

COORDINATES OF THE STRUCTURES

The optimized Cartesian coordinates of all structures obtained at the DFT level used in this work are provided below:

Coordinates for PCM

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.944615	-0.037710	-0.139285
2	6	0	0.450545	-0.037710	-0.139285
3	6	0	1.148083	1.170041	-0.139285
4	6	0	0.450429	2.378550	-0.140484
5	6	0	-0.944396	2.378472	-0.140963
6	6	0	-1.641997	1.170266	-0.139967
7	1	0	1.000053	-0.990223	-0.137970
8	1	0	2.247763	1.170121	-0.138651
9	1	0	-1.494518	3.330753	-0.141916
10	1	0	-2.741601	1.170449	-0.140147
11	8	0	-1.659555	-1.276160	-0.138700
12	1	0	-1.820211	-1.553007	0.766366
13	7	0	1.185911	3.651330	-0.140563
14	1	0	0.937948	4.179650	0.671466
15	6	0	0.840800	4.416605	-1.347275
16	8	0	1.373351	5.489030	-1.616722
17	1	0	0.066245	3.959857	-1.998859

COF-PEDOT Coordinates:

Center	Atomic	Atomic	Coordinates (Angstroms)		
Number	Number	Type	X	Y	Z

1	8	0	-7.420191	0.124538	-1.058035
2	5	0	-4.900996	6.348859	-1.216795
3	8	0	-9.480348	-1.037373	-1.027558
4	6	0	-7.257979	2.657791	-1.082169
5	5	0	-5.023932	-6.147110	-1.060278
6	8	0	-9.455085	1.330129	-1.074450
7	6	0	-7.311558	-2.411214	-1.064460
8	5	0	-8.075812	1.331731	-1.068497
9	5	0	-8.101565	-1.068740	-1.049107
10	5	0	-10.158036	0.153789	-1.045509
11	8	0	-5.537588	7.569325	-1.308264
12	6	0	-7.883538	3.903594	-1.237113
13	6	0	-5.107308	3.785218	-0.993606
14	1	0	-8.971346	3.949996	-1.331544
15	1	0	-4.018923	3.738263	-0.894527
16	6	0	-5.912897	-2.392700	-1.194142
17	6	0	-7.231440	-4.833509	-0.948449
18	1	0	-5.400952	-1.432986	-1.299213
19	1	0	-7.746631	-5.792634	-0.855416
20	6	0	-5.859798	2.615793	-0.952306
21	6	0	-7.130681	5.073241	-1.275198
22	1	0	-5.365367	1.650830	-0.814698
23	1	0	-7.627290	6.038736	-1.398113

24	6	0	-7.961379	-3.648703	-0.946948
25	6	0	-5.182832	-3.576885	-1.193641
26	1	0	-9.049789	-3.676731	-0.852081
27	1	0	-4.094000	-3.546661	-1.293173
28	6	0	-5.832495	-4.815630	-1.066965
29	6	0	-5.731890	5.031995	-1.160519
30	5	0	-4.826149	8.738523	-1.338814
31	8	0	-3.648824	-6.141695	-1.115816
32	8	0	-3.525428	6.324899	-1.177674
33	8	0	-5.676977	-7.360782	-0.998708
34	5	0	-2.928286	-7.312781	-1.118472
35	8	0	5.762105	-7.470423	-1.377693
36	6	0	1.453370	-7.338869	-1.258783
37	5	0	8.251807	-1.193764	-1.226665
38	8	0	3.677408	-8.582972	-1.367290
39	6	0	5.953310	-4.924673	-1.296934
40	8	0	3.753074	-6.218170	-1.287215
41	5	0	5.128763	-6.246866	-1.321347
42	5	0	5.045096	-8.637124	-1.402602
43	5	0	3.011129	-7.376269	-1.306411
44	8	0	-3.614496	-8.509256	-1.075944
45	8	0	7.594335	0.013577	-1.197612
46	6	0	0.721388	-8.536112	-1.284161
47	6	0	-0.639487	-6.106463	-1.140673
48	1	0	1.255370	-9.487740	-1.339508
49	1	0	-1.171846	-5.153458	-1.077111
50	6	0	5.305713	-3.680022	-1.252339
51	6	0	8.091059	-3.769994	-1.295388

52	1	0	4.213700	-3.645260	-1.234548
53	1	0	9.183195	-3.804402	-1.311445
54	6	0	7.356890	-4.951756	-1.318658
55	6	0	6.039313	-2.499067	-1.231202
56	1	0	7.872205	-5.914694	-1.353758
57	1	0	5.523558	-1.536415	-1.197614
58	6	0	0.751525	-6.124274	-1.185253
59	6	0	-0.668234	-8.519646	-1.237946
60	1	0	1.310077	-5.185030	-1.161424
61	1	0	-1.226613	-9.458598	-1.255939
62	6	0	-1.370082	-7.306043	-1.167599
63	6	0	7.443085	-2.525672	-1.251830
64	5	0	-4.981754	-8.540093	-1.011644
65	5	0	8.277600	1.206649	-1.175427
66	8	0	9.630760	-1.190952	-1.232746
67	8	0	-3.458947	8.689795	-1.288685
68	5	0	-2.788668	7.485686	-1.218876
69	8	0	5.905863	7.533476	-1.061915
70	6	0	1.594539	7.464611	-1.134388
71	8	0	3.876815	6.312224	-1.113914
72	8	0	3.838485	8.678790	-1.072172
73	6	0	6.053886	4.982753	-1.112188
74	5	0	5.207239	8.711654	-1.049749
75	5	0	5.252913	6.319477	-1.094862
76	5	0	3.153021	7.481868	-1.105463
77	6	0	0.878588	6.256605	-1.167826
78	6	0	-0.514032	8.668119	-1.159962
79	1	0	1.426212	5.310749	-1.173906

80	1	0	-1.061911	9.613392	-1.159813
81	6	0	7.457807	4.982839	-1.101350
82	6	0	6.092442	2.555477	-1.159981
83	1	0	7.992043	5.935786	-1.078328
84	1	0	5.558273	1.602607	-1.183247
85	6	0	0.876178	8.670321	-1.130850
86	6	0	-0.512911	6.253235	-1.193764
87	1	0	1.421156	9.617024	-1.106280
88	1	0	-1.055505	5.304481	-1.223870
89	6	0	5.382127	3.750515	-1.141683
90	6	0	8.168779	3.786798	-1.120742
91	1	0	4.289531	3.737289	-1.150778
92	1	0	9.261472	3.800076	-1.113322
93	6	0	7.496544	2.555014	-1.150406
94	6	0	-1.230132	7.460999	-1.189434
95	8	0	9.656118	1.174852	-1.177907
96	5	0	10.334593	-0.015461	-1.207012
97	1	0	-11.359162	0.166833	-1.036376
98	1	0	-5.394579	9.794377	-1.409084
99	1	0	5.789238	9.761936	-1.019894
100	1	0	11.535618	-0.028228	-1.210023
101	1	0	5.610008	-9.695832	-1.454880
102	1	0	-5.564470	-9.589583	-0.967202
103	6	0	7.173829	1.018775	2.077908
104	6	0	8.567352	1.016685	2.682804
105	6	0	8.629794	3.323114	2.607368
106	6	0	7.192122	3.325255	1.983284
107	6	0	6.659800	-0.228462	1.924354

108	6	0	9.027392	-0.232033	2.951989
109	1	0	9.121468	4.258091	2.777617
110	1	0	6.734330	4.261640	1.741394
111	1	0	9.929299	-0.454538	3.482988
112	6	0	5.214247	-0.544417	1.497470
113	16	0	3.969295	0.667203	1.131721
114	6	0	4.698194	-1.791543	1.349686
115	6	0	2.668398	-0.539423	1.073102
116	6	0	3.199681	-1.788594	1.099953
117	6	0	4.732073	-4.098250	1.265300
118	6	0	3.186096	-4.095201	1.007728
119	8	0	5.395174	-3.022703	1.419703
120	8	0	2.512909	-3.017017	0.939442
121	8	0	6.551223	2.249418	1.754941
122	8	0	9.231552	2.245412	2.918477
123	16	0	7.902980	-1.439797	2.297122
124	1	0	5.246925	-5.035023	1.313067
125	1	0	2.679965	-5.029962	0.885431
126	6	0	1.163782	-0.217667	1.008156
127	6	0	-1.409116	-0.211350	1.212306
128	6	0	0.632608	1.031627	0.987242
129	6	0	-0.881765	1.035372	1.107402
130	16	0	-0.137793	-1.423943	0.956934
131	6	0	0.655002	3.338051	0.892678
132	6	0	-0.907365	3.341940	1.016659
133	8	0	-1.581695	2.266827	1.115357
134	8	0	1.331119	2.259587	0.884238
135	1	0	1.170142	4.272460	0.812661

136	1	0	-1.424035	4.278927	1.018548
137	6	0	-2.886222	-0.525917	1.513795
138	6	0	-5.459127	-0.519162	1.717833
139	6	0	-3.413778	-1.772575	1.618601
140	6	0	-4.928195	-1.768597	1.738642
141	6	0	-3.388566	-4.079155	1.709116
142	6	0	-4.950958	-4.075060	1.832859
143	16	0	-4.157331	0.686832	1.769274
144	8	0	-2.714050	-3.004135	1.610630
145	8	0	-5.626915	-2.996480	1.841438
146	1	0	-2.872033	-5.016214	1.707207
147	1	0	-5.466249	-5.009423	1.912584
148	6	0	-6.963610	-0.196802	1.652841
149	6	0	-9.536500	-0.189813	1.856788
150	6	0	-7.494448	1.052664	1.632001
151	6	0	-9.008839	1.056790	1.752091
152	6	0	-7.471489	3.359103	1.537667
153	6	0	-9.033864	3.363374	1.661610
154	1	0	-6.956115	4.293396	1.457772
155	1	0	-9.550299	4.300493	1.663570
156	16	0	-8.265493	-1.402706	1.601437
157	1	0	-10.562793	-0.408200	2.066357
158	8	0	-9.708467	2.288419	1.760192
159	8	0	-6.795632	2.280466	1.529121

