Electronic Supplementary Material (ESI) for RSC Advances.

Supporting Information

Theoretical framework for achieving High Voc in Non-fused non-fullerene terthiophene-based end-capped modified derivatives for potential applications in organic photovoltaics

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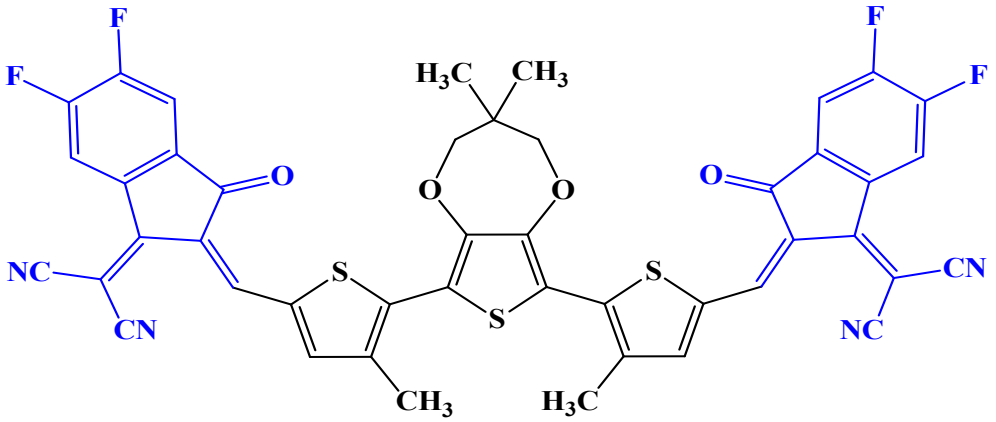
A3T-5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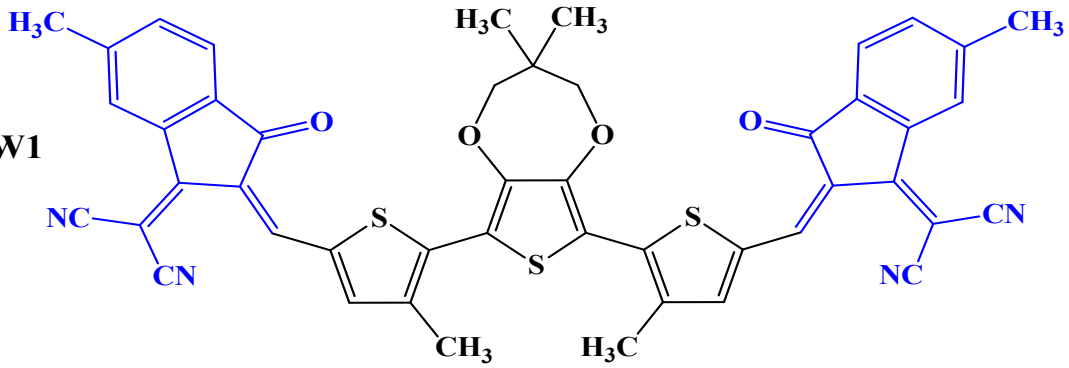
A3T-W1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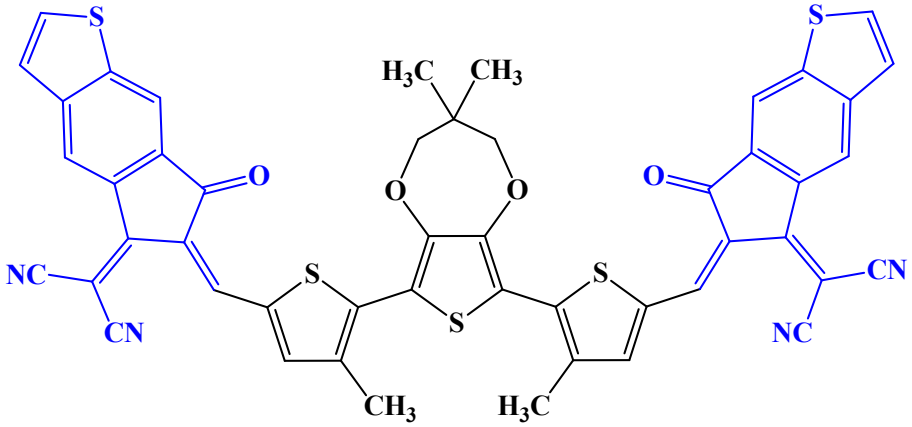

