Electronic Supplementary Material (ESI) for Dalton Transactions

Supporting Information

Synthesis, characterization and coordination properties of bis(alkyl)selenosalen ligands

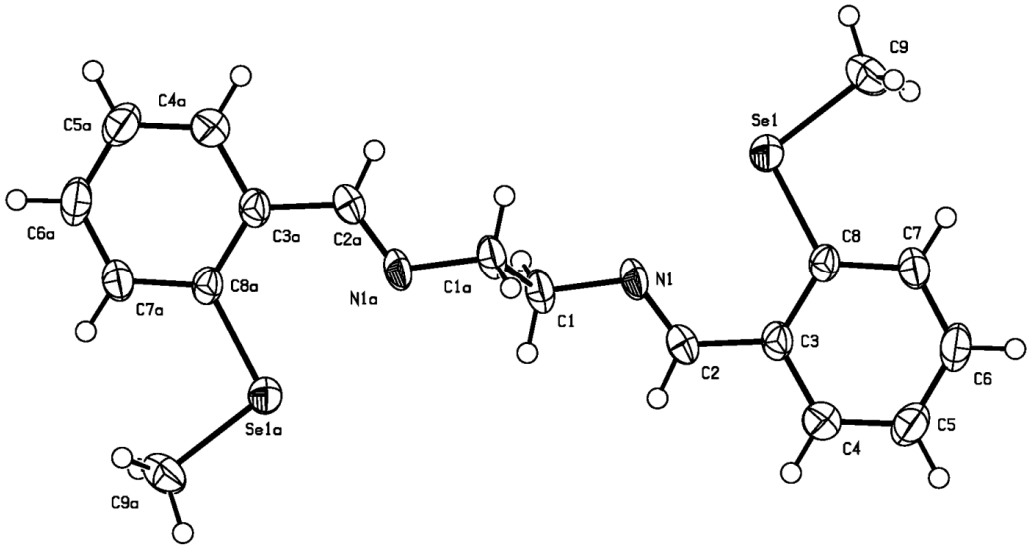
Snigdha Panda,* G. Rama Krishna, C. Malla Reddy, Sanjio S. Zade*

Department of Chemical Sciences, Indian Institute of Science Education and Research, Kolkata, PO: BCKV campus main office, Mohanpur 741252, Nadia, West Bengal, India.

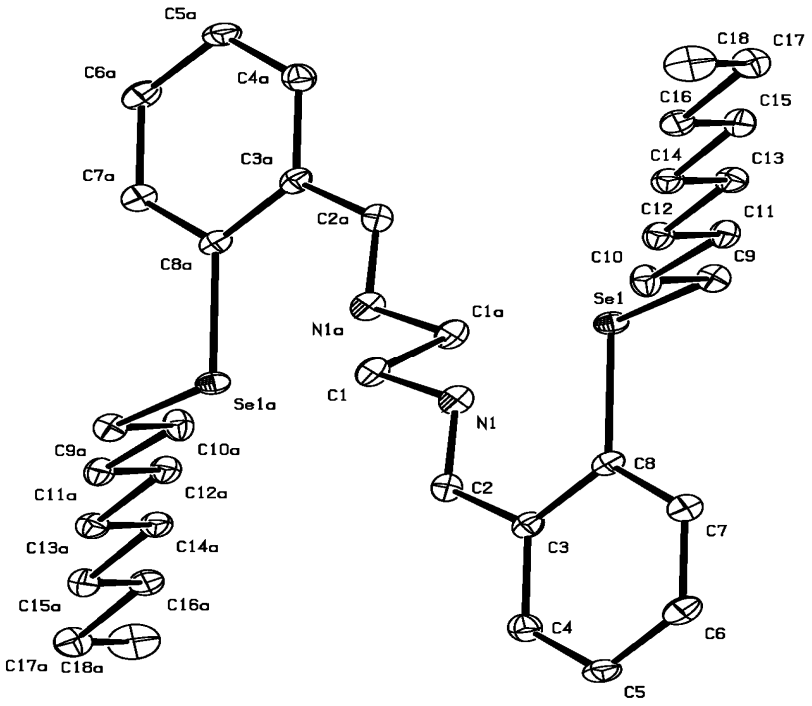
Email: snigdha@iiserkol.ac.in, sanjiozade@iiserkol.ac.in

Fax: +91-33-25873020

Table of contents



(a)



(b)

Figure S1. ORTEP representation of podand (a) **4** and (b) **5** (H atoms are omitted for clarity)**.** Thermal ellipsoids are drawn at 50% probability. Atoms labeled with the suffix *a* are generated by the symmetry operator (– x – 1, – y + 2, – z + 1) and (– x + 2, – y +1, – z +1) for compound **4** and **5** respectively.

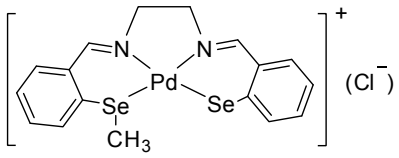
Table S1. Calculated absolute energies in Hartrees at B3LYP/6-31G(d)/sdd(Pt).

Compound	B3LYP/6-31G(d)/sdd(Pt)	ZPVE	G°	Single Point-methanol solvent[a]	BSSE correction
7.Cl	-6153.5805458	0.305681	-6153.329762	-6153.637818	0.0082990
11	-6653.6738131	0.344196	-6653.392577	-6653.732627	0.0088066
12	-6653.6435974	0.344527	-6653.360162	-6653.72491	0.0161592
13	-6653.6558426	0.344597	-6653.369423	-6653.699281	0.0098653
S_N2-TS	-6653.6280570	0.343515	-6653.345590	-6653.698264	0.0087355
TS1	-6653.5979661	0.341515	-6653.316017	-6653.646654	0.0093467
TS2	-6653.5988415	0.341721	-6653.317897	-6653.646852	0.0091860

[a]Gas phase geometries are taken for single point calculation in methanol solvent at B3LYP/6-31G(d)/sdd(Pt).

Coordinates of the optimized geometries

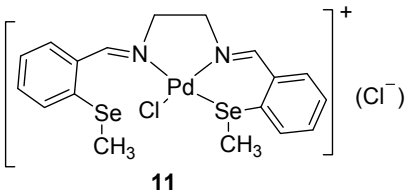
7.Cl



7.Cl

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	-0.337981	0.495126	0.051869
2	34	0	1.575033	-1.032748	0.173296
3	6	0	3.097824	1.549024	-0.194799
4	6	0	4.133845	-0.530206	-0.918886
5	1	0	4.108570	-1.617759	-0.963924
6	6	0	3.049447	0.141030	-0.353047
7	6	0	4.271519	2.225942	-0.591320
8	1	0	4.324720	3.303261	-0.453552
9	6	0	5.344313	1.553985	-1.165296
10	1	0	6.229712	2.104036	-1.470169
11	6	0	5.269417	0.173229	-1.334765
12	1	0	6.099522	-0.374441	-1.771349
13	6	0	2.056494	2.425874	0.328132
14	1	0	2.396161	3.443622	0.549396
15	7	0	0.810953	2.164359	0.516199
16	6	0	-0.081770	3.216636	1.017485
17	1	0	0.407421	4.199477	0.999686
18	1	0	-0.344884	2.975022	2.054292
19	6	0	-1.349948	3.234749	0.160023
20	1	0	-2.079948	3.937548	0.582660
21	1	0	-1.093769	3.573054	-0.852268
22	7	0	-1.903599	1.875715	0.073390
23	6	0	-3.190176	1.737317	0.053918
24	1	0	-3.781330	2.655244	0.147866
25	6	0	-3.989680	0.541764	-0.075476
26	6	0	-4.481062	-1.812260	-0.407837
27	1	0	-4.134652	-2.828125	-0.573408
28	6	0	-3.518811	-0.784784	-0.294250
29	6	0	-5.389701	0.766267	0.018518
30	1	0	-5.738366	1.783449	0.183066
31	6	0	-6.308882	-0.257437	-0.091776
32	1	0	-7.372413	-0.055044	-0.012951
33	6	0	-5.840466	-1.563001	-0.309768
34	1	0	-6.542897	-2.387120	-0.400936
35	34	0	-1.729432	-1.378212	-0.489432
36	6	0	1.813888	-0.993112	2.138226
37	1	0	2.729613	-1.559667	2.313277
38	1	0	0.947354	-1.514315	2.549036
39	1	0	1.849361	0.038733	2.489638
40	17	0	3.595500	-3.324163	0.646512

