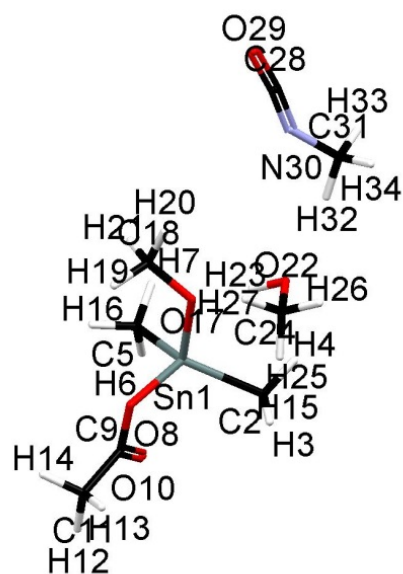
Number	Label	X	Y	Z
1	Sn1	-0.75	0	0
2	C2	-0.6561	-1.4045	1.579
3	H3	-0.8894	-2.3978	1.1861
4	H4	0.3579	-1.406	1.9835
5	C5	-1.1584	0.0382	-2.0768
6	H6	-0.5918	-0.7513	-2.5753
7	H7	-0.8385	1.0052	-2.4752
8	O8	-2.4741	1.0849	0.5834
9	C9	-3.5658	0.3661	0.4933
10	O10	-3.5433	-0.8168	0.1152
11	C11	-4.8437	1.0769	0.8782
12	H12	-5.6997	0.4085	0.7807
13	H13	-4.7706	1.435	1.9099
14	H14	-4.9853	1.9534	0.2381
15	H15	-1.3854	-1.1448	2.3489
16	H16	-2.2259	-0.0966	-2.2547
17	C22	2.4006	0.0344	0.2138
18	O23	1.31	-0.0312	-0.5157
19	N24	2.7644	-0.8372	1.0802
20	C25	4.0265	-0.6292	1.7858
21	H26	4.2884	-1.5491	2.3173
22	H27	4.856	-0.3714	1.1138
23	H28	3.951	0.1739	2.5329
24	O29	3.1538	1.1823	0.0206
25	C31	3.1148	1.8075	-1.2788
26	H32	3.4998	1.1238	-2.0414
27	H33	2.1034	2.1185	-1.5494
28	H34	3.7657	2.679	-1.2013
29	O17	0.0427	1.923	0.7883
30	C18	-0.3909	2.7588	1.9032
31	H19	0.0441	2.3843	2.832
32	H20	-0.0697	3.7832	1.7088
33	H21	-1.4747	2.6939	1.9286
34	H30	1.0006	2.0096	0.6549



Tables S4. Coordinates of the structures shown in Figure 15.

a) Coordinates for structure (1)

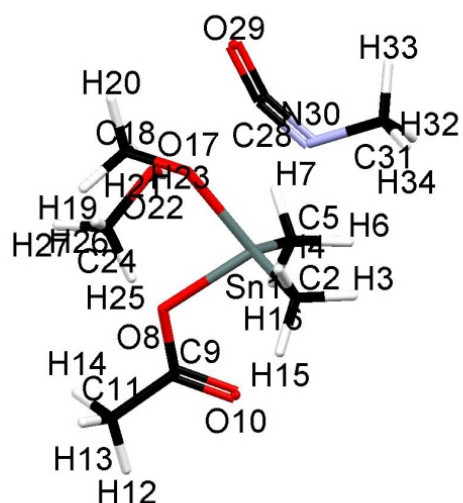
Number	Label	X	Y	Z
1	Sn1	-2.2126	-0.1149	0
2	C2	-2.3307	0.398	-2.0483
3	H3	-2.1694	-0.4877	-2.666
4	H4	-3.3161	0.8183	-2.2629
5	C5	-2.937	-1.8887	0.9113
6	H6	-2.7094	-2.7467	0.2752
7	H7	-4.0186	-1.818	1.051
8	O8	-0.3885	0.4159	0.8316
9	C9	0.4453	-0.4578	0.3237
10	O10	0.0041	-1.3201	-0.4634
11	C11	1.8883	-0.3547	0.7273
12	H12	2.4746	-1.1448	0.2591
13	H13	2.2796	0.6235	0.4311
14	H14	1.97	-0.4237	1.8161
15	H15	-1.5655	1.1425	-2.2828
16	H16	-2.4588	-2.0285	1.8843
17	O17	-3.1635	1.399	0.8506
18	C18	-3.3685	1.4905	2.2606
19	H19	-2.417	1.5853	2.8004
20	H20	-3.9721	2.3812	2.4672
21	H21	-3.9069	0.6158	2.6495
22	O22	-4.0257	3.6373	-0.4498
23	H23	-3.6971	2.8214	-0.0048
24	C24	-2.9914	4.616	-0.4273
25	H25	-2.0914	4.2749	-0.958
26	H26	-3.368	5.5113	-0.9305
27	H27	-2.7079	4.8906	0.5986
28	C28	-9.3257	-0.1881	0.8178
29	O29	-9.7216	0.2954	1.8314
30	N30	-8.8304	-0.7306	-0.1268
31	C31	-8.9236	-0.9377	-1.5538
32	H32	-8.0993	-1.5766	-1.8733
33	H33	-9.8693	-1.426	-1.805
34	H34	-8.858	0.0179	-2.0813



b) Coordinates for structure (2)

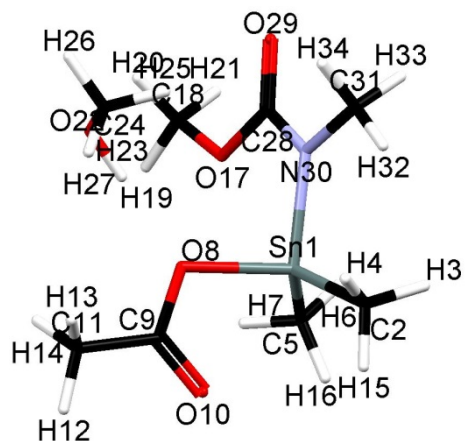
Coordinates for structure (2)

Number	Label	X	Y	Z
1	Sn1	-1.5805	-0.0287	0
2	C2	-1.5799	0.4075	2.0727
3	H3	-1.2412	-0.4673	2.6335
4	H4	-0.8923	1.2357	2.2626
5	C5	-1.8485	-1.8452	-1.0621
6	H6	-1.5592	-2.6869	-0.4277
7	H7	-1.2144	-1.843	-1.9523
8	O8	-3.1829	1.123	-0.6947
9	C9	-4.3491	0.6818	-0.2842
10	O10	-4.4509	-0.3247	0.4342
11	C11	-5.5422	1.4883	-0.7423
12	H12	-6.4703	1.0305	-0.3991
13	H13	-5.4679	2.5069	-0.3477
14	H14	-5.5451	1.5614	-1.8341
15	H15	-2.5845	0.6801	2.4006
16	H16	-2.894	-1.9567	-1.3542
17	O17	-0.4008	1.3011	-1.0045
18	C18	-0.6215	1.8119	-2.324
19	H19	-1.4055	2.574	-2.3019
20	H20	0.315	2.2637	-2.6673
21	H21	-0.9079	1.0161	-3.0206
22	O22	0.3451	3.5865	0.5603
23	H23	0.0307	2.8219	0.0403
24	C24	-0.75	4.4705	0.7993
25	H25	-1.546	3.9875	1.3814
26	H26	-0.3658	5.3171	1.3743
27	H27	-1.1788	4.8516	-0.1371
28	C28	1.3162	0.3299	-0.6941
29	O29	2.1488	0.8585	-1.3499
30	N30	0.7893	-0.4828	0.1087
31	C31	1.6176	-1.4883	0.8044
32	H32	1.1878	-2.4776	0.6308
33	H33	2.6519	-1.4801	0.4508
34	H34	1.6026	-1.2817	1.8776



c) Coordinates for structure (3)

Number	Label	X	Y	Z
1	Sn1	0.584	-1.0093	-0.1701
2	C2	1.5991	-1.577	-1.9444
3	H3	1.1354	-2.4659	-2.3803
4	H4	1.5732	-0.7647	-2.6755
5	C5	0.6895	-2.1698	1.5973
6	H6	-0.1733	-2.8381	1.6461
7	H7	0.6819	-1.5117	2.4684
8	O8	0.9945	0.9792	0.1972
9	C9	2.2567	1.0819	0.5799
10	O10	2.9551	0.063	0.6594
11	C11	2.748	2.4681	0.8941
12	H12	3.7874	2.4361	1.2196
13	H13	2.6578	3.1003	0.0055
14	H14	2.1257	2.9118	1.677
15	H15	2.6393	-1.8034	-1.7009
16	H16	1.61	-2.7577	1.5925
17	O17	-1.7605	-0.1654	1.3797
18	C18	-2.6403	0.2286	2.4469
19	H19	-2.0104	0.2889	3.334
20	H20	-3.0889	1.2019	2.2347
21	H21	-3.4267	-0.5162	2.5916
22	C28	-2.3177	-0.3145	0.1406
23	O29	-3.5141	-0.1149	-0.0792
24	N30	-1.3788	-0.696	-0.7593
25	C31	-1.8508	-0.8653	-2.1394
26	H32	-1.0162	-1.1571	-2.778
27	H33	-2.6207	-1.6422	-2.2009
28	H34	-2.2723	0.0682	-2.528
29	O22	-0.8214	3.2093	-0.1276
30	H23	-0.2214	2.4488	-0.0237
31	C24	-0.7429	3.6716	-1.4758
32	H25	-1.0488	2.8969	-2.1913
33	H26	-1.426	4.5197	-1.5699
34	H27	0.2696	4.0105	-1.7332



d) Coordinates for structure (4)

Number	Label	X	Y	Z
1	Sn1	-0.2778	-0.4167	0
2	C2	-1.154	-1.8195	1.3331
3	H3	-0.396	-2.4667	1.7787
4	H4	-1.6934	-1.29	2.1216
5	C5	-0.4252	-0.2807	-2.1094
6	H6	0.376	0.3626	-2.4793
7	H7	-1.3947	0.1321	-2.3933
8	O8	-1.276	1.3637	0.5281
9	C9	-2.5687	1.3581	0.3024
10	O10	-3.1549	0.3685	-0.1612
11	C11	-3.2834	2.6474	0.6429
12	H12	-4.3588	2.5409	0.4966
13	H13	-3.0747	2.9284	1.6795
14	H14	-2.9061	3.453	0.0044
15	H15	-1.8646	-2.4362	0.7767
16	H16	-0.3075	-1.2789	-2.5392
17	O17	1.8889	1.8568	-0.6911
18	C18	2.3308	3.0687	-1.3413
19	H19	2.3089	2.846	-2.407
20	H20	1.6526	3.8918	-1.1077
21	H21	3.345	3.3189	-1.0236
22	C22	1.8216	1.885	0.6546
23	O23	2.1007	2.8599	1.3351
24	N24	1.3966	0.6465	1.139
25	C25	1.2954	0.5799	2.6123
26	H26	1.067	-0.4484	2.8982
27	H27	2.2402	0.874	3.0762
28	H28	0.5014	1.2365	2.9767
29	O29	1.7186	-1.3361	-0.1267
30	C31	2.1416	-2.6708	0.1218
31	H32	1.9746	-2.9669	1.1664
32	H33	1.5956	-3.3652	-0.528
33	H34	3.2119	-2.7634	-0.0981
34	H30	1.939	-0.3406	0.634