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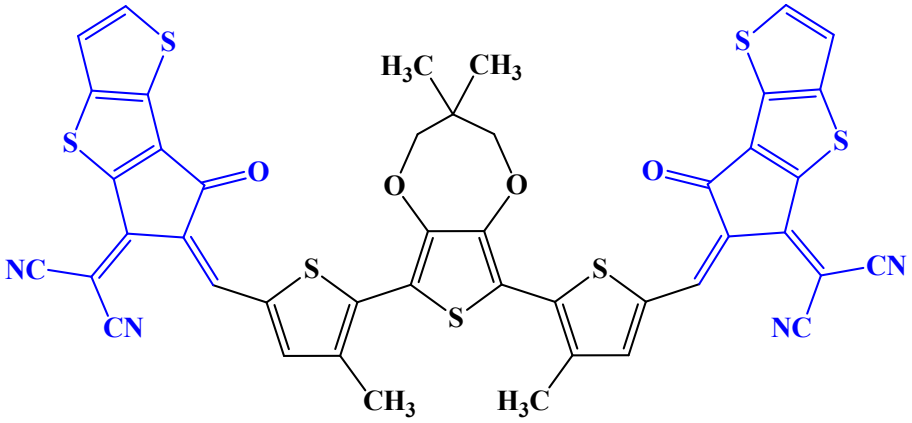

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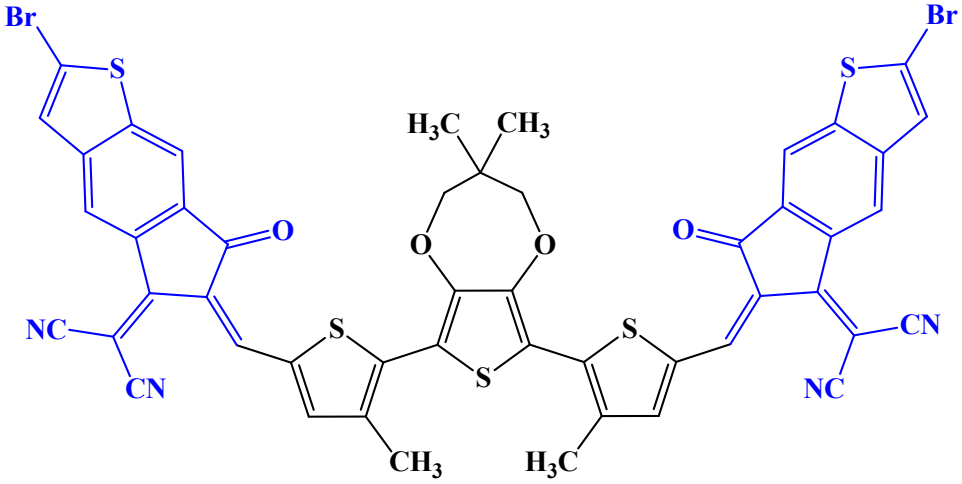