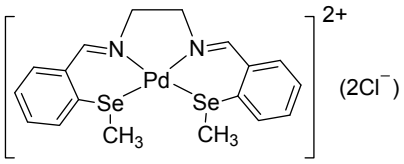
11



11

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	34	0	-1.860866	-1.042222	-0.242614
2	6	0	-2.398243	-1.524357	-2.087261
3	1	0	-2.632899	-0.615546	-2.641624
4	1	0	-1.529344	-2.029811	-2.507289
5	6	0	0.041740	3.284616	0.103287
6	1	0	0.530231	3.261429	1.084875
7	1	0	-0.478991	4.243630	-0.007811
8	6	0	-3.372131	0.140210	0.155376
9	6	0	-3.300926	1.535570	0.402215
10	6	0	-2.139758	2.411556	0.351398
11	1	0	-2.370483	3.446582	0.622515
12	6	0	-4.603445	-0.513541	0.266939
13	1	0	-4.630642	-1.596219	0.141639
14	6	0	-5.716851	1.562933	0.824587
15	1	0	-6.614669	2.117306	1.081306
16	6	0	-4.495975	2.215337	0.738673
17	1	0	-4.447950	3.284037	0.932591
18	6	0	-5.765741	0.189657	0.587720
19	1	0	-6.705312	-0.350209	0.664514
20	7	0	-0.914937	2.160311	0.037854
21	34	0	2.171620	0.034475	1.808866
22	6	0	2.890119	-0.908282	3.386427
23	1	0	2.281305	-0.564534	4.225784
24	1	0	3.933927	-0.637594	3.554911
25	6	0	1.103551	3.116064	-0.983839
26	1	0	1.838057	3.930434	-0.925861
27	1	0	0.627639	3.138300	-1.972086
28	6	0	3.557774	-0.348142	0.534700
29	6	0	3.788059	0.496474	-0.580871
30	6	0	2.992302	1.679231	-0.903868
31	1	0	3.563118	2.538920	-1.279949
32	6	0	4.408691	-1.443894	0.724190
33	1	0	4.240856	-2.120424	1.553463
34	6	0	5.722231	-0.845230	-1.220688
35	1	0	6.553949	-1.032118	-1.892659
36	6	0	4.891679	0.249249	-1.418285
37	1	0	5.075609	0.924680	-2.250493
38	6	0	5.468048	-1.697949	-0.144679
39	1	0	6.100372	-2.564521	0.027790
40	7	0	1.720304	1.804857	-0.780182
41	1	0	-3.240627	-2.204752	-1.973322
42	1	0	2.776950	-1.988548	3.283629
43	46	0	0.003394	0.447717	-0.638682
44	17	0	1.039572	-1.316247	-1.793186
45	17	0	-3.372348	-3.558212	0.333483

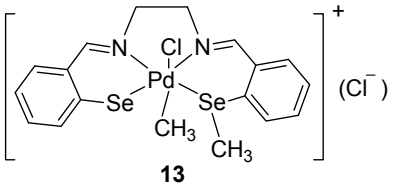
12



12

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	34	0	-1.760051	-0.832615	0.522991
2	6	0	-1.444257	-2.244817	-0.836869
3	1	0	-1.510445	-1.804298	-1.831531
4	1	0	-0.448540	-2.661022	-0.669612
5	6	0	-0.635565	3.592883	0.751957
6	1	0	-0.409596	3.479161	1.819302
7	1	0	-1.234397	4.503606	0.619439
8	6	0	-3.306501	0.022968	-0.308806
9	6	0	-3.532510	1.421211	-0.345359
10	6	0	-2.628180	2.477601	0.087295
11	1	0	-3.106851	3.455918	0.210008
12	6	0	-4.309868	-0.842436	-0.751187
13	1	0	-4.189179	-1.910945	-0.614010
14	6	0	-5.738997	1.027213	-1.326875
15	1	0	-6.673582	1.417994	-1.717250
16	6	0	-4.767654	1.892177	-0.843245
17	1	0	-4.949014	2.964123	-0.852984
18	6	0	-5.504074	-0.346363	-1.277779
19	1	0	-6.260631	-1.046582	-1.619349
20	7	0	-1.364922	2.400934	0.308867
21	34	0	1.705997	-0.885081	-0.346213
22	6	0	1.692592	-1.850072	1.391182
23	1	0	0.708528	-2.309542	1.498325
24	1	0	1.880221	-1.141311	2.197867
25	6	0	0.669183	3.699220	-0.038593
26	1	0	1.271773	4.537348	0.334284
27	1	0	0.434795	3.886574	-1.094321
28	6	0	3.432278	-0.000440	-0.097204
29	6	0	3.666315	1.391437	0.036462
30	6	0	2.694451	2.477690	0.049227
31	1	0	3.156840	3.471413	0.051890
32	6	0	4.514154	-0.884654	-0.147698
33	1	0	4.317072	-1.944004	-0.324297
34	6	0	6.075262	0.945915	0.131295
35	1	0	7.091208	1.317903	0.223192
36	6	0	5.005967	1.830812	0.145375
37	1	0	5.196267	2.896886	0.242199
38	6	0	5.824286	-0.417155	-0.021552
39	1	0	6.644615	-1.128088	-0.060255
40	7	0	1.408949	2.430384	0.043802
41	1	0	-2.198608	-3.003995	-0.635053
42	1	0	2.449293	-2.627096	1.288969
43	46	0	0.024577	0.823221	0.090837
44	17	0	2.794361	-3.604633	-1.138453
45	17	0	-3.500947	-2.912950	1.649616

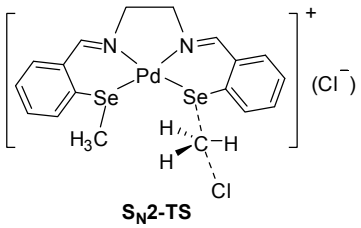
13



13

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	34	0	-1.569858	1.197519	0.101712
2	6	0	-1.945014	1.660791	1.985220
3	1	0	-1.923202	0.742923	2.571841
4	1	0	-1.152117	2.349931	2.275979
5	6	0	0.379995	-2.878158	-1.362214
6	1	0	0.949006	-2.483210	-2.212258
7	1	0	-0.113637	-3.810388	-1.668151
8	6	0	-3.086863	-0.023861	-0.192039
9	6	0	-3.013491	-1.307070	-0.789473
10	6	0	-1.837222	-2.092063	-1.178434
11	1	0	-2.100115	-3.018756	-1.702193
12	6	0	-4.335085	0.519322	0.118417
13	1	0	-4.396802	1.534702	0.490644
14	6	0	-5.462837	-1.453974	-0.695730
15	1	0	-6.371149	-2.014766	-0.893808
16	6	0	-4.225841	-1.987142	-1.034061
17	1	0	-4.180678	-2.970966	-1.493567
18	6	0	-5.514015	-0.191033	-0.114319
19	1	0	-6.466064	0.262967	0.144189
20	7	0	-0.598741	-1.867030	-0.955060
21	34	0	1.635738	0.906414	-1.213920
22	6	0	1.206625	0.755269	1.920673
23	6	0	1.353321	-3.150499	-0.197189
24	1	0	2.086586	-3.911521	-0.499259
25	1	0	0.793406	-3.497769	0.676417
26	6	0	3.406062	0.733430	-0.512649
27	6	0	3.977456	-0.469044	-0.015793
28	6	0	3.260125	-1.738795	0.010510
29	1	0	3.877465	-2.635654	-0.135393
30	6	0	4.225060	1.873419	-0.585548
31	1	0	3.798463	2.799800	-0.957105
32	6	0	6.120537	0.652521	0.300716
33	1	0	7.158784	0.621711	0.616690
34	6	0	5.332981	-0.488242	0.368334
35	1	0	5.760497	-1.421061	0.729650
36	6	0	5.558371	1.837714	-0.186419
37	1	0	6.160253	2.740006	-0.252771
38	7	0	1.991905	-1.882026	0.126240
39	1	0	-2.901118	2.177123	1.999953
40	46	0	0.327374	-0.413384	0.448420
41	17	0	-0.757133	-1.712517	2.201252
42	1	0	2.202742	0.334352	2.061760
43	1	0	1.269432	1.800044	1.614574
44	1	0	0.599893	0.617923	2.813855
45	17	0	-3.037214	3.476779	-0.450169

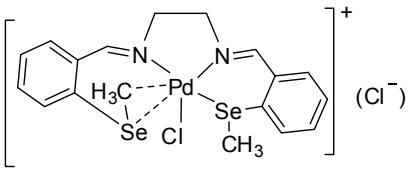
S_N2-TS



S_N2-TS

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	34	0	-1.844914	-0.975796	0.359704
2	6	0	-1.663635	-2.253286	-1.146157
3	1	0	-1.545700	-1.702188	-2.079419
4	1	0	-0.773954	-2.842591	-0.920512
5	6	0	0.047069	3.217093	-0.164307
6	1	0	0.363707	3.200074	0.889782
7	1	0	-0.399928	4.193407	-0.390174
8	6	0	-3.327731	0.087052	-0.359024
9	6	0	-3.306574	1.484572	-0.594846
10	6	0	-2.180355	2.401958	-0.457299
11	1	0	-2.463780	3.459187	-0.436436
12	6	0	-4.520044	-0.622659	-0.521960
13	1	0	-4.545497	-1.676367	-0.246511
14	6	0	-5.678448	1.394106	-1.197153
15	1	0	-6.581377	1.904510	-1.518293
16	6	0	-4.506264	2.111225	-0.997880
17	1	0	-4.500718	3.185903	-1.161548
18	6	0	-5.681029	0.021241	-0.956163
19	1	0	-6.591877	-0.558031	-1.076796
20	7	0	-0.927808	2.131374	-0.377975
21	34	0	1.646380	-1.380951	0.605979
22	6	0	2.093021	0.335516	2.211943
23	6	0	1.265732	2.967184	-1.048133
24	1	0	2.050099	3.692831	-0.807623
25	1	0	0.992346	3.074416	-2.106150
26	6	0	3.254108	-1.148513	-0.416559
27	6	0	3.688692	0.050801	-1.038231
28	6	0	2.974265	1.323493	-1.112901
29	1	0	3.592624	2.149825	-1.479949
30	6	0	4.082501	-2.277578	-0.468116
31	1	0	3.750440	-3.193471	0.010783
32	6	0	5.760643	-1.067922	-1.716213
33	1	0	6.724182	-1.028593	-2.214463
34	6	0	4.954379	0.060553	-1.665985
35	1	0	5.297603	0.982758	-2.128265
36	6	0	5.317514	-2.246750	-1.113112
37	1	0	5.932301	-3.141861	-1.137318
38	7	0	1.746579	1.586912	-0.836230
39	1	0	-2.551072	-2.882803	-1.106143
40	46	0	0.119701	0.362572	-0.218935
41	17	0	2.095388	2.762889	3.023864
42	1	0	2.628960	0.923526	1.494611
43	1	0	2.658550	-0.164317	2.990670
44	1	0	1.055758	0.542476	2.404058
45	17	0	-3.567344	-3.217248	1.289636

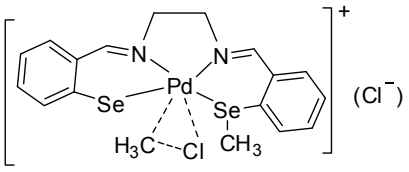
TS1



TS1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	34	0	-2.246805	1.694272	-0.385611
2	6	0	-0.418766	1.699244	-1.994901
3	6	0	-3.541514	0.254542	-0.301869
4	46	0	-0.216675	0.102135	-0.150190
5	1	0	-1.025060	1.331866	-2.813509
6	1	0	0.600386	1.317229	-2.023696
7	1	0	-0.447237	2.777296	-1.854619
8	6	0	-3.728282	-0.534043	0.858652
9	6	0	-4.429246	0.111347	-1.373876
10	7	0	0.698672	1.177291	1.485823
11	7	0	-1.588078	-0.437630	1.972643
12	34	0	1.897701	-1.261339	0.142327
13	17	0	-1.020814	-1.409815	-1.794294
14	6	0	-2.856758	-0.416547	2.049506
15	6	0	-4.818080	-1.413179	0.918135
16	1	0	-4.288799	0.723900	-2.257971
17	6	0	-5.480484	-0.803237	-1.317033
18	6	0	-0.118811	1.321255	2.700534
19	6	0	1.902536	1.624177	1.501413
20	6	0	-0.775633	-0.019949	3.093532
21	6	0	2.068528	-2.364496	-1.476875
22	6	0	2.998687	0.266790	-0.326710
23	1	0	-3.367368	-0.262935	3.015366
24	6	0	-5.679055	-1.567580	-0.166439
25	1	0	-4.975619	-1.996606	1.822475
26	1	0	-6.149784	-0.907294	-2.166412
27	1	0	-0.912106	2.043618	2.480179
28	1	0	0.492952	1.696113	3.531140
29	6	0	2.882754	1.454955	0.425106
30	1	0	2.249417	2.176341	2.382094
31	1	0	0.002060	-0.768819	3.282019
32	1	0	-1.353872	0.132979	4.020042
33	1	0	1.288572	-3.119779	-1.386048
34	1	0	3.062543	-2.806044	-1.427213
35	1	0	1.883591	-1.758176	-2.361944
36	6	0	3.984235	0.164967	-1.307358
37	1	0	-6.501738	-2.274485	-0.110415
38	6	0	3.777693	2.510749	0.184902
39	1	0	4.129657	-0.766509	-1.838749
40	6	0	4.826261	1.246528	-1.572898
41	6	0	4.729178	2.422051	-0.826107
42	1	0	3.707336	3.410604	0.791231
43	1	0	5.583897	1.151846	-2.345289
44	1	0	5.400645	3.253333	-1.017373
45	17	0	4.358667	-2.454623	0.902738

TS2



TS2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	-0.326854	-0.403344	0.164261
2	34	0	1.584182	1.149420	0.098313
3	6	0	3.160782	-1.403151	-0.520090
4	6	0	4.268087	0.461044	0.587901
5	1	0	4.230412	1.481001	0.961156
6	6	0	3.116218	-0.093171	0.026529
7	6	0	4.395540	-2.083360	-0.493393
8	1	0	4.442857	-3.083756	-0.916621
9	6	0	5.540663	-1.526278	0.065493
10	1	0	6.471267	-2.086091	0.070158
11	6	0	5.471918	-0.250336	0.614628
12	1	0	6.349712	0.211125	1.057467
13	6	0	2.068605	-2.205051	-1.086961
14	1	0	2.396839	-3.176988	-1.482211
15	7	0	0.825525	-1.914072	-1.120566
16	6	0	-0.143072	-2.885990	-1.611963
17	1	0	0.330802	-3.841580	-1.884038
18	1	0	-0.628821	-2.469547	-2.502875
19	6	0	-1.212702	-3.136569	-0.529655
20	1	0	-1.944690	-3.868277	-0.898344
21	1	0	-0.726892	-3.537312	0.367151
22	7	0	-1.862993	-1.874649	-0.165933
23	6	0	-3.142680	-1.777475	-0.207569
24	1	0	-3.719995	-2.685622	-0.422284
25	6	0	-3.940520	-0.575387	-0.000132
26	6	0	-4.407815	1.800668	-0.059119
27	1	0	-4.077608	2.817679	-0.245968
28	6	0	-3.490479	0.750084	-0.254908
29	6	0	-5.273945	-0.790633	0.411168
30	1	0	-5.607344	-1.812201	0.581386
31	6	0	-6.154475	0.261653	0.609625
32	1	0	-7.170648	0.073294	0.941944
33	6	0	-5.711065	1.567257	0.366727
34	1	0	-6.384432	2.408030	0.510485
35	34	0	-1.793130	1.243712	-0.979540
36	6	0	1.557769	1.637534	-1.817262
37	1	0	2.545337	2.041738	-2.030836
38	1	0	0.808751	2.423858	-1.916365
39	1	0	1.298067	0.761693	-2.411728
40	17	0	0.486992	-1.459667	2.305049
41	6	0	-0.995778	0.344500	2.540663
42	1	0	-1.073603	-0.082339	3.530443
43	1	0	-1.938951	0.399331	2.009427
44	1	0	-0.356650	1.216585	2.467086
45	17	0	3.249189	3.574122	0.152342

CH_3Cl

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	0.000000	-1.139252
2	1	0	1.033881	0.000000	-1.485487
3	1	0	-0.516941	0.895367	-1.485487
4	1	0	-0.516941	-0.895367	-1.485487
5	17	0	0.000000	0.000000	0.664234