P@COF-PEDOT Coordinates

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	8	0	-7.257384	-0.466730	-1.210814
2	5	0	-5.085377	5.872095	-1.346361
3	8	0	-9.249257	-1.743764	-1.157480
4	6	0	-7.236499	2.068170	-1.216447
5	5	0	-4.505872	-6.581614	-1.308359
6	8	0	-9.357191	0.623844	-1.188432
7	6	0	-7.005425	-2.989708	-1.238705
8	5	0	-7.980341	0.701091	-1.202555
9	5	0	-7.870679	-1.696598	-1.200221
10	5	0	-9.991497	-0.591475	-1.157109
11	8	0	-5.783106	7.067136	-1.418909
12	6	0	-7.929809	3.278839	-1.351907
13	6	0	-5.149525	3.305529	-1.144578
14	1	0	-9.018271	3.267045	-1.431396
15	1	0	-4.060338	3.315176	-1.059401
16	6	0	-5.613491	-2.888704	-1.392049
17	6	0	-6.782000	-5.401863	-1.143492
18	1	0	-5.160846	-1.901217	-1.498011
19	1	0	-7.237703	-6.389148	-1.049708
20	6	0	-5.837319	2.099365	-1.105067
21	6	0	-7.242387	4.486236	-1.389301
22	1	0	-5.291289	1.162370	-0.982420
23	1	0	-7.790837	5.423640	-1.496945

24	6	0	-7.579308	-4.262925	-1.119854
25	6	0	-4.816449	-4.026878	-1.414915
26	1	0	-8.661114	-4.354961	-1.006579
27	1	0	-3.734737	-3.932780	-1.533654
28	6	0	-5.389701	-5.301171	-1.287320
29	6	0	-5.842194	4.517870	-1.292357
30	5	0	-5.153004	8.286945	-1.449341
31	8	0	-3.134130	-6.496413	-1.393778
32	8	0	-3.705113	5.912074	-1.322504
33	8	0	-5.088078	-7.830935	-1.244453
34	5	0	-2.349312	-7.625721	-1.424551
35	8	0	6.321428	-7.335186	-1.939565
36	6	0	2.018528	-7.417353	-1.683686
37	5	0	8.506540	-0.954219	-1.802657
38	8	0	4.293674	-8.548361	-1.873109
39	6	0	6.391531	-4.786555	-1.838954
40	8	0	4.256782	-6.182368	-1.770944
41	5	0	5.631170	-6.144416	-1.850080
42	5	0	5.660470	-8.534399	-1.952845
43	5	0	3.572515	-7.375654	-1.778631
44	8	0	-2.965373	-8.859869	-1.378083
45	8	0	7.789517	0.216599	-1.734588
46	6	0	1.349916	-8.650082	-1.699973
47	6	0	-0.130224	-6.297984	-1.493995
48	1	0	1.930415	-9.570684	-1.780425
49	1	0	-0.709235	-5.376132	-1.406831
50	6	0	5.687961	-3.575776	-1.758896
51	6	0	8.469483	-3.532200	-1.896255

52	1	0	4.598387	-3.593593	-1.704118
53	1	0	9.559531	-3.513538	-1.949322
54	6	0	7.792415	-4.746643	-1.907909
55	6	0	6.364239	-2.362937	-1.748282
56	1	0	8.350473	-5.682516	-1.971020
57	1	0	5.805724	-1.427462	-1.686203
58	6	0	1.257368	-6.242199	-1.577572
59	6	0	-0.035357	-8.706926	-1.614710
60	1	0	1.766100	-5.276340	-1.560561
61	1	0	-0.543729	-9.672489	-1.627206
62	6	0	-0.797102	-7.533439	-1.513218
63	6	0	7.764825	-2.322228	-1.816359
64	5	0	-4.326725	-8.967814	-1.283359
65	5	0	8.411874	1.442449	-1.721833
66	8	0	9.882685	-0.882071	-1.857612
67	8	0	-3.779996	8.337525	-1.418671
68	8	0	5.720326	7.622687	-1.416058
69	6	0	1.422268	7.334314	-1.354249
70	8	0	3.756381	6.295094	-1.408508
71	8	0	3.597524	8.659785	-1.345820
72	6	0	5.998043	5.087429	-1.510290
73	5	0	4.961331	8.761994	-1.367126
74	5	0	5.129113	6.376935	-1.439856
75	5	0	2.972228	7.427379	-1.365106
76	6	0	0.756928	6.095437	-1.373030
77	6	0	-0.738364	8.448032	-1.340812
78	1	0	1.332972	5.167860	-1.379040
79	1	0	-1.323287	9.369397	-1.330913

80	6	0	7.398258	5.163882	-1.556123
81	6	0	6.163929	2.669355	-1.601868
82	1	0	7.880198	6.143010	-1.538416
83	1	0	5.681960	1.690511	-1.619563
84	6	0	0.647099	8.507056	-1.336253
85	6	0	-0.627933	6.028953	-1.376967
86	1	0	1.148928	9.476000	-1.322986
87	1	0	-1.123514	5.056000	-1.395917
88	6	0	5.392536	3.822272	-1.534284
89	6	0	8.170191	4.009472	-1.623510
90	1	0	4.304004	3.750241	-1.500135
91	1	0	9.258703	4.081101	-1.658360
92	6	0	7.564164	2.745015	-1.647254
93	6	0	-1.405596	7.205170	-1.360269
94	8	0	9.789464	1.482660	-1.774871
95	5	0	10.524963	0.328405	-1.842931
96	1	0	-11.189955	-0.645737	-1.130044
97	1	0	-5.793102	9.299245	-1.503495
98	1	0	5.488788	9.839807	-1.347312
99	1	0	11.722972	0.377268	-1.889182
100	1	0	6.273263	-9.562805	-2.033997
101	1	0	-4.847310	-10.047951	-1.236210
102	6	0	6.909057	1.199316	2.869733
103	6	0	8.239968	1.267143	3.565704
104	6	0	8.310440	3.549528	3.228715
105	6	0	6.960154	3.480285	2.524699
106	6	0	6.397561	-0.055892	2.823639
107	6	0	8.668860	0.061388	4.009217

108	1	0	8.795916	4.499965	3.328732
109	1	0	6.525009	4.382793	2.144494
110	1	0	9.529059	-0.099699	4.628336
111	6	0	5.001688	-0.423393	2.337580
112	16	0	3.801850	0.729949	1.726010
113	6	0	4.490327	-1.678979	2.319501
114	6	0	2.510597	-0.483337	1.736161
115	6	0	3.030854	-1.713634	1.969938
116	6	0	4.501647	-3.975251	2.551942
117	6	0	3.019344	-4.011327	2.196567
118	8	0	5.171777	-2.874456	2.606454
119	8	0	2.348028	-2.941884	1.929209
120	8	0	6.319746	2.371310	2.367551
121	8	0	8.892936	2.503392	3.710654
122	16	0	7.590022	-1.216761	3.430332
123	1	0	5.007612	-4.895747	2.764924
124	1	0	2.514363	-4.956324	2.167043
125	6	0	1.030954	-0.188459	1.532066
126	6	0	-1.530185	-0.200017	1.595149
127	6	0	0.491677	1.034775	1.295563
128	6	0	-1.010784	1.026074	1.337588
129	16	0	-0.244612	-1.417179	1.589071
130	6	0	0.475616	3.303009	0.854987
131	6	0	-1.048349	3.291444	0.908104
132	8	0	-1.725592	2.217420	1.134518
133	8	0	1.181032	2.237107	1.042236
134	1	0	0.968366	4.233713	0.646800
135	1	0	-1.579206	4.208219	0.744734

136	6	0	-3.000743	-0.496925	1.860779
137	6	0	-5.566304	-0.515867	1.942942
138	6	0	-3.516118	-1.725342	2.116090
139	6	0	-5.017642	-1.736615	2.163661
140	6	0	-3.474542	-3.995771	2.532808
141	6	0	-4.998356	-4.007018	2.581126
142	16	0	-4.294101	0.714678	1.874375
143	8	0	-2.799180	-2.918475	2.312319
144	8	0	-5.702416	-2.940297	2.404539
145	1	0	-2.942503	-4.913472	2.686930
146	1	0	-5.505774	-4.932477	2.768137
147	6	0	-7.052986	-0.236678	1.771375
148	6	0	-9.615971	-0.255372	1.857465
149	6	0	-7.601191	0.984484	1.552858
150	6	0	-9.103734	0.972432	1.603869
151	6	0	-7.621870	3.255171	1.140055
152	6	0	-9.145599	3.243062	1.191628
153	1	0	-7.115214	4.181006	0.953152
154	1	0	-9.677777	4.161152	1.040094
155	16	0	-8.325331	-1.466599	1.839518
156	1	0	-10.649235	-0.467039	2.049228
157	8	0	-9.820999	2.165865	1.411540
158	8	0	-6.916995	2.188504	1.313224
159	15	0	-2.991611	7.145491	-1.364446

S@COF-PEDOT Coordinates

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	8	0	-7.384155	-0.125394	-1.032388
2	5	0	-4.999170	6.152328	-1.158002
3	8	0	-9.418891	-1.331366	-1.006038
4	6	0	-7.276309	2.410852	-1.041915
5	5	0	-4.854035	-6.344104	-1.074419
6	8	0	-9.444442	1.036366	-1.039115
7	6	0	-7.221209	-2.658153	-1.053785
8	5	0	-8.065513	1.067506	-1.034939
9	5	0	-8.039785	-1.333038	-1.029557
10	5	0	-10.121978	-0.154924	-1.016144
11	8	0	-5.661903	7.359376	-1.241507
12	6	0	-7.928645	3.643838	-1.188758
13	6	0	-5.150172	3.583597	-0.949545
14	1	0	-9.017331	3.667455	-1.281507
15	1	0	-4.060891	3.559413	-0.852153
16	6	0	-5.823452	-2.608902	-1.185169
17	6	0	-7.089029	-5.078807	-0.952049
18	1	0	-5.332344	-1.637836	-1.285288
19	1	0	-7.583412	-6.049283	-0.863960
20	6	0	-5.877366	2.398087	-0.914111
21	6	0	-7.201084	4.829560	-1.220977
22	1	0	-5.362172	1.443161	-0.782790
23	1	0	-7.718446	5.784884	-1.337599

24	6	0	-7.844191	-3.909953	-0.942672
25	6	0	-5.068174	-3.777144	-1.192540
26	1	0	-8.931614	-3.961862	-0.846561
27	1	0	-3.980383	-3.723003	-1.293305
28	6	0	-5.690958	-5.030249	-1.072271
29	6	0	-5.801569	4.817647	-1.108353
30	5	0	-4.975730	8.543717	-1.266139
31	8	0	-3.479439	-6.308884	-1.131706
32	8	0	-3.623350	6.157639	-1.120804
33	8	0	-5.480830	-7.571836	-1.019103
34	5	0	-2.733972	-7.464217	-1.142145
35	8	0	5.957425	-7.433985	-1.413543
36	6	0	1.647033	-7.395537	-1.288283
37	5	0	8.312242	-1.106374	-1.229031
38	8	0	3.897068	-8.591017	-1.406946
39	6	0	6.094139	-4.885234	-1.318143
40	8	0	3.922146	-6.225643	-1.313140
41	5	0	5.298085	-6.224637	-1.349221
42	5	0	5.265551	-8.615626	-1.444347
43	5	0	3.205166	-7.399251	-1.338148
44	8	0	-3.394320	-8.675356	-1.105728
45	8	0	7.629086	0.086403	-1.192065
46	6	0	0.940844	-8.608031	-1.319715
47	6	0	-0.471588	-6.208994	-1.160256
48	1	0	1.495020	-9.547653	-1.381319
49	1	0	-1.024159	-5.268008	-1.090431
50	6	0	5.420078	-3.655034	-1.265429
51	6	0	8.206648	-3.685015	-1.312613

52	1	0	4.327598	-3.643798	-1.246021
53	1	0	9.299247	-3.695904	-1.330286
54	6	0	7.497944	-4.882091	-1.341843
55	6	0	6.128228	-2.458765	-1.238335
56	1	0	8.033728	-5.833538	-1.383243
57	1	0	5.592008	-1.507604	-1.198449
58	6	0	0.919422	-6.196717	-1.206741
59	6	0	-0.448745	-8.621632	-1.271604
60	1	0	1.457749	-5.245869	-1.178142
61	1	0	-0.986896	-9.572220	-1.294365
62	6	0	-1.176342	-7.423785	-1.193251
63	6	0	7.532216	-2.455146	-1.260938
64	5	0	-4.760510	-8.735875	-1.039837
65	5	0	8.286655	1.293701	-1.163787
66	8	0	9.690808	-1.073962	-1.236882
67	8	0	-3.607729	8.524022	-1.218067
68	8	0	5.780027	7.567455	-1.010198
69	6	0	1.471070	7.406592	-1.077487
70	8	0	3.777547	6.303303	-1.066710
71	8	0	3.688563	8.668220	-1.011077
72	6	0	5.982612	5.020828	-1.075581
73	5	0	5.056330	8.730292	-0.990236
74	5	0	5.153200	6.339948	-1.049400
75	5	0	3.028864	7.457091	-1.050480
76	6	0	0.781127	6.183728	-1.117062
77	6	0	-0.662845	8.564743	-1.093289
78	1	0	1.348889	5.249883	-1.129384
79	1	0	-1.230857	9.498036	-1.086901

80	6	0	7.386223	5.050951	-1.066562
81	6	0	6.073114	2.595255	-1.137621
82	1	0	7.899944	6.014983	-1.038658
83	1	0	5.559458	1.631303	-1.165767
84	6	0	0.727038	8.596582	-1.065965
85	6	0	-0.610015	6.150676	-1.141216
86	1	0	1.251636	9.554593	-1.036565
87	1	0	-1.132193	5.190698	-1.176168
88	6	0	5.337376	3.774663	-1.111412
89	6	0	8.122637	3.870562	-1.093870
90	1	0	4.245303	3.738067	-1.119169
91	1	0	9.214804	3.907222	-1.087788
92	6	0	7.476916	2.624842	-1.129868
93	6	0	-1.352950	7.342739	-1.128892
94	8	0	9.665533	1.291482	-1.168238
95	5	0	10.369321	0.116179	-1.205185
96	1	0	-11.323093	-0.167688	-1.005379
97	1	0	-5.566758	9.587532	-1.329496
98	1	0	5.615726	9.792620	-0.954992
99	1	0	11.570339	0.129184	-1.209826
100	1	0	5.852949	-9.661657	-1.503548
101	1	0	-5.320535	-9.797858	-1.000780
102	6	0	7.191787	1.063274	2.089821
103	6	0	8.585893	1.087541	2.692888
104	6	0	8.598780	3.395179	2.630863
105	6	0	7.160508	3.370128	2.008666
106	6	0	6.704390	-0.193782	1.929640
107	6	0	9.072972	-0.152571	2.954169

108	1	0	9.070544	4.339476	2.805941
109	1	0	6.682409	4.297874	1.772850
110	1	0	9.980195	-0.358774	3.482688
111	6	0	5.265336	-0.538168	1.502789
112	16	0	3.994183	0.648589	1.145746
113	6	0	4.775921	-1.795191	1.348382
114	6	0	2.719364	-0.585290	1.081756
115	6	0	3.277336	-1.822918	1.100612
116	6	0	4.859111	-4.100111	1.250461
117	6	0	3.313059	-4.128711	0.994914
118	8	0	5.499227	-3.011511	1.410293
119	8	0	2.616822	-3.064829	0.933808
120	8	0	6.542490	2.282144	1.774865
121	8	0	9.223940	2.328834	2.934883
122	16	0	7.973775	-1.380333	2.293706
123	1	0	5.393989	-5.025892	1.292081
124	1	0	2.826906	-5.073381	0.867808
125	6	0	1.208107	-0.295495	1.020643
126	6	0	-1.364043	-0.345532	1.228160
127	6	0	0.650250	0.942224	1.007725
128	6	0	-0.863683	0.912800	1.129866
129	16	0	-0.067387	-1.529082	0.964052
130	6	0	0.623072	3.249109	0.926624
131	6	0	-0.938841	3.218778	1.052649
132	8	0	-1.589833	2.128897	1.145931
133	8	0	1.322135	2.185456	0.911000
134	1	0	1.117952	4.194798	0.851406
135	1	0	-1.475472	4.144445	1.060688

136	6	0	-2.833638	-0.693446	1.529717
137	6	0	-5.405804	-0.743044	1.737124
138	6	0	-3.334204	-1.951717	1.627912
139	6	0	-4.848187	-1.980909	1.749937
140	6	0	-3.259433	-4.257714	1.704902
141	6	0	-4.821377	-4.287839	1.830691
142	16	0	-4.130083	0.490264	1.793931
143	8	0	-2.608253	-3.167924	1.611832
144	8	0	-5.520282	-3.224067	1.846454
145	1	0	-2.722939	-5.183456	1.696843
146	1	0	-5.316410	-5.233483	1.905617
147	6	0	-6.916941	-0.452642	1.675968
148	6	0	-9.489098	-0.502005	1.883286
149	6	0	-7.474466	0.785256	1.663124
150	6	0	-8.988425	0.756212	1.785198
151	6	0	-7.501078	3.092166	1.582253
152	6	0	-9.063009	3.062217	1.708243
153	1	0	-7.005961	4.037744	1.507156
154	1	0	-9.599406	3.988021	1.716353
155	16	0	-8.192751	-1.685862	1.619198
156	1	0	-10.510176	-0.743563	2.092904
157	8	0	-9.714277	1.972490	1.801410
158	8	0	-6.802272	2.028336	1.566523
159	16	0	-2.911697	7.334176	-1.156171

Si@COF-PEDOT Coordinates

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	8	0	-7.391201	-0.079361	-1.036856
2	5	0	-4.981028	6.188615	-1.168246
3	8	0	-9.430764	-1.277137	-1.009787
4	6	0	-7.273181	2.456421	-1.048928
5	5	0	-4.886031	-6.308207	-1.071955
6	8	0	-9.446810	1.090644	-1.045271
7	6	0	-7.238409	-2.612774	-1.055645
8	5	0	-8.067768	1.116258	-1.040786
9	5	0	-8.051669	-1.284363	-1.032963
10	5	0	-10.129124	-0.097895	-1.021260
11	8	0	-5.638894	7.398225	-1.253138
12	6	0	-7.920531	3.691863	-1.197183
13	6	0	-5.142381	3.620723	-0.957221
14	1	0	-9.009091	3.719751	-1.290225
15	1	0	-4.053230	3.592269	-0.859535
16	6	0	-5.840434	-2.569262	-1.186733
17	6	0	-7.115963	-5.033835	-0.951421
18	1	0	-5.345410	-1.600276	-1.287715
19	1	0	-7.614256	-6.002230	-0.862471
20	6	0	-5.874332	2.438175	-0.920765
21	6	0	-7.188213	4.874624	-1.230424
22	1	0	-5.363004	1.481325	-0.788348
23	1	0	-7.701711	5.831897	-1.348143

24	6	0	-7.866433	-3.861952	-0.943417
25	6	0	-5.089845	-3.740530	-1.192732
26	1	0	-8.954079	-3.909402	-0.847522
27	1	0	-4.001821	-3.690855	-1.293283
28	6	0	-5.717679	-4.991005	-1.071347
29	6	0	-5.788784	4.857213	-1.117442
30	5	0	-4.947970	8.579780	-1.278801
31	8	0	-3.511292	-6.278559	-1.128939
32	8	0	-3.605206	6.188446	-1.130713
33	8	0	-5.517759	-7.533359	-1.015550
34	5	0	-2.770461	-7.436882	-1.138021
35	8	0	5.921053	-7.441781	-1.407299
36	6	0	1.610819	-7.385920	-1.283145
37	5	0	8.301183	-1.123480	-1.228620
38	8	0	3.856070	-8.590533	-1.400039
39	6	0	6.067964	-4.893503	-1.314449
40	8	0	3.890612	-6.225185	-1.308624
41	5	0	5.266553	-6.229734	-1.344366
42	5	0	5.224453	-8.620669	-1.437076
43	5	0	3.168937	-7.395934	-1.332620
44	8	0	-3.435670	-8.645326	-1.100539
45	8	0	7.622807	0.072064	-1.193033
46	6	0	0.899781	-8.595603	-1.313522
47	6	0	-0.503057	-6.190761	-1.156845
48	1	0	1.450198	-9.537502	-1.374036
49	1	0	-1.051866	-5.247497	-1.088111
50	6	0	5.398830	-3.660557	-1.263150
51	6	0	8.185269	-3.701760	-1.309614

52	1	0	4.306398	-3.644920	-1.244024
53	1	0	9.277819	-3.717050	-1.327006
54	6	0	7.471776	-4.896013	-1.337805
55	6	0	6.111765	-2.467110	-1.237094
56	1	0	8.003750	-5.849643	-1.378108
57	1	0	5.579354	-1.513767	-1.198305
58	6	0	0.888003	-6.184110	-1.202998
59	6	0	-0.489863	-8.603583	-1.265741
60	1	0	1.430131	-5.235399	-1.175230
61	1	0	-1.031817	-9.552027	-1.287671
62	6	0	-1.212670	-7.402749	-1.188783
63	6	0	7.515762	-2.469145	-1.259353
64	5	0	-4.802108	-8.700298	-1.034925
65	5	0	8.285206	1.276743	-1.165817
66	8	0	9.679870	-1.096605	-1.236163
67	8	0	-3.580071	8.554648	-1.230371
68	8	0	5.803722	7.560652	-1.019209
69	6	0	1.494171	7.417002	-1.087401
70	8	0	3.796202	6.304484	-1.074935
71	8	0	3.716690	8.669794	-1.021722
72	6	0	5.996108	5.013168	-1.081960
73	5	0	5.084689	8.726401	-1.000605
74	5	0	5.171986	6.335629	-1.057321
75	5	0	3.052149	7.461280	-1.060060
76	6	0	0.799339	6.196875	-1.125907
77	6	0	-0.635078	8.583684	-1.104906
78	1	0	1.363354	5.260749	-1.137141
79	1	0	-1.199344	9.519254	-1.099605

80	6	0	7.399827	5.037671	-1.072624
81	6	0	6.076897	2.587190	-1.141518
82	1	0	7.917403	5.999663	-1.045571
83	1	0	5.559385	1.625277	-1.168814
84	6	0	0.754915	8.609977	-1.077270
85	6	0	-0.591919	6.169377	-1.150372
86	1	0	1.283343	9.565906	-1.048712
87	1	0	-1.117933	5.211467	-1.184480
88	6	0	5.345888	3.769565	-1.116687
89	6	0	8.131507	3.854310	-1.098553
90	1	0	4.253679	3.737341	-1.124678
91	1	0	9.223811	3.886597	-1.092238
92	6	0	7.480804	2.611154	-1.133447
93	6	0	-1.330070	7.364423	-1.139441
94	8	0	9.664065	1.268990	-1.169925
95	5	0	10.363143	0.090837	-1.205505
96	1	0	-11.330283	-0.105831	-1.010779
97	1	0	-5.534792	9.625891	-1.343363
98	1	0	5.648334	9.786512	-0.966300
99	1	0	11.564204	0.099020	-1.209862
100	1	0	5.807666	-9.669106	-1.495071
101	1	0	-5.366397	-9.759986	-0.994930
102	6	0	7.188631	1.054011	2.087753
103	6	0	8.582676	1.073300	2.691140
104	6	0	8.604834	3.380803	2.626778
105	6	0	7.166623	3.360888	2.004250
106	6	0	6.696235	-0.201242	1.928726
107	6	0	9.064714	-0.168490	2.953798

108	1	0	9.080338	4.323378	2.801015
109	1	0	6.692306	4.290304	1.767376
110	1	0	9.970974	-0.377794	3.482751
111	6	0	5.255916	-0.540288	1.501868
112	16	0	3.989620	0.651195	1.143307
113	6	0	4.761501	-1.795494	1.348614
114	6	0	2.709878	-0.577626	1.080253
115	6	0	3.262877	-1.817462	1.100502
116	6	0	4.835470	-4.100827	1.253051
117	6	0	3.289378	-4.123485	0.997151
118	8	0	5.479908	-3.014641	1.411938
119	8	0	2.597429	-3.056883	0.934794
120	8	0	6.544304	2.275155	1.771400
121	8	0	9.225637	2.312269	2.932034
122	16	0	7.960763	-1.392504	2.294309
123	1	0	5.366621	-5.028703	1.295742
124	1	0	2.799471	-5.066327	0.870882
125	6	0	1.199810	-0.281835	1.018472
126	6	0	-1.372570	-0.321346	1.225403
127	6	0	0.646925	0.958098	1.004161
128	6	0	-0.867144	0.934869	1.125958
129	16	0	-0.080608	-1.510353	0.962817
130	6	0	0.629019	3.264989	0.920714
131	6	0	-0.933034	3.241050	1.046384
132	8	0	-1.588415	2.153884	1.140609
133	8	0	1.323814	2.198526	0.906342
134	1	0	1.127706	4.208609	0.844660
135	1	0	-1.465950	4.168870	1.053351

136	6	0	-2.843622	-0.663057	1.526950
137	6	0	-5.416017	-0.702129	1.733770
138	6	0	-3.349255	-1.919211	1.626297
139	6	0	-4.863372	-1.942206	1.747976
140	6	0	-3.283751	-4.225410	1.705643
141	6	0	-4.845834	-4.249142	1.831076
142	16	0	-4.135374	0.526110	1.789642
143	8	0	-2.628183	-3.138335	1.611629
144	8	0	-5.540471	-3.182561	1.845587
145	1	0	-2.750972	-5.153303	1.698655
146	1	0	-5.344674	-5.192717	1.906838
147	6	0	-6.925962	-0.405732	1.671946
148	6	0	-9.498347	-0.444569	1.878677
149	6	0	-7.478515	0.834378	1.657709
150	6	0	-8.992608	0.811530	1.779438
151	6	0	-7.495855	3.141294	1.574492
152	6	0	-9.057924	3.117737	1.700126
153	1	0	-6.996932	4.084801	1.498559
154	1	0	-9.590606	4.045692	1.707164
155	16	0	-8.206694	-1.633883	1.616111
156	1	0	-10.520436	-0.681817	2.088287
157	8	0	-9.713580	2.030725	1.794236
158	8	0	-6.801317	2.074654	1.560013
159	14	0	-2.888832	7.362083	-1.167096

PCL-COF-PEDOT Coordinates

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	8	0	-6.810835	1.224572	-1.387604
2	5	0	-3.497310	7.039127	-0.868102
3	8	0	-9.035010	0.391674	-1.235813
4	6	0	-6.277811	3.694012	-1.154248
5	5	0	-5.583799	-5.344145	-1.525736
6	8	0	-8.618981	2.717927	-0.999705
7	6	0	-7.143767	-1.285617	-1.507953
8	5	0	-7.267771	2.502999	-1.182813
9	5	0	-7.681851	0.156544	-1.372093
10	5	0	-9.496630	1.662892	-1.028094
11	8	0	-3.986836	8.315290	-0.670844
12	6	0	-6.744649	5.000728	-0.969448
13	6	0	-4.015304	4.545792	-1.209015
14	1	0	-7.813154	5.169241	-0.875133
15	1	0	-2.948674	4.373804	-1.316820
16	6	0	-5.769971	-1.522030	-1.633776
17	6	0	-7.523397	-3.674905	-1.494394
18	1	0	-5.085567	-0.679419	-1.674825
19	1	0	-8.203194	-4.520068	-1.435958
20	6	0	-4.900014	3.481102	-1.276815
21	6	0	-5.858586	6.063561	-0.889672
22	1	0	-4.528391	2.469545	-1.408246
23	1	0	-6.227008	7.073551	-0.735956

24	6	0	-8.014674	-2.380137	-1.452313
25	6	0	-5.275166	-2.815296	-1.673773
26	1	0	-9.081085	-2.200774	-1.355108
27	1	0	-4.207070	-2.977929	-1.768009
28	6	0	-6.145879	-3.908970	-1.587314
29	6	0	-4.478314	5.851116	-1.001642
30	5	0	-3.128888	9.371467	-0.517299
31	8	0	-4.227276	-5.560402	-1.403697
32	8	0	-2.133573	6.842680	-0.920344
33	8	0	-6.430025	-6.438338	-1.563926
34	5	0	-3.711934	-6.831905	-1.374423
35	8	0	4.844126	-8.074531	-0.952451
36	6	0	0.589830	-7.478794	-1.071827
37	5	0	8.029818	-2.191531	-0.684335
38	8	0	2.650912	-8.967586	-1.111464
39	6	0	5.288016	-5.575850	-0.890651
40	8	0	2.968148	-6.615778	-0.942688
41	5	0	4.334601	-6.789381	-0.931896
42	5	0	4.007390	-9.152996	-1.050723
43	5	0	2.120383	-7.695523	-1.039846
44	8	0	-4.568053	-7.910755	-1.484852
45	8	0	7.596059	-0.899686	-0.860221
46	6	0	-0.278582	-8.545869	-1.328972
47	6	0	-1.321095	-5.996628	-0.932093
48	1	0	0.132864	-9.539527	-1.479572
49	1	0	-1.717607	-5.003963	-0.744732
50	6	0	4.804148	-4.264853	-0.998508
51	6	0	7.531884	-4.694733	-0.683257

52	1	0	3.735397	-4.102866	-1.109390
53	1	0	8.597557	-4.854810	-0.550543
54	6	0	6.665772	-5.774612	-0.740650
55	6	0	5.672800	-3.186545	-0.956375
56	1	0	7.049122	-6.787855	-0.664556
57	1	0	5.291037	-2.171935	-1.030374
58	6	0	0.047112	-6.204853	-0.863595
59	6	0	-1.646925	-8.337512	-1.405285
60	1	0	0.715089	-5.373894	-0.653307
61	1	0	-2.314228	-9.167095	-1.619179
62	6	0	-2.187885	-7.059119	-1.220548
63	6	0	7.048413	-3.386311	-0.789372
64	5	0	-5.921364	-7.708470	-1.565094
65	5	0	8.475902	0.156305	-0.765877
66	8	0	9.370034	-2.427467	-0.438624
67	8	0	-1.777025	9.168404	-0.568307
68	5	0	-1.262475	7.904169	-0.781977
69	8	0	7.325364	6.790473	-0.996521
70	6	0	3.057660	7.364616	-0.985142
71	8	0	5.124195	5.908295	-1.127658
72	8	0	5.449237	8.250651	-0.920900
73	6	0	7.033534	4.253430	-1.075545
74	5	0	6.805686	8.056031	-0.928253
75	5	0	6.482513	5.697192	-1.083816
76	5	0	4.593581	7.169491	-1.021996
77	6	0	2.200936	6.277734	-1.210420
78	6	0	1.127940	8.784574	-0.645258
79	1	0	2.621377	5.307424	-1.458645

80	1	0	0.704209	9.760622	-0.428811
81	6	0	8.399267	3.992948	-0.906174
82	6	0	6.611783	1.873661	-1.103727
83	1	0	9.093305	4.825395	-0.829385
84	1	0	5.917311	1.041312	-1.178114
85	6	0	2.502645	8.619561	-0.709242
86	6	0	0.825488	6.447205	-1.148029
87	1	0	3.162431	9.466161	-0.542825
88	1	0	0.167214	5.602612	-1.336353
89	6	0	6.144252	3.176138	-1.183749
90	6	0	8.861713	2.689330	-0.820463
91	1	0	5.085982	3.363854	-1.334721
92	1	0	9.918674	2.490448	-0.670322
93	6	0	7.971905	1.610451	-0.909324
94	6	0	0.267789	7.699506	-0.858469
95	8	0	9.817420	-0.098536	-0.553533
96	5	0	10.251466	-1.381789	-0.371579
97	1	0	-10.664989	1.861516	-0.895131
98	1	0	-3.561616	10.468860	-0.339225
99	1	0	7.539142	8.995771	-0.868794
100	1	0	11.405760	-1.594494	-0.152162
101	1	0	4.458296	-10.256943	-1.081773
102	1	0	-6.657574	-8.645362	-1.629638
103	6	0	6.419245	0.523085	2.175091
104	6	0	7.818515	0.488112	2.416309
105	6	0	7.832242	2.771790	2.354866
106	6	0	6.525968	2.806939	2.131408
107	6	0	5.827454	-0.712755	2.136962

108	6	0	8.292964	-0.775747	2.560912
109	1	0	8.439008	3.661195	2.425764
110	1	0	5.967485	3.720142	2.000525
111	1	0	9.307857	-1.077658	2.773194
112	6	0	4.433445	-1.000939	1.946744
113	16	0	3.248497	0.270315	1.728637
114	6	0	3.806319	-2.218132	1.968009
115	6	0	1.919930	-0.871434	1.689106
116	6	0	2.403287	-2.147622	1.808941
117	6	0	3.635915	-4.493130	2.122017
118	6	0	2.320543	-4.433058	1.955990
119	8	0	4.462362	-3.397363	2.152199
120	8	0	1.615018	-3.260647	1.789217
121	8	0	5.735463	1.684312	2.011176
122	8	0	8.570166	1.619466	2.498961
123	16	0	7.033702	-1.947776	2.416161
124	1	0	4.176304	-5.419831	2.240192
125	1	0	1.684995	-5.305043	1.924634
126	6	0	0.558053	-0.440236	1.573189
127	6	0	-1.957709	-0.245511	1.449814
128	6	0	0.107704	0.812437	1.253595
129	6	0	-1.296948	0.922366	1.178763
130	16	0	-0.801596	-1.509569	1.819973
131	6	0	0.274787	3.034173	0.717559
132	6	0	-1.047463	3.138240	0.651646
133	8	0	-1.917126	2.086343	0.832021
134	8	0	0.938010	1.859829	0.986785
135	1	0	0.944611	3.868777	0.569770

136	1	0	-1.553739	4.071987	0.457013
137	6	0	-3.371409	-0.488661	1.465955
138	6	0	-5.879221	-0.326925	1.688354
139	6	0	-4.012382	-1.698671	1.459847
140	6	0	-5.410826	-1.611070	1.600653
141	6	0	-4.189680	-3.984924	1.549825
142	6	0	-5.505055	-3.892134	1.696897
143	16	0	-4.545074	0.799415	1.588869
144	8	0	-3.366428	-2.899845	1.322887
145	8	0	-6.207405	-2.715085	1.651115
146	1	0	-3.647232	-4.917426	1.579874
147	1	0	-6.141245	-4.748083	1.866464
148	6	0	-7.241621	0.107085	1.828203
149	6	0	-9.718410	0.288222	2.138092
150	6	0	-7.702199	1.396108	1.925816
151	6	0	-9.105602	1.499087	2.104235
152	6	0	-7.558900	3.677546	2.060173
153	6	0	-8.871556	3.768541	2.228482
154	1	0	-6.895562	4.528176	2.048067
155	1	0	-9.378002	4.709491	2.383466
156	16	0	-8.588157	-1.000111	1.961292
157	1	0	-10.773177	0.087906	2.251844
158	8	0	-9.737654	2.702127	2.223179
159	8	0	-6.894307	2.488873	1.842783
160	6	0	-0.951187	-1.551058	-1.623967
161	6	0	0.363089	-1.975773	-1.453589
162	6	0	1.407685	-1.072892	-1.572722
163	6	0	1.147882	0.269709	-1.841963

164	6	0	-0.167237	0.684488	-2.048646
165	6	0	-1.208391	-0.227322	-1.956366
166	1	0	0.556454	-3.015641	-1.213527
167	1	0	2.432873	-1.399526	-1.426575
168	1	0	-0.389354	1.734348	-2.207984
169	1	0	-2.238753	0.090013	-2.076122
170	8	0	-2.005385	-2.415514	-1.477584
171	1	0	-2.134362	-2.639513	-0.547708
172	7	0	2.210901	1.194526	-1.824637
173	1	0	2.873175	1.123940	-1.061820
174	6	0	2.268775	2.329965	-2.559272
175	8	0	3.054720	3.233645	-2.368934
176	1	0	1.527478	2.352490	-3.376737

PCL-P@COF-PEDOT Coordinates

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	8	0	6.519512	2.451918	1.773314
2	5	0	2.057682	7.000216	-0.347303
3	8	0	8.821748	2.338538	2.354497
4	6	0	5.324960	4.641913	1.332890
5	5	0	6.966431	-4.146360	1.819353
6	8	0	7.761825	4.451956	2.071665
7	6	0	7.502065	0.157719	2.115374
8	5	0	6.575793	3.822949	1.745978
9	5	0	7.632293	1.696439	2.081706
10	5	0	8.882510	3.706776	2.338617
11	8	0	2.089251	8.370498	-0.182798
12	6	0	5.326762	6.038571	1.406465
13	6	0	3.151985	4.738183	0.268287
14	1	0	6.188594	6.545031	1.831360
15	1	0	2.316064	4.225989	-0.198530
16	6	0	6.248182	-0.411073	1.875615
17	6	0	8.441481	-2.067230	2.257985
18	1	0	5.405193	0.246409	1.691588
19	1	0	9.301981	-2.718924	2.381397
20	6	0	4.208222	3.999873	0.779150
21	6	0	4.256115	6.774896	0.921272
22	1	0	4.199895	2.916993	0.699340
23	1	0	4.270300	7.859121	0.976486

24	6	0	8.596679	-0.690606	2.323601
25	6	0	6.080165	-1.784366	1.844186
26	1	0	9.575375	-0.257470	2.509684
27	1	0	5.098381	-2.204704	1.652423
28	6	0	7.181690	-2.631520	2.017965
29	6	0	3.161387	6.138602	0.321619
30	5	0	1.318184	9.254377	-0.887899
31	8	0	5.681136	-4.641605	1.767578
32	8	0	1.112820	6.412095	-1.152714
33	8	0	8.015669	-5.021713	1.604036
34	5	0	5.424279	-5.888096	1.261226
35	8	0	-2.854254	-7.857874	-0.289531
36	6	0	1.258056	-6.833046	0.381835
37	5	0	-7.032788	-3.118477	1.830901
38	8	0	-0.549228	-8.272970	-0.665058
39	6	0	-3.697124	-5.734784	0.808137
40	8	0	-1.228143	-6.301797	0.481493
41	5	0	-2.553858	-6.650514	0.320117
42	5	0	-1.861690	-8.641074	-0.808228
43	5	0	-0.224507	-7.136328	0.049062
44	8	0	6.480347	-6.710009	0.922926
45	8	0	-6.842553	-1.761281	1.921125
46	6	0	2.285771	-7.631369	-0.135562
47	6	0	2.920793	-5.526702	1.562449
48	1	0	2.031784	-8.460280	-0.789664
49	1	0	3.176520	-4.707978	2.227487
50	6	0	-3.474293	-4.384697	1.103527
51	6	0	-6.051909	-5.413013	1.266274

52	1	0	-2.466028	-3.984228	1.036990
53	1	0	-7.060713	-5.809333	1.333560
54	6	0	-5.002367	-6.235840	0.894524
55	6	0	-4.532522	-3.552488	1.436733
56	1	0	-5.185462	-7.280047	0.658447
57	1	0	-4.358883	-2.496136	1.621024
58	6	0	1.595649	-5.783969	1.247583
59	6	0	3.613729	-7.373662	0.180022
60	1	0	0.803017	-5.180076	1.681805
61	1	0	4.403401	-7.994264	-0.234359
62	6	0	3.950276	-6.305569	1.017187
63	6	0	-5.836382	-4.054823	1.523933
64	5	0	7.768612	-6.293500	1.164138
65	5	0	-7.901691	-0.908946	2.144686
66	8	0	-8.299644	-3.634315	2.031926
67	8	0	0.418836	8.829401	-1.821619
68	8	0	-7.821541	5.869752	1.862095
69	6	0	-3.905316	6.802231	0.337229
70	8	0	-5.587112	5.246678	1.374121
71	8	0	-6.271509	7.494504	1.059327
72	6	0	-7.167336	3.383450	1.970749
73	5	0	-7.515853	7.165926	1.536672
74	5	0	-6.858546	4.883176	1.754970
75	5	0	-5.295671	6.521792	0.961165
76	6	0	-2.943862	5.783663	0.343372
77	6	0	-2.398200	8.173168	-0.977504
78	1	0	-3.151236	4.842389	0.840374
79	1	0	-2.185881	9.104866	-1.493773

80	6	0	-8.453858	2.904044	2.251873
81	6	0	-6.372597	1.102156	1.873926
82	1	0	-9.267167	3.611077	2.392014
83	1	0	-5.564427	0.396697	1.704828
84	6	0	-3.604016	8.005608	-0.309990
85	6	0	-1.729165	5.952806	-0.303577
86	1	0	-4.335008	8.809255	-0.308481
87	1	0	-0.992799	5.154356	-0.279928
88	6	0	-6.126325	2.462596	1.793184
89	6	0	-8.696303	1.540194	2.330992
90	1	0	-5.122926	2.809528	1.570875
91	1	0	-9.699008	1.172934	2.529602
92	6	0	-7.658852	0.618507	2.134003
93	6	0	-1.453269	7.142569	-0.979820
94	8	0	-9.155756	-1.439755	2.371239
95	5	0	-9.347736	-2.793198	2.296370
96	1	0	9.915588	4.257653	2.568787
97	1	0	1.450359	10.426528	-0.708670
98	1	0	-8.342984	8.017302	1.660083
99	1	0	-10.439817	-3.246064	2.464305
100	1	0	-2.135916	-9.643512	-1.394586
101	1	0	8.674919	-7.045453	0.973516
102	6	0	-7.048865	-0.505181	-1.330484
103	6	0	-8.443198	-0.679597	-1.121668
104	6	0	-8.661394	1.593938	-1.038774
105	6	0	-7.359952	1.758283	-1.231429
106	6	0	-6.355833	-1.677866	-1.483780
107	6	0	-8.813418	-1.985838	-1.117985

108	1	0	-9.344873	2.419027	-0.911281
109	1	0	-6.880037	2.723218	-1.272786
110	1	0	-9.809775	-2.387093	-1.006532
111	6	0	-4.942628	-1.834530	-1.682272
112	16	0	-3.853878	-0.466499	-1.626974
113	6	0	-4.236739	-2.981369	-1.931478
114	6	0	-2.458562	-1.470784	-1.955747
115	6	0	-2.848743	-2.778251	-2.082586
116	6	0	-3.920291	-5.198547	-2.393612
117	6	0	-2.613604	-5.007639	-2.541383
118	8	0	-4.805997	-4.218244	-2.029240
119	8	0	-1.983013	-3.802394	-2.338394
120	8	0	-6.465547	0.720404	-1.370927
121	8	0	-9.290272	0.372389	-0.954078
122	16	0	-7.461731	-3.027939	-1.380196
123	1	0	-4.395855	-6.156936	-2.538047
124	1	0	-1.930875	-5.786590	-2.847321
125	6	0	-1.132910	-0.928955	-2.022031
126	6	0	1.364311	-0.558018	-1.933249
127	6	0	-0.765303	0.386755	-1.918624
128	6	0	0.627715	0.596371	-1.869237
129	16	0	0.294355	-1.932395	-2.114152
130	6	0	-1.079785	2.652056	-1.817779
131	6	0	0.233806	2.855197	-1.786368
132	8	0	1.168544	1.844253	-1.742559
133	8	0	-1.661553	1.410434	-1.819056
134	1	0	-1.806580	3.450380	-1.841506
135	1	0	0.681333	3.838893	-1.808455

136	6	0	2.786059	-0.708631	-1.828003
137	6	0	5.276980	-0.363673	-1.581283
138	6	0	3.503696	-1.869831	-1.713470
139	6	0	4.895121	-1.678829	-1.588738
140	6	0	3.851550	-4.137073	-1.670435
141	6	0	5.162871	-3.951659	-1.579987
142	16	0	3.869183	0.661602	-1.750381
143	8	0	2.931560	-3.112669	-1.682554
144	8	0	5.768855	-2.723438	-1.487101
145	1	0	3.390787	-5.112472	-1.721044
146	1	0	5.871445	-4.767067	-1.581826
147	6	0	6.599846	0.173963	-1.428099
148	6	0	9.040872	0.538681	-1.028234
149	6	0	6.962948	1.494340	-1.363789
150	6	0	8.345906	1.699973	-1.125858
151	6	0	6.683845	3.760525	-1.472485
152	6	0	7.977112	3.953805	-1.237716
153	1	0	5.986141	4.566651	-1.639394
154	1	0	8.423385	4.936343	-1.200907
155	16	0	8.013027	-0.829493	-1.216728
156	1	0	10.098192	0.417736	-0.847189
157	8	0	8.886085	2.950755	-0.996272
158	8	0	6.083031	2.525659	-1.505374
159	15	0	-0.005330	7.237719	-2.090928
160	6	0	1.851095	-1.455248	1.357596
161	6	0	0.495620	-1.711848	1.180198
162	6	0	-0.420039	-0.670487	1.177636
163	6	0	0.008260	0.636762	1.398757

164	6	0	1.360572	0.880389	1.633437
165	6	0	2.277023	-0.154970	1.601015
166	1	0	0.156463	-2.723697	0.977829
167	1	0	-1.456474	-0.883776	0.939908
168	1	0	1.702666	1.895985	1.812586
169	1	0	3.333789	0.035207	1.740884
170	8	0	2.794289	-2.431199	1.286035
171	1	0	2.467723	-3.174244	0.767484
172	7	0	-0.869365	1.733882	1.322040
173	1	0	-0.487585	2.610970	0.995917
174	6	0	-2.210607	1.724717	1.479494
175	8	0	-2.921182	2.682667	1.249420
176	1	0	-2.611284	0.768001	1.850159

PCL-S@COF-PEDOT Coordinates

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	8	0	6.691394	1.840652	1.759533
2	5	0	3.045910	6.966259	-0.568210
3	8	0	8.931628	1.348934	2.381510
4	6	0	5.904459	4.181122	1.213928
5	5	0	6.162712	-4.765897	1.765828
6	8	0	8.265341	3.602532	2.000892
7	6	0	7.276590	-0.583400	2.124326
8	5	0	6.991654	3.177996	1.678787
9	5	0	7.654338	0.912777	2.094322
10	5	0	9.231741	2.683701	2.325310
11	8	0	3.208342	8.290264	-0.405033
12	6	0	6.149233	5.557901	1.194888
13	6	0	3.765089	4.584002	0.157259
14	1	0	7.090387	5.933244	1.586346
15	1	0	2.837087	4.205060	-0.257125
16	6	0	5.956784	-0.959503	1.853792
17	6	0	7.877297	-2.920447	2.269573
18	1	0	5.217505	-0.186052	1.672184
19	1	0	8.627575	-3.693548	2.408449
20	6	0	4.686479	3.707712	0.707094
21	6	0	5.215005	6.436779	0.665532
22	1	0	4.488550	2.639950	0.708148
23	1	0	5.413038	7.504211	0.651279

24	6	0	8.230045	-1.582626	2.352793
25	6	0	5.593093	-2.293713	1.794895
26	1	0	9.256557	-1.296959	2.563660
27	1	0	4.563449	-2.563638	1.579378
28	6	0	6.558397	-3.291768	1.981320
29	6	0	4.017809	5.961287	0.116205
30	5	0	2.514035	9.446142	-0.784344
31	8	0	4.839240	-5.096057	1.593281
32	8	0	2.053835	6.380498	-1.371742
33	8	0	7.114176	-5.766890	1.676451
34	5	0	4.472100	-6.345014	1.165808
35	8	0	-3.936467	-7.840332	-0.208697
36	6	0	0.262983	-7.091505	0.323005
37	5	0	-7.462697	-2.470945	1.687633
38	8	0	-1.678781	-8.517247	-0.506933
39	6	0	-4.545650	-5.575190	0.778515
40	8	0	-2.166618	-6.388620	0.431336
41	5	0	-3.518275	-6.632462	0.320772
42	5	0	-3.020595	-8.765256	-0.632552
43	5	0	-1.241725	-7.338378	0.064764
44	8	0	5.444096	-7.308299	0.973748
45	8	0	-7.049167	-1.161707	1.748027
46	6	0	1.225375	-8.060785	0.013254
47	6	0	2.018883	-5.672400	1.200295
48	1	0	0.909734	-8.992774	-0.446874
49	1	0	2.335613	-4.741790	1.660735
50	6	0	-4.132415	-4.267089	1.058009
51	6	0	-6.832958	-4.908219	1.197249

52	1	0	-3.077097	-4.019245	0.988492
53	1	0	-7.890373	-5.150703	1.249400
54	6	0	-5.908711	-5.883087	0.858186
55	6	0	-5.059837	-3.285661	1.366628
56	1	0	-6.237505	-6.894483	0.636745
57	1	0	-4.737389	-2.262330	1.534601
58	6	0	0.680746	-5.895144	0.920963
59	6	0	2.565528	-7.842743	0.299604
60	1	0	-0.063535	-5.145281	1.173915
61	1	0	3.305921	-8.602735	0.066457
62	6	0	2.978948	-6.643451	0.891185
63	6	0	-6.424426	-3.591726	1.435488
64	5	0	6.752346	-7.025153	1.279192
65	5	0	-7.952657	-0.140332	1.931855
66	8	0	-8.802297	-2.761387	1.860229
67	8	0	1.457432	9.492238	-1.571785
68	8	0	-6.758036	6.514095	1.913557
69	6	0	-2.834779	7.042225	0.223793
70	8	0	-4.713075	5.610164	1.115452
71	8	0	-5.033284	7.960591	1.142302
72	6	0	-6.522922	3.969623	1.751746
73	5	0	-6.281618	7.776394	1.684001
74	5	0	-5.982969	5.409948	1.606129
75	5	0	-4.234572	6.868474	0.875750
76	6	0	-1.913449	5.982830	0.224764
77	6	0	-1.292450	8.337838	-1.141508
78	1	0	-2.109441	5.074520	0.786932
79	1	0	-1.014764	9.261668	-1.635915

80	6	0	-7.860153	3.705854	2.074476
81	6	0	-6.118390	1.591428	1.597605
82	1	0	-8.534373	4.535296	2.269348
83	1	0	-5.442875	0.763700	1.401710
84	6	0	-2.491111	8.220513	-0.444739
85	6	0	-0.726899	6.073091	-0.479364
86	1	0	-3.178160	9.061245	-0.424535
87	1	0	-0.044928	5.227416	-0.509639
88	6	0	-5.659995	2.894400	1.511420
89	6	0	-8.324017	2.399761	2.137639
90	1	0	-4.626491	3.101175	1.264528
91	1	0	-9.366011	2.198891	2.369017
92	6	0	-7.457754	1.323887	1.902241
93	6	0	-0.429302	7.244955	-1.173069
94	8	0	-9.282589	-0.447339	2.142464
95	5	0	-9.699575	-1.750141	2.082418
96	1	0	10.339125	3.054245	2.569988
97	1	0	2.938753	10.481066	-0.334622
98	1	0	-6.955194	8.724687	1.949702
99	1	0	-10.856256	-2.008366	2.226982
100	1	0	-3.391388	-9.789032	-1.120513
101	1	0	7.578508	-7.881180	1.184877
102	6	0	-7.049644	0.096371	-1.416401
103	6	0	-8.465180	0.067359	-1.299951
104	6	0	-8.451073	2.348886	-1.178490
105	6	0	-7.130802	2.378902	-1.296367
106	6	0	-6.474539	-1.141772	-1.544714
107	6	0	-8.970432	-1.191465	-1.352964

108	1	0	-9.051616	3.239325	-1.073760
109	1	0	-6.553444	3.289783	-1.291347
110	1	0	-10.008604	-1.486257	-1.315883
111	6	0	-5.074708	-1.451160	-1.634685
112	16	0	-3.846776	-0.220455	-1.435217
113	6	0	-4.483418	-2.665279	-1.864617
114	6	0	-2.549249	-1.368166	-1.690858
115	6	0	-3.073422	-2.619748	-1.888412
116	6	0	-4.380541	-4.878001	-2.433870
117	6	0	-3.053263	-4.836244	-2.459933
118	8	0	-5.177504	-3.820986	-2.075118
119	8	0	-2.311743	-3.728192	-2.119290
120	8	0	-6.341311	1.255371	-1.405662
121	8	0	-9.207015	1.199594	-1.156415
122	16	0	-7.721969	-2.366847	-1.551085
123	1	0	-4.949005	-5.760350	-2.687284
124	1	0	-2.437639	-5.671998	-2.757293
125	6	0	-1.171368	-0.973884	-1.710033
126	6	0	1.354773	-0.866377	-1.743512
127	6	0	-0.662576	0.298025	-1.651382
128	6	0	0.742357	0.356075	-1.680289
129	16	0	0.140466	-2.130722	-1.809352
130	6	0	-0.714392	2.592467	-1.667280
131	6	0	0.615001	2.642660	-1.697917
132	8	0	1.424554	1.536929	-1.627823
133	8	0	-1.429268	1.424946	-1.557947
134	1	0	-1.348286	3.464902	-1.754962
135	1	0	1.176066	3.557950	-1.821580

136	6	0	2.761253	-1.133464	-1.690570
137	6	0	5.277644	-0.973016	-1.538262
138	6	0	3.396031	-2.345638	-1.606806
139	6	0	4.801521	-2.258394	-1.531872
140	6	0	3.571737	-4.631348	-1.609349
141	6	0	4.895988	-4.545638	-1.567408
142	16	0	3.944676	0.152971	-1.642018
143	8	0	2.732711	-3.539732	-1.553456
144	8	0	5.594431	-3.366974	-1.457047
145	1	0	3.034898	-5.565357	-1.674545
146	1	0	5.543186	-5.408684	-1.621535
147	6	0	6.634315	-0.521032	-1.410809
148	6	0	9.091421	-0.299086	-1.010375
149	6	0	7.082326	0.775071	-1.398027
150	6	0	8.474791	0.899935	-1.162174
151	6	0	6.953921	3.046982	-1.617889
152	6	0	8.256804	3.165029	-1.387565
153	1	0	6.312233	3.887819	-1.831587
154	1	0	8.768331	4.115845	-1.402070
155	16	0	7.976855	-1.604154	-1.148073
156	1	0	10.138996	-0.480917	-0.823405
157	8	0	9.095316	2.117228	-1.088252
158	8	0	6.271962	1.854105	-1.588456
159	16	0	0.979442	7.308981	-2.225431
160	6	0	1.338298	-1.154011	1.279528
161	6	0	-0.045738	-1.173777	1.424657
162	6	0	-0.743731	0.014800	1.577343
163	6	0	-0.059506	1.226067	1.637400

164	6	0	1.330648	1.239478	1.539331
165	6	0	2.025156	0.055915	1.347466
166	1	0	-0.573035	-2.118904	1.376182
167	1	0	-1.827205	0.012311	1.610844
168	1	0	1.866987	2.180230	1.604005
169	1	0	3.099134	0.051883	1.225238
170	8	0	2.045244	-2.298730	1.080533
171	1	0	1.627302	-2.830904	0.391174
172	7	0	-0.794650	2.416943	1.779639
173	1	0	-0.614798	3.174101	1.132676
174	6	0	-1.754086	2.671900	2.709635
175	8	0	-2.439483	3.667934	2.710409
176	1	0	-1.818458	1.895704	3.497555

PCL-Si@COF-PEDOT Coordinates

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	8	0	-6.770345	1.121187	-1.123395
2	5	0	-3.773536	7.132517	-0.879401
3	8	0	-8.958451	0.202235	-0.946500
4	6	0	-6.311698	3.583844	-0.707119
5	5	0	-5.442620	-5.413154	-1.713230
6	8	0	-8.580331	2.481341	-0.398899
7	6	0	-7.043229	-1.380216	-1.463494
8	5	0	-7.246181	2.350180	-0.730724
9	5	0	-7.608131	0.030742	-1.174285
10	5	0	-9.435305	1.416835	-0.531872
11	8	0	-4.205084	8.304697	-0.281579
12	6	0	-6.783172	4.823200	-0.258571
13	6	0	-4.187083	4.620266	-1.224558
14	1	0	-7.805859	4.897958	0.098756
15	1	0	-3.182259	4.556500	-1.634359
16	6	0	-5.669053	-1.585103	-1.635411
17	6	0	-7.387689	-3.770599	-1.584214
18	1	0	-5.000420	-0.729104	-1.625288
19	1	0	-8.051884	-4.628859	-1.548362
20	6	0	-4.994257	3.494035	-1.173035
21	6	0	-5.962054	5.940590	-0.272804
22	1	0	-4.617903	2.533069	-1.511510
23	1	0	-6.332298	6.897883	0.082195

24	6	0	-7.896529	-2.489037	-1.457548
25	6	0	-5.159238	-2.867155	-1.764198
26	1	0	-8.961877	-2.333145	-1.319663
27	1	0	-4.088539	-3.021804	-1.863324
28	6	0	-6.010443	-3.978793	-1.722805
29	6	0	-4.657420	5.860379	-0.773820
30	5	0	-3.507004	9.488857	-0.254411
31	8	0	-4.086387	-5.639473	-1.801808
32	8	0	-2.589405	7.087132	-1.564197
33	8	0	-6.292056	-6.496293	-1.569889
34	5	0	-3.571414	-6.899552	-1.613306
35	8	0	4.985777	-7.984317	-0.960384
36	6	0	0.735245	-7.497881	-1.361336
37	5	0	7.964806	-1.996818	-0.736949
38	8	0	2.813656	-8.940417	-1.058149
39	6	0	5.364384	-5.473559	-1.082946
40	8	0	3.092176	-6.590154	-1.288977
41	5	0	4.452098	-6.717372	-1.123456
42	5	0	4.171786	-9.083735	-0.936259
43	5	0	2.265927	-7.686324	-1.241317
44	8	0	-4.433821	-7.966934	-1.454832
45	8	0	7.463933	-0.715801	-0.806749
46	6	0	-0.142704	-8.573753	-1.187665
47	6	0	-1.161568	-6.039050	-1.716003
48	1	0	0.261649	-9.560924	-0.983642
49	1	0	-1.565798	-5.053061	-1.928841
50	6	0	4.827289	-4.180617	-1.162665
51	6	0	7.573150	-4.516821	-0.835213

52	1	0	3.754050	-4.050840	-1.274520
53	1	0	8.643595	-4.640234	-0.701180
54	6	0	6.747062	-5.625325	-0.921474
55	6	0	5.657578	-3.074741	-1.071229
56	1	0	7.165955	-6.625365	-0.857503
57	1	0	5.240051	-2.072458	-1.103760
58	6	0	0.208944	-6.228198	-1.634308
59	6	0	-1.513215	-8.384177	-1.275538
60	1	0	0.887672	-5.396643	-1.796660
61	1	0	-2.191366	-9.221908	-1.142427
62	6	0	-2.041996	-7.114013	-1.536833
63	6	0	7.038818	-3.225534	-0.902201
64	5	0	-5.788842	-7.763672	-1.465080
65	5	0	8.293005	0.368880	-0.644552
66	8	0	9.322049	-2.179712	-0.543192
67	8	0	-2.326160	9.641225	-0.918761
68	8	0	6.981137	6.919453	-0.121469
69	6	0	2.800634	7.643397	-0.822386
70	8	0	4.818417	6.115298	-0.690788
71	8	0	5.121948	8.397641	-0.098694
72	6	0	6.714146	4.432110	-0.577218
73	5	0	6.460626	8.171083	0.078064
74	5	0	6.153773	5.869434	-0.472489
75	5	0	4.293035	7.377949	-0.525911
76	6	0	2.021525	6.664213	-1.450643
77	6	0	0.874449	9.113571	-0.786529
78	1	0	2.463922	5.715687	-1.737537
79	1	0	0.426336	10.067069	-0.520776

80	6	0	8.088089	4.194185	-0.451555
81	6	0	6.351948	2.046720	-0.782000
82	1	0	8.760449	5.035623	-0.311327
83	1	0	5.675426	1.203117	-0.886968
84	6	0	2.209160	8.871181	-0.499419
85	6	0	0.690612	6.902459	-1.755657
86	1	0	2.808252	9.639405	-0.019031
87	1	0	0.130504	6.128653	-2.271533
88	6	0	5.854022	3.340134	-0.752268
89	6	0	8.586511	2.902330	-0.492897
90	1	0	4.785734	3.515363	-0.844874
91	1	0	9.651744	2.721764	-0.386035
92	6	0	7.725143	1.809569	-0.650682
93	6	0	0.102995	8.126287	-1.412741
94	8	0	9.650890	0.170202	-0.488007
95	5	0	10.152922	-1.100372	-0.418035
96	1	0	-10.598336	1.559031	-0.310671
97	1	0	-3.953172	10.401419	0.375575
98	1	0	7.176531	9.065298	0.411989
99	1	0	11.322708	-1.268276	-0.247713
100	1	0	4.643133	-10.171532	-0.801115
101	1	0	-6.529660	-8.694088	-1.368679
102	6	0	6.405711	0.419153	2.361588
103	6	0	7.807294	0.427255	2.593572
104	6	0	7.715549	2.704458	2.748587
105	6	0	6.406561	2.698352	2.537184
106	6	0	5.872586	-0.833628	2.204671
107	6	0	8.340884	-0.820725	2.623448

108	1	0	8.279581	3.610648	2.907968
109	1	0	5.804985	3.593062	2.508889
110	1	0	9.369307	-1.092793	2.809210
111	6	0	4.499648	-1.171503	1.953684
112	16	0	3.275808	0.051738	1.694401
113	6	0	3.929930	-2.416608	1.907045
114	6	0	2.008300	-1.142431	1.554685
115	6	0	2.537354	-2.400568	1.680273
116	6	0	3.851321	-4.699760	2.001284
117	6	0	2.542212	-4.691412	1.784613
118	8	0	4.629379	-3.572404	2.084208
119	8	0	1.795745	-3.545476	1.613077
120	8	0	5.667952	1.559072	2.309507
121	8	0	8.508412	1.580849	2.771876
122	16	0	7.135797	-2.031245	2.373592
123	1	0	4.424930	-5.605782	2.125342
124	1	0	1.944205	-5.587113	1.712387
125	6	0	0.632503	-0.774985	1.386593
126	6	0	-1.892867	-0.741820	1.221799
127	6	0	0.107437	0.459871	1.112202
128	6	0	-1.300983	0.474466	1.014197
129	16	0	-0.662428	-1.947108	1.529885
130	6	0	0.112634	2.713874	0.699837
131	6	0	-1.214276	2.728539	0.610585
132	8	0	-2.004708	1.611389	0.743671
133	8	0	0.858973	1.586045	0.936012
134	1	0	0.720516	3.600309	0.589822
135	1	0	-1.791633	3.625650	0.438113

136	6	0	-3.296203	-1.030856	1.306255
137	6	0	-5.779363	-0.914591	1.727502
138	6	0	-3.911185	-2.254194	1.344961
139	6	0	-5.299402	-2.189338	1.586331
140	6	0	-4.054104	-4.538582	1.376812
141	6	0	-5.363250	-4.475253	1.592682
142	16	0	-4.478701	0.235460	1.538228
143	8	0	-3.250911	-3.439103	1.184864
144	8	0	-6.078496	-3.305652	1.661133
145	1	0	-3.502092	-5.465468	1.328962
146	1	0	-5.982269	-5.348217	1.737209
147	6	0	-7.131586	-0.495811	1.974574
148	6	0	-9.587388	-0.344840	2.431882
149	6	0	-7.578263	0.777617	2.227249
150	6	0	-8.969044	0.862110	2.493019
151	6	0	-7.407627	3.025611	2.631012
152	6	0	-8.707710	3.097968	2.883785
153	1	0	-6.734938	3.866223	2.699694
154	1	0	-9.193972	4.010360	3.195361
155	16	0	-8.476415	-1.608105	2.060096
156	1	0	-10.635139	-0.555366	2.585164
157	8	0	-9.584220	2.045535	2.780056
158	8	0	-6.771397	1.874650	2.213983
159	14	0	-1.660677	8.443763	-1.888242
160	6	0	1.081367	-1.834299	-1.661963
161	6	0	2.164004	-0.988425	-1.870118
162	6	0	1.955589	0.347308	-2.169006
163	6	0	0.659990	0.846479	-2.296996

164	6	0	-0.421785	-0.015799	-2.130952
165	6	0	-0.214503	-1.349521	-1.813162
166	1	0	3.166566	-1.374665	-1.727141
167	1	0	2.806265	1.017258	-2.240695
168	1	0	-1.433379	0.364336	-2.238657
169	1	0	-1.061827	-2.011381	-1.661403
170	8	0	1.338445	-3.121465	-1.294473
171	1	0	0.693085	-3.408517	-0.638906
172	7	0	0.429082	2.215836	-2.539122
173	1	0	-0.281951	2.678842	-1.989055
174	6	0	1.178793	3.022154	-3.329484
175	8	0	1.051711	4.226338	-3.393323
176	1	0	1.922090	2.468514	-3.929487