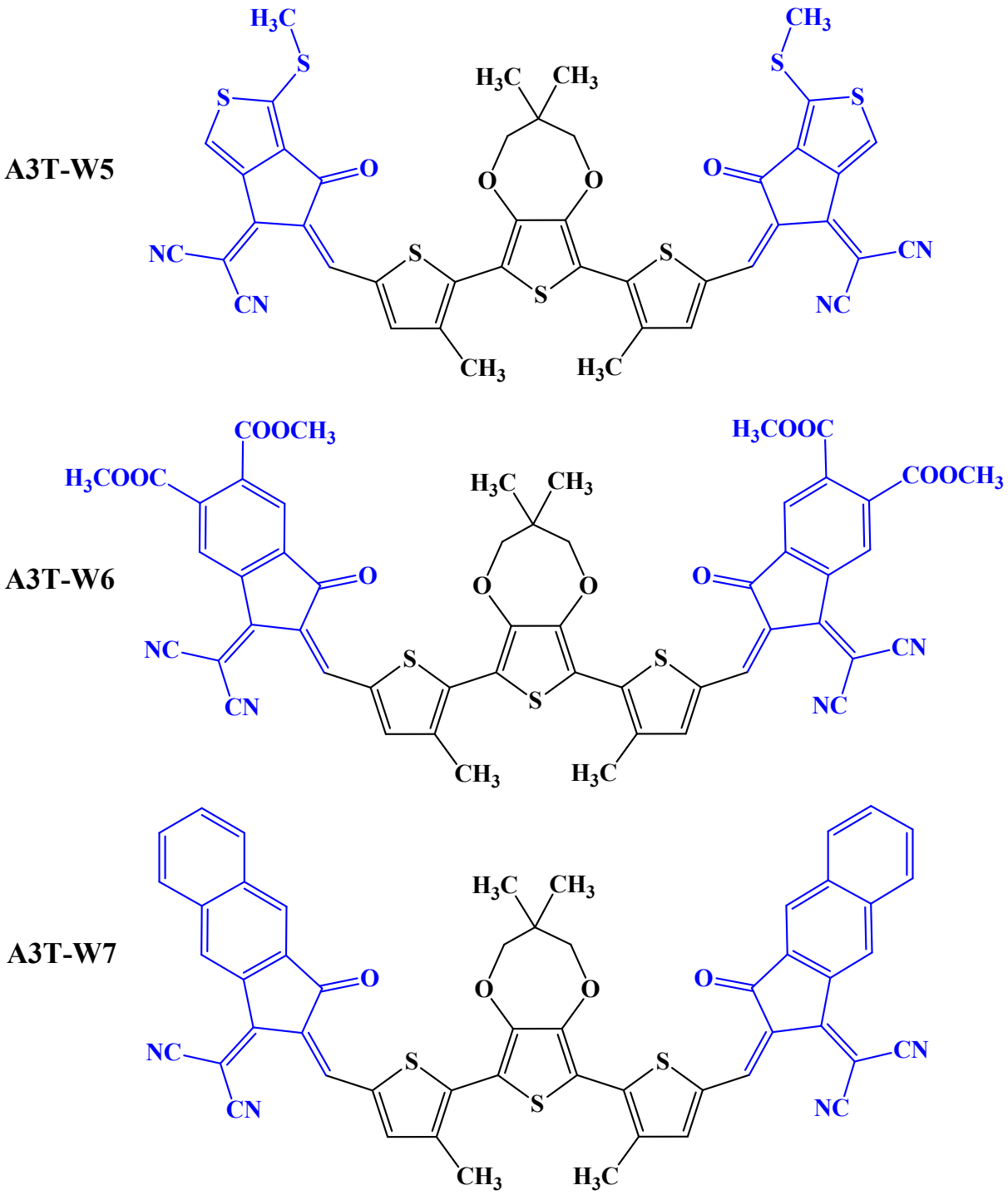
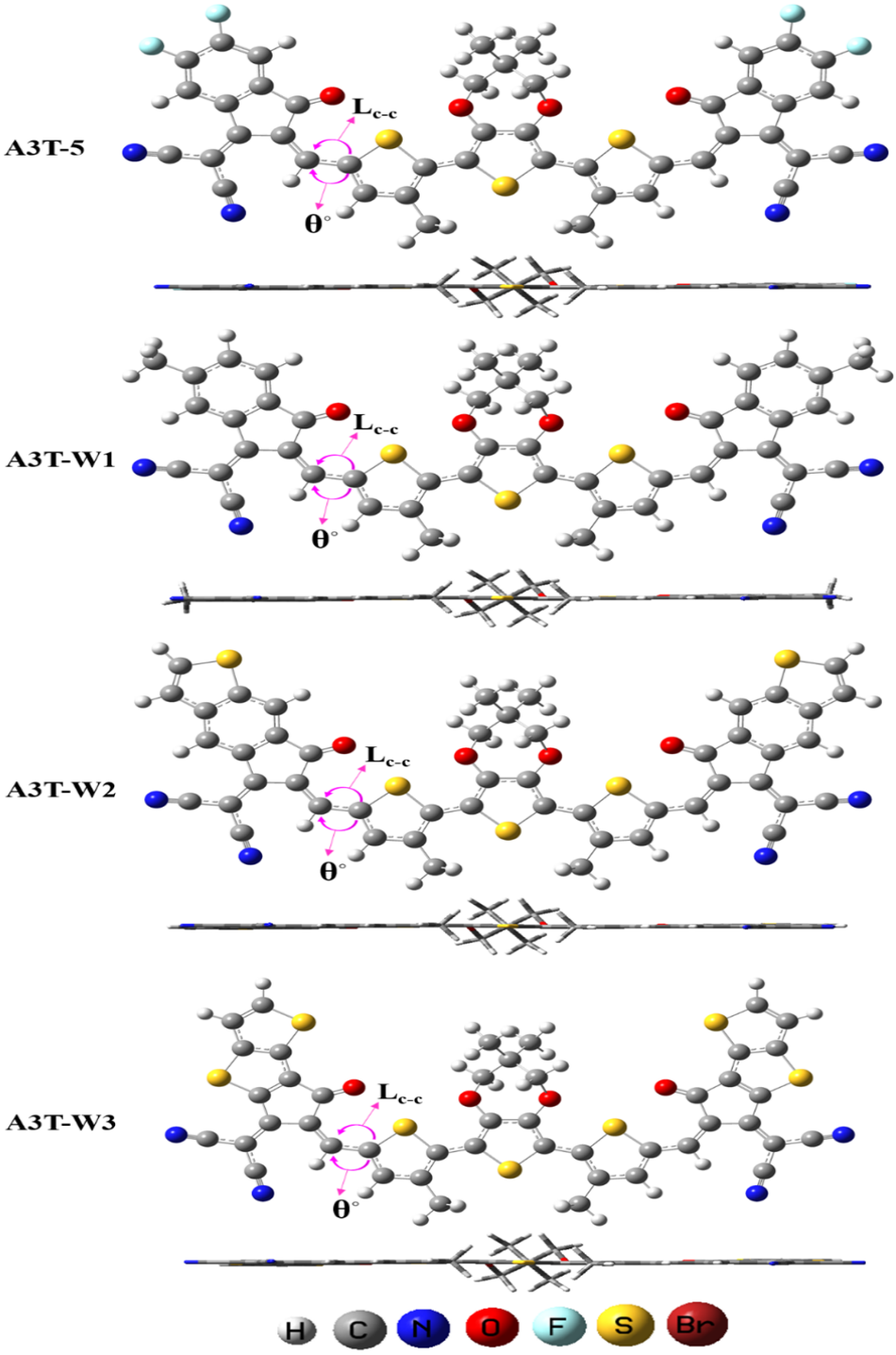


Figure S1. Structural configuration of A3T-5 and newly proposed molecules under study.


A3T-5
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θ°
A3T-W1
L_{c-c}
θ°
A3T-W2
L_{c-c}
θ°
A3T-W3
L_{c-c}
θ°
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N
O
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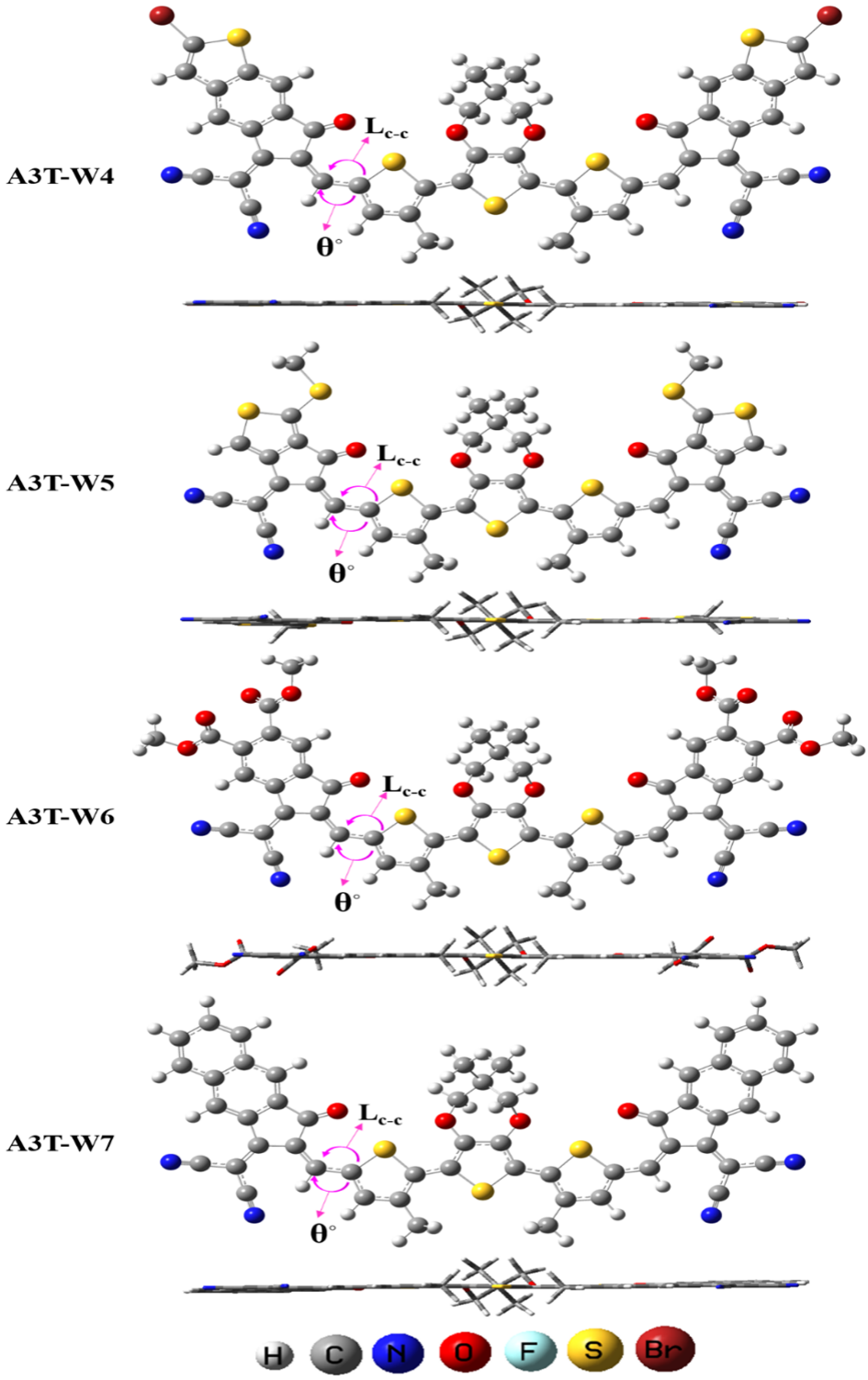

Figure S2. The optimal geometries of all examined compounds in front and side view.

Table S1: Cartesian coordinates of internally optimized geometries of all molecules (reference **A3T-5** and investigated molecules **A3T-W1** to **A3T-W7**) along X, Y and Z axis at CAM-B3LYP/6-31G (d, p) level of density functional theory (DFT).

Cartesian coordinates of Reference Molecule (A3T-5)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.275345	-1.610056	-0.003529
2	6	0	-0.671198	-0.366345	-0.008283
3	6	0	0.728429	-0.373062	0.010917
4	6	0	1.286641	-1.637865	0.029855
5	16	0	-0.007343	-2.812336	0.035896
6	8	0	1.377671	0.809329	-0.010934
7	8	0	-1.428677	0.796417	-0.201997
8	6	0	1.385510	2.099454	0.077844
9	6	0	-1.197404	2.070595	-0.108479
10	6	0	0.022668	2.668302	0.262074
11	6	0	-0.019790	3.796660	1.286096
12	6	0	-0.112659	3.477306	-1.038274
13	1	0	-0.350350	3.398942	2.246713
14	1	0	-0.815908	4.406325	0.854112
15	1	0	0.856323	4.426315	1.460004
16	1	0	-0.878648	4.082481	-1.527964
17	1	0	0.185967	2.665810	-1.701200
18	1	0	0.760952	4.105967	-0.847166
19	6	0	5.170024	-1.861361	0.054677
20	6	0	4.658564	-3.158465	0.107194
21	6	0	3.267019	-3.253765	0.103995

22	6	0	2.679841	-1.980628	0.050966
23	16	0	3.866700	-0.707511	0.004316
24	1	0	5.311009	-4.023620	0.147386
25	6	0	-2.671695	-1.950669	-0.029457
26	6	0	-3.252669	-3.228261	-0.062698
27	6	0	-4.645542	-3.141201	-0.070000
28	6	0	-5.165172	-1.848142	-0.039811
29	16	0	-3.870771	-0.686569	-0.008173
30	1	0	-5.291574	-4.011575	-0.096596
31	6	0	2.546651	-4.566104	0.154887
32	6	0	-2.536309	-4.543406	-0.086230
33	1	0	1.902356	-4.644836	1.035675
34	1	0	3.264845	-5.386168	0.199363
35	1	0	1.922536	-4.724963	-0.729908
36	1	0	-3.258143	-5.360016	-0.134095
37	1	0	-1.929002	-4.694646	0.811340
38	1	0	-1.876143	-4.634958	-0.953749
39	6	0	-6.572888	-1.651587	-0.045662
40	6	0	6.573942	-1.655140	0.051471
41	6	0	-7.372667	-0.539017	-0.022439
42	6	0	-8.835774	-0.509987	-0.035468
43	6	0	-9.244394	0.910934	0.004326
44	6	0	-8.096751	1.713604	0.039056
45	6	0	-6.895488	0.858507	0.024628
46	6	0	-9.709007	-1.573888	-0.077607
47	6	0	-11.125755	-1.419140	-0.086275
48	6	0	-9.300813	-2.938709	-0.117626
49	7	0	-8.999274	-4.061100	-0.151153

50	7	0	-12.284470	-1.329202	-0.094513
51	8	0	-5.741011	1.247476	0.049427
52	1	0	-7.085470	-2.606432	-0.073961
53	6	0	-10.503199	1.516481	0.011651
54	6	0	-10.552169	2.899434	0.053659
55	6	0	-9.393952	3.686051	0.087876
56	6	0	-8.143297	3.097722	0.081056
57	1	0	-11.436165	0.971039	-0.013236
58	1	0	-7.239845	3.694806	0.107210
59	6	0	7.368871	-0.537496	0.010147
60	6	0	8.830730	-0.504556	0.017276
61	6	0	9.236178	0.917631	-0.030127
62	6	0	8.086149	1.716245	-0.068564
63	6	0	6.887087	0.856912	-0.047853
64	6	0	9.708862	-1.565253	0.057298
65	6	0	11.124888	-1.404885	0.059025
66	6	0	9.307565	-2.931971	0.099521
67	7	0	9.013103	-4.056280	0.134193
68	7	0	12.283387	-1.310820	0.061501
69	8	0	5.731707	1.244842	-0.075671
70	6	0	10.492962	1.526928	-0.041643
71	6	0	10.538009	2.909932	-0.091552
72	6	0	9.377691	3.692525	-0.129707
73	6	0	8.128904	3.100055	-0.118689
74	1	0	11.427552	0.984413	-0.013891
75	1	0	7.223886	3.694517	-0.147456
76	1	0	7.093566	-2.605752	0.091787
77	9	0	-9.529519	5.006849	0.126992

78	9	0	-11.726878	3.520403	0.062276
79	9	0	9.508469	5.014026	-0.176652
80	9	0	11.711256	3.534257	-0.104173
81	1	0	-1.441277	2.480178	-1.066428
82	1	0	-1.925062	2.447169	0.579712
83	1	0	1.994217	2.384646	0.910335
84	1	0	1.810846	2.504590	-0.816502

Cartesian coordinates of Designed Molecule A3T-W1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.265856	-1.444856	0.096566
2	6	0	-0.705728	-0.176768	0.046338
3	6	0	0.709029	-0.177382	-0.040796
4	6	0	1.268100	-1.445973	-0.090320
5	16	0	0.000643	-2.642475	0.003670
6	8	0	1.474529	0.936018	-0.064526
7	8	0	-1.470332	0.937274	0.069038
8	6	0	0.994222	2.015320	0.749005
9	6	0	-0.989121	2.015379	-0.745557
10	6	0	0.002908	2.911111	0.001288
11	6	0	-0.714275	3.782399	1.035304
12	6	0	0.720739	3.780837	-1.033593
13	1	0	-1.252737	3.168491	1.762023

14	1	0	-1.437895	4.440603	0.547178
15	1	0	-0.003532	4.413111	1.577391
16	1	0	0.010455	4.411556	-1.576268
17	1	0	1.258700	3.165820	-1.759743
18	1	0	1.444879	4.438958	-0.546134
19	6	0	5.160449	-1.646258	-0.087794
20	6	0	4.653255	-2.945234	-0.129151
21	6	0	3.262613	-3.045414	-0.173649
22	6	0	2.664297	-1.775851	-0.140129
23	16	0	3.852289	-0.496878	-0.117806
24	1	0	5.307649	-3.810073	-0.135205
25	6	0	-2.662369	-1.773463	0.145740
26	6	0	-3.261971	-3.042395	0.179580
27	6	0	-4.652441	-2.940811	0.133441
28	6	0	-5.158500	-1.641391	0.090618
29	16	0	-3.849099	-0.493361	0.121405
30	1	0	-5.307642	-3.805042	0.139184
31	6	0	2.567910	-4.372192	-0.254437
32	6	0	-2.568753	-4.369867	0.261806
33	1	0	2.234132	-4.717761	0.729380
34	1	0	3.251748	-5.122757	-0.654905
35	1	0	1.696226	-4.345109	-0.911052
36	1	0	-3.253775	-5.119465	0.662063
37	1	0	-1.697671	-4.343329	0.919238
38	1	0	-2.234414	-4.716368	-0.721492
39	6	0	-6.560866	-1.429832	0.054116
40	6	0	6.562810	-1.434931	-0.053487
41	6	0	-7.359946	-0.312956	0.017030

42	6	0	-8.823898	-0.292447	0.013514
43	6	0	-9.239543	1.131475	-0.061712
44	6	0	-8.092603	1.934751	-0.095220
45	6	0	-6.890366	1.086945	-0.039867
46	6	0	-9.689285	-1.367038	0.073491
47	6	0	-11.109411	-1.243282	0.058571
48	6	0	-9.274453	-2.727865	0.162273
49	7	0	-8.993797	-3.854125	0.237317
50	7	0	-12.271161	-1.198816	0.048574
51	8	0	-5.737777	1.484343	-0.017152
52	1	0	-7.081077	-2.380391	0.059459
53	6	0	-10.494636	1.740052	-0.099620
54	6	0	-10.585519	3.134870	-0.162688
55	6	0	-9.416523	3.909317	-0.193363
56	6	0	-8.160888	3.316104	-0.165057
57	1	0	-11.406941	1.160942	-0.084477
58	1	0	-7.248993	3.901492	-0.200394
59	6	0	7.360114	-0.316846	-0.018028
60	6	0	8.824083	-0.292453	-0.018267
61	6	0	9.235850	1.132590	0.057185
62	6	0	8.086894	1.932766	0.092536
63	6	0	6.886858	1.081736	0.039006
64	6	0	9.692583	-1.364423	-0.081495
65	6	0	11.112323	-1.236023	-0.071446
66	6	0	9.281659	-2.726440	-0.169876
67	7	0	9.004025	-3.853464	-0.244667
68	7	0	12.273970	-1.188175	-0.066024
69	8	0	5.732945	1.475618	0.020967

70	6	0	10.489540	1.744816	0.087051
71	6	0	10.576748	3.139752	0.148947
72	6	0	9.405628	3.911375	0.177322
73	6	0	8.151649	3.314672	0.157047
74	1	0	11.403348	1.168349	0.065779
75	1	0	7.238257	3.897971	0.187968
76	1	0	7.083635	-2.385122	-0.059405
77	1	0	-0.521488	1.589209	-1.638608
78	1	0	-1.871168	2.580213	-1.053756
79	1	0	0.526254	1.590437	1.642494
80	1	0	1.876744	2.579737	1.056607
81	6	0	-11.933550	3.800624	-0.184427
82	6	0	11.921980	3.808681	0.208385
83	1	0	9.489366	4.993186	0.212147
84	1	0	-9.502999	4.990541	-0.237696
85	1	0	-11.896812	4.756920	-0.709874
86	1	0	-12.680507	3.169904	-0.670034
87	1	0	-12.283788	3.997028	0.834233
88	1	0	12.687913	3.207719	-0.284988
89	1	0	11.898392	4.792302	-0.265202
90	1	0	12.235782	3.951295	1.247684

Cartesian coordinates of Designed Molecