Electronic Supplementary Material (ESI) for Journal of Materials Chemistry C

Oligofuran-Containing Molecules for Organic Electronics

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DS-2F syn-syn

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.482171	0.528003	-0.000018
2	6	0	0.375069	1.900158	-0.000060
3	6	0	1.701531	2.402575	0.000023
4	6	0	2.549824	1.315517	-0.000029
5	8	0	1.801262	0.162809	-0.000019
6	1	0	-0.547301	2.462351	-0.000089
7	1	0	2.006878	3.439980	0.000057
8	6	0	-0.482197	-0.527482	-0.000008
9	6	0	-0.374907	-1.899638	0.000033
10	8	0	-1.801278	-0.162432	0.000000
11	6	0	-1.701297	-2.402210	-0.000062
12	1	0	0.547540	-2.461701	0.000060
13	6	0	-2.549704	-1.315219	0.000009
14	1	0	-2.006580	-3.439633	-0.000107
15	6	0	-3.980239	-1.216037	0.000026
16	1	0	-4.489838	-2.176679	0.000002
17	6	0	3.980363	1.216211	-0.000037
18	1	0	4.490120	2.176758	-0.000021
19	6	0	4.683251	0.059360	-0.000049
20	1	0	4.120331	-0.872046	-0.000050
21	6	0	-4.683301	-0.059298	0.000054
22	1	0	-4.120488	0.872182	0.000062
23	6	0	-6.136688	0.090369	0.000062
24	6	0	-6.682781	1.388893	0.000025
25	6	0	-7.033791	-0.997500	0.000107
26	6	0	-8.060209	1.596139	0.000028
27	1	0	-6.009072	2.242768	-0.000008
28	6	0	-8.409081	-0.790792	0.000110
29	1	0	-6.652305	-2.014506	0.000145
30	6	0	-8.932108	0.506462	0.000070
31	1	0	-8.452601	2.609706	-0.000002
32	1	0	-9.079703	-1.646265	0.000146
33	1	0	-10.007252	0.663200	0.000073
34	6	0	6.136632	-0.090512	-0.000049
35	6	0	6.682502	-1.389124	0.000010
36	6	0	7.033913	0.997209	-0.000106
37	6	0	8.059902	-1.596605	0.000017
38	1	0	6.008652	-2.242888	0.000053
39	6	0	8.409166	0.790271	-0.000100
40	1	0	6.652594	2.014279	-0.000162
41	6	0	8.931977	-0.507072	-0.000037
42	1	0	8.452123	-2.610237	0.000064
43	1	0	9.079937	1.645628	-0.000146
44	1	0	10.007097	-0.663977	-0.000033

DS-2F syn-anti

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.693934	1.025117	0.000009
2	6	0	0.783157	2.398508	0.000071
3	6	0	2.167660	2.706983	0.000058
4	6	0	2.852734	1.510426	0.000027
5	8	0	1.947465	0.475881	-0.000009
6	1	0	-0.049936	3.086170	0.000104
7	1	0	2.617426	3.690419	0.000084
8	6	0	-0.411325	0.117718	-0.000030
9	6	0	-0.502084	-1.256833	-0.000111
10	8	0	-1.663123	0.663930	0.000002
11	6	0	-1.884505	-1.567305	-0.000090
12	1	0	0.330000	-1.945861	-0.000162
13	6	0	-2.571692	-0.370762	-0.000043
14	1	0	-2.326952	-2.553688	-0.000128
15	6	0	-3.955705	0.014849	-0.000016
16	1	0	-4.119343	1.089682	0.000003
17	6	0	4.254626	1.209141	0.000018
18	1	0	4.895147	2.087869	0.000037
19	6	0	4.788075	-0.034873	-0.000007
20	1	0	4.100268	-0.878292	-0.000008
21	6	0	-5.004487	-0.840276	-0.000005
22	1	0	-4.795684	-1.909772	0.000000
23	6	0	-6.423943	-0.493226	0.000017
24	6	0	-7.375786	-1.531577	0.000161
25	6	0	-6.901176	0.833671	-0.000102
26	6	0	-8.742446	-1.261805	0.000198
27	1	0	-7.030247	-2.563019	0.000250
28	6	0	-8.265484	1.102824	-0.000065
29	1	0	-6.198854	1.662155	-0.000234
30	6	0	-9.195551	0.058056	0.000086
31	1	0	-9.453777	-2.083548	0.000312
32	1	0	-8.607956	2.134409	-0.000160
33	1	0	-10.260541	0.273092	0.000112
34	6	0	6.206677	-0.385209	-0.000022
35	6	0	6.567739	-1.746806	0.000081
36	6	0	7.245813	0.568052	-0.000139
37	6	0	7.903382	-2.142332	0.000079
38	1	0	5.782419	-2.499256	0.000167
39	6	0	8.579321	0.173372	-0.000140
40	1	0	7.008919	1.628147	-0.000239
41	6	0	8.917703	-1.183797	-0.000030
42	1	0	8.152036	-3.200397	0.000163
43	1	0	9.361753	0.927919	-0.000232
44	1	0	9.960775	-1.488008	-0.000033

DS-2F anti-ant

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.606375	0.379111	-0.000033
2	6	0	0.871699	1.730722	0.000034
3	6	0	2.282536	1.862022	0.000082
4	6	0	2.811492	0.587690	0.000029
5	8	0	1.777975	-0.322669	-0.000048
6	1	0	0.134318	2.520296	0.000050
7	1	0	2.847206	2.783867	0.000145
8	6	0	-0.606375	-0.379110	-0.000120
9	6	0	-0.871698	-1.730722	-0.000341
10	8	0	-1.777975	0.322669	0.000014
11	6	0	-2.282535	-1.862022	-0.000361
12	1	0	-0.134316	-2.520294	-0.000482
13	6	0	-2.811492	-0.587692	-0.000136
14	1	0	-2.847204	-2.783868	-0.000524
15	6	0	-4.135349	-0.029397	-0.000029
16	1	0	-4.162053	1.057539	0.000127
17	6	0	4.135348	0.029395	0.000029
18	1	0	4.162052	-1.057540	-0.000033
19	6	0	5.283598	0.745474	0.000082
20	1	0	5.210505	1.832739	0.000107
21	6	0	-5.283598	-0.745476	-0.000097
22	1	0	-5.210506	-1.832740	-0.000207
23	6	0	-6.648489	-0.223714	-0.000010
24	6	0	-7.722090	-1.135635	0.000192
25	6	0	-6.957184	1.152291	-0.000126
26	6	0	-9.044569	-0.698291	0.000299
27	1	0	-7.507680	-2.202008	0.000274
28	6	0	-8.277523	1.588790	-0.000019
29	1	0	-6.157247	1.886954	-0.000323
30	6	0	-9.330209	0.667679	0.000198
31	1	0	-9.852477	-1.425299	0.000459
32	1	0	-8.489188	2.654936	-0.000115
33	1	0	-10.360220	1.013435	0.000276
34	6	0	6.648489	0.223714	0.000082
35	6	0	7.722089	1.135635	-0.000148
36	6	0	6.957185	-1.152292	0.000303
37	6	0	9.044569	0.698292	-0.000178
38	1	0	7.507679	2.202008	-0.000313
39	6	0	8.277524	-1.588789	0.000272
40	1	0	6.157248	-1.886954	0.000522
41	6	0	9.330209	-0.667678	0.000029
42	1	0	9.852476	1.425301	-0.000361
43	1	0	8.489189	-2.654935	0.000449
44	1	0	10.360220	-1.013433	0.000009

DS-2T syn-syn

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.634410	-0.341531	0.000092
2	6	0	0.890727	-1.700324	0.000221
3	6	0	2.267504	-2.017807	0.000247
4	6	0	3.102183	-0.914966	0.000034
5	16	0	2.145449	0.559548	-0.000075
6	1	0	0.103610	-2.446954	0.000334
7	1	0	2.651172	-3.032961	0.000369
8	6	0	-0.634409	0.341533	0.000052
9	6	0	-0.890727	1.700325	-0.000018
10	16	0	-2.145449	-0.559548	0.000030
11	6	0	-2.267505	2.017808	-0.000019
12	1	0	-0.103612	2.446956	-0.000027
13	6	0	-3.102182	0.914965	-0.000035
14	1	0	-2.651175	3.032961	-0.000036
15	6	0	4.543323	-0.930381	-0.000030
16	1	0	4.967935	-1.933046	-0.000180
17	6	0	5.364907	0.144821	0.000076
18	1	0	4.913731	1.137220	0.000220
19	6	0	-4.543323	0.930380	-0.000052
20	1	0	-4.967935	1.933045	-0.000029
21	6	0	-5.364907	-0.144821	-0.000056
22	1	0	-4.913731	-1.137220	-0.000043
23	6	0	6.826361	0.140712	0.000014
24	6	0	7.506054	1.374394	0.000132
25	6	0	7.603436	-1.035886	-0.000165
26	6	0	8.897661	1.434972	0.000074
27	1	0	6.926696	2.294955	0.000259
28	6	0	8.992738	-0.975346	-0.000216
29	1	0	7.117281	-2.007211	-0.000263
30	6	0	9.649666	0.259492	-0.000097
31	1	0	9.394770	2.401483	0.000161
32	1	0	9.569158	-1.896871	-0.000350
33	1	0	10.735331	0.302104	-0.000144
34	6	0	-6.826361	-0.140713	-0.000037
35	6	0	-7.506054	-1.374395	-0.000085
36	6	0	-7.603436	1.035885	0.000019
37	6	0	-8.897661	-1.434972	-0.000076
38	1	0	-6.926696	-2.294955	-0.000139
39	6	0	-8.992738	0.975346	0.000035
40	1	0	-7.117281	2.007211	0.000051
41	6	0	-9.649666	-0.259493	-0.000014
42	1	0	-9.394770	-2.401484	-0.000120
43	1	0	-9.569158	1.896871	0.000080
44	1	0	-10.735331	-0.302105	-0.000012

DS-2T syn-anti

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.738484	0.775077	-0.000590
2	6	0	1.154092	2.093593	-0.002381
3	6	0	2.559152	2.245760	-0.002824
4	6	0	3.257483	1.052370	-0.001411
5	16	0	2.132450	-0.299147	0.000570
6	1	0	0.461386	2.928674	-0.003331
7	1	0	3.059607	3.208732	-0.004150
8	6	0	-0.601842	0.244994	0.000370
9	6	0	-1.015741	-1.076622	0.002456
10	16	0	-1.999938	1.304322	-0.001020
11	6	0	-2.417597	-1.240073	0.002974
12	1	0	-0.319084	-1.908553	0.003765
13	6	0	-3.120951	-0.048263	0.001205
14	1	0	-2.901220	-2.210675	0.004895
15	6	0	4.690306	0.895473	-0.001406
16	1	0	5.231824	1.840273	-0.002823
17	6	0	5.376601	-0.270853	0.000134
18	1	0	4.808641	-1.201349	0.001451
19	6	0	-4.543332	0.212456	0.000998
20	1	0	-4.828167	1.262683	0.001746
21	6	0	-5.511834	-0.733166	-0.000290
22	1	0	-5.209698	-1.779775	-0.002078
23	6	0	6.827866	-0.444797	0.000238
24	6	0	7.351893	-1.752264	0.001528
25	6	0	7.743017	0.627918	-0.000869
26	6	0	8.725623	-1.982773	0.001680
27	1	0	6.664379	-2.595111	0.002408
28	6	0	9.114564	0.397786	-0.000718
29	1	0	7.379217	1.651286	-0.001816
30	6	0	9.615716	-0.908021	0.000552
31	1	0	9.100664	-3.002844	0.002681
32	1	0	9.799373	1.241905	-0.001578
33	1	0	10.688052	-1.082793	0.000672
34	6	0	-6.957590	-0.517302	-0.000010
35	6	0	-7.807904	-1.640328	-0.005667
36	6	0	-7.557468	0.758895	0.005743
37	6	0	-9.193754	-1.500352	-0.005909
38	1	0	-7.367511	-2.634847	-0.010052
39	6	0	-8.941027	0.898666	0.005484
40	1	0	-6.936962	1.650222	0.010803
41	6	0	-9.768741	-0.228859	-0.000376
42	1	0	-9.824724	-2.385253	-0.010401
43	1	0	-9.378861	1.893475	0.010042
44	1	0	-10.849205	-0.114757	-0.000490

DS-2T anti-anti

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.695685	-0.188395	0.001406
2	6	0	-1.255614	-1.454924	0.002619
3	6	0	-2.667246	-1.459624	0.002288
4	6	0	-3.232174	-0.196528	0.000791
5	16	0	-1.965676	1.021394	-0.000354
6	1	0	-0.657196	-2.360207	0.003959
7	1	0	-3.257125	-2.369619	0.003294
8	6	0	0.695685	0.188395	0.001408
9	6	0	1.255614	1.454924	0.002632
10	16	0	1.965676	-1.021394	-0.000363
11	6	0	2.667246	1.459624	0.002300
12	1	0	0.657196	2.360207	0.003980
13	6	0	3.232174	0.196528	0.000794
14	1	0	3.257126	2.369618	0.003313
15	6	0	-4.615760	0.223688	0.000078
16	1	0	-4.778961	1.299489	-0.000561
17	6	0	-5.686436	-0.604465	0.000099
18	1	0	-5.507542	-1.678968	0.000523
19	6	0	4.615760	-0.223688	0.000077
20	1	0	4.778961	-1.299489	-0.000561
21	6	0	5.686436	0.604465	0.000096
22	1	0	5.507542	1.678968	0.000524
23	6	0	-7.097558	-0.222656	-0.000482
24	6	0	-8.072395	-1.239537	-0.000975
25	6	0	-7.545524	1.114413	-0.000570
26	6	0	-9.432781	-0.939956	-0.001582
27	1	0	-7.749769	-2.278348	-0.000899
28	6	0	-8.903615	1.413503	-0.001182
29	1	0	-6.826216	1.928150	-0.000099
30	6	0	-9.856516	0.389582	-0.001697
31	1	0	-10.161994	-1.745836	-0.001962
32	1	0	-9.223266	2.452369	-0.001229
33	1	0	-10.916465	0.628219	-0.002161
34	6	0	7.097558	0.222656	-0.000482
35	6	0	8.072395	1.239537	-0.000986
36	6	0	7.545524	-1.114413	-0.000559
37	6	0	9.432781	0.939957	-0.001592
38	1	0	7.749769	2.278348	-0.000919
39	6	0	8.903615	-1.413503	-0.001171
40	1	0	6.826216	-1.928150	-0.000079
41	6	0	9.856516	-0.389582	-0.001697
42	1	0	10.161994	1.745836	-0.001980
43	1	0	9.223266	-2.452369	-0.001209
44	1	0	10.916465	-0.628219	-0.002160

DS-4F

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.857357	0.173768	0.000088
2	6	0	-2.533295	1.510590	0.000007
3	6	0	-1.115169	1.584499	-0.000033
4	6	0	-0.654241	0.288361	-0.000027
5	8	0	-1.713374	-0.582473	0.000061
6	1	0	-3.236274	2.330787	-0.000010
7	1	0	-0.501492	2.473492	-0.000085
8	6	0	-4.099628	-0.534750	0.000156
9	6	0	-4.420214	-1.874220	0.000326
10	8	0	-5.241170	0.214808	-0.000015
11	6	0	-5.835399	-1.947299	0.000305
12	1	0	-3.716276	-2.693731	0.000466
13	6	0	-6.311307	-0.652300	0.000117
14	1	0	-6.437641	-2.845065	0.000447
15	6	0	0.654241	-0.288363	-0.000072
16	6	0	1.115171	-1.584500	-0.000077
17	8	0	1.713373	0.582473	-0.000141
18	6	0	2.533296	-1.510590	-0.000102
19	1	0	0.501495	-2.473495	-0.000039
20	6	0	2.857357	-0.173768	-0.000168
21	1	0	3.236276	-2.330786	-0.000086
22	6	0	4.099628	0.534750	-0.000215
23	6	0	4.420214	1.874221	-0.000377
24	8	0	5.241170	-0.214808	-0.000010
25	6	0	5.835399	1.947299	-0.000330
26	1	0	3.716277	2.693732	-0.000530
27	6	0	6.311307	0.652300	-0.000135
28	1	0	6.437641	2.845066	-0.000460
29	6	0	-7.611097	-0.039923	0.000018
30	1	0	-7.593171	1.047174	-0.000131
31	6	0	7.611096	0.039923	-0.000010
32	1	0	7.593170	-1.047174	0.000144
33	6	0	8.787509	0.708662	-0.000037
34	1	0	8.758699	1.797986	-0.000078
35	6	0	-8.787509	-0.708661	0.000066
36	1	0	-8.758699	-1.797986	0.000097
37	6	0	10.130134	0.132043	0.000024
38	6	0	11.239689	0.999823	0.000376
39	6	0	10.382847	-1.255267	-0.000254
40	6	0	12.543365	0.509193	0.000483
41	1	0	11.068548	2.074005	0.000577
42	6	0	11.684407	-1.744951	-0.000141
43	1	0	9.553807	-1.956941	-0.000600
44	6	0	12.773504	-0.867204	0.000233
45	1	0	13.380050	1.202892	0.000760
46	1	0	11.852646	-2.818789	-0.000363
47	1	0	13.788700	-1.254264	0.000316
48	6	0	-10.130134	-0.132043	0.000042
49	6	0	-11.239690	-0.999823	-0.000322
50	6	0	-10.382847	1.255267	0.000368
51	6	0	-12.543365	-0.509193	-0.000399
52	1	0	-11.068548	-2.074005	-0.000560
53	6	0	-11.684407	1.744951	0.000287

54	1	0	-9.553807	1.956941	0.000729
55	6	0	-12.773505	0.867204	-0.000103
56	1	0	-13.380051	-1.202892	-0.000688
57	1	0	-11.852646	2.818789	0.000545
58	1	0	-13.788701	1.254264	-0.000161

DS-4T

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.228982	0.193122	0.000031
2	6	0	-2.666810	1.455889	0.000058
3	6	0	-1.253857	1.454264	0.000068
4	6	0	-0.694755	0.190117	0.000039
5	16	0	-1.963414	-1.028591	0.000000
6	1	0	-3.260739	2.363789	0.000080
7	1	0	-0.658132	2.361001	0.000098
8	6	0	-4.620008	-0.182960	0.000020
9	6	0	-5.181214	-1.449088	0.000022
10	16	0	-5.888532	1.028427	-0.000009
11	6	0	-6.592704	-1.452109	0.000013
12	1	0	-4.584204	-2.355292	0.000038
13	6	0	-7.156035	-0.188132	-0.000007
14	1	0	-7.183666	-2.361364	0.000020
15	6	0	0.694755	-0.190117	0.000040
16	6	0	1.253857	-1.454264	0.000072
17	16	0	1.963414	1.028591	0.000001
18	6	0	2.666810	-1.455889	0.000066
19	1	0	0.658132	-2.361001	0.000104
20	6	0	3.228982	-0.193122	0.000038
21	1	0	3.260739	-2.363789	0.000093
22	6	0	4.620008	0.182960	0.000030
23	6	0	5.181214	1.449088	0.000048
24	16	0	5.888532	-1.028427	-0.000021
25	6	0	6.592704	1.452110	0.000036
26	1	0	4.584204	2.355292	0.000079
27	6	0	7.156035	0.188132	0.000002
28	1	0	7.183666	2.361364	0.000055
29	6	0	-8.538995	0.234059	-0.000022
30	1	0	-8.700736	1.310049	-0.000025
31	6	0	-9.610647	-0.592828	-0.000024
32	1	0	-9.433069	-1.667549	-0.000017
33	6	0	8.538995	-0.234059	-0.000020
34	1	0	8.700736	-1.310049	-0.000021
35	6	0	9.610647	0.592828	-0.000026
36	1	0	9.433069	1.667549	-0.000017
37	6	0	-11.021252	-0.209244	-0.000029
38	6	0	-11.997267	-1.224964	-0.000045
39	6	0	-11.467334	1.128443	-0.000018
40	6	0	-13.357259	-0.923620	-0.000049
41	1	0	-11.675964	-2.264175	-0.000053
42	6	0	-12.825018	1.429273	-0.000023
43	1	0	-10.746988	1.941250	-0.000005
44	6	0	-13.779163	0.406496	-0.000039

45	1	0	-14.087553	-1.728494	-0.000062
46	1	0	-13.143384	2.468515	-0.000014
47	1	0	-14.838793	0.646511	-0.000043
48	6	0	11.021252	0.209244	-0.000032
49	6	0	11.997267	1.224964	-0.000063
50	6	0	11.467334	-1.128443	-0.000005
51	6	0	13.357259	0.923620	-0.000069
52	1	0	11.675964	2.264174	-0.000083
53	6	0	12.825018	-1.429273	-0.000011
54	1	0	10.746988	-1.941250	0.000021
55	6	0	13.779163	-0.406496	-0.000043
56	1	0	14.087553	1.728494	-0.000094
57	1	0	13.143384	-2.468515	0.000009
58	1	0	14.838793	-0.646511	-0.000048

D2F-Ant

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.739460	-0.250883	-0.000095
2	6	0	-2.632322	-1.079208	-0.000151
3	6	0	-1.308684	-0.559950	-0.000140
4	6	0	-1.118577	0.872822	-0.000077
5	6	0	-2.282004	1.705063	-0.000029
6	6	0	-3.539662	1.172255	-0.000034
7	6	0	-0.178487	-1.392980	-0.000190
8	6	0	0.178487	1.392980	-0.000064
9	6	0	1.308684	0.559951	-0.000113
10	6	0	1.118577	-0.872821	-0.000178
11	6	0	2.282004	-1.705063	-0.000223
12	1	0	2.147778	-2.784212	-0.000268
13	6	0	3.539662	-1.172255	-0.000209
14	6	0	3.739460	0.250884	-0.000152
15	6	0	2.632322	1.079208	-0.000100
16	1	0	-0.316290	-2.472483	-0.000234
17	1	0	-2.757563	-2.159011	-0.000207
18	1	0	-2.147778	2.784212	0.000019
19	1	0	-4.408930	1.820320	0.000010
20	1	0	0.316290	2.472483	-0.000013
21	1	0	4.408930	-1.820319	-0.000244
22	1	0	2.757563	2.159012	-0.000043
23	6	0	5.085598	0.796915	-0.000121
24	6	0	5.598488	2.073621	-0.000064
25	8	0	6.127784	-0.100496	0.000096
26	6	0	7.014385	1.958534	-0.000117
27	1	0	5.027217	2.991153	-0.000092
28	6	0	7.292772	0.613449	0.000050
29	1	0	7.742219	2.756816	-0.000186
30	6	0	-5.085598	-0.796915	-0.000060
31	6	0	-5.598487	-2.073621	0.000042
32	8	0	-6.127784	0.100496	0.000108
33	6	0	-7.014384	-1.958535	-0.000011
34	1	0	-5.027216	-2.991153	0.000076
35	6	0	-7.292772	-0.613449	0.000071
36	1	0	-7.742219	-2.756817	-0.000036
37	6	0	8.515569	-0.137828	0.000155
38	6	0	8.798206	-1.480238	0.000274
39	8	0	9.679785	0.584317	-0.000013
40	6	0	10.223583	-1.589619	0.000297
41	1	0	8.074591	-2.282218	0.000341
42	6	0	10.705731	-0.315814	0.000260
43	1	0	10.808835	-2.498573	0.000390
44	1	0	11.697607	0.109063	0.000281
45	6	0	-8.515569	0.137828	0.000122
46	6	0	-8.798206	1.480238	0.000150
47	8	0	-9.679784	-0.584318	0.000003
48	6	0	-10.223583	1.589618	0.000163
49	1	0	-8.074592	2.282218	0.000161
50	6	0	-10.705732	0.315813	0.000216
51	1	0	-10.808835	2.498572	0.000193
52	1	0	-11.697607	-0.109064	0.000267

D2T-Ant

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.738757	0.194755	0.239600
2	6	0	-2.745813	-0.746913	0.043174
3	6	0	-1.366778	-0.394500	0.022756
4	6	0	-0.995832	0.991124	0.194477
5	6	0	-2.041497	1.947786	0.383770
6	6	0	-3.354071	1.569434	0.408407
7	6	0	-0.355526	-1.348271	-0.169592
8	6	0	0.355514	1.348296	0.169559
9	6	0	1.366767	0.394525	-0.022793
10	6	0	0.995820	-0.991099	-0.194511
11	6	0	2.041487	-1.947759	-0.383792
12	1	0	1.772243	-2.992369	-0.519952
13	6	0	3.354061	-1.569405	-0.408427
14	6	0	3.738750	-0.194725	-0.239633
15	6	0	2.745800	0.746939	-0.043212
16	1	0	-0.630508	-2.392814	-0.301368
17	1	0	-3.011412	-1.787159	-0.124733
18	1	0	-1.772248	2.992393	0.519938
19	1	0	-4.125347	2.314905	0.580260
20	1	0	0.630495	2.392839	0.301337
21	1	0	4.125332	-2.314886	-0.580260
22	1	0	3.011388	1.787191	0.124678
23	6	0	5.147711	0.199263	-0.279191
24	6	0	5.692041	1.422372	-0.609309
25	16	0	6.427138	-0.928501	0.141924
26	6	0	7.106655	1.460495	-0.543458
27	1	0	5.089038	2.263947	-0.932134
28	6	0	7.676983	0.263574	-0.161765
29	1	0	7.694741	2.334823	-0.802210
30	6	0	9.076548	-0.070897	0.002102
31	6	0	9.676098	-1.312299	0.034373
32	16	0	10.284889	1.188387	0.205810
33	6	0	11.087750	-1.258545	0.209983
34	1	0	9.119776	-2.235882	-0.085881
35	6	0	11.563552	0.019891	0.309818
36	1	0	11.722579	-2.136997	0.250966
37	1	0	12.585670	0.349346	0.438911
38	6	0	-5.147715	-0.199240	0.279184
39	6	0	-5.692023	-1.422351	0.609353
40	16	0	-6.427155	0.928502	-0.141877
41	6	0	-7.106632	-1.460502	0.543486
42	1	0	-5.088992	-2.263899	0.932196
43	6	0	-7.676980	-0.263570	0.161839
44	1	0	-7.694694	-2.334850	0.802223
45	6	0	-9.076555	0.070857	-0.002023
46	6	0	-9.676144	1.312255	-0.034029
47	16	0	-10.284830	-1.188402	-0.206114
48	6	0	-11.087782	1.258493	-0.209707
49	1	0	-9.119866	2.235833	0.086457
50	6	0	-11.563532	-0.019940	-0.309892
51	1	0	-11.722648	2.136928	-0.250492
52	1	0	-12.585630	-0.349404	-0.439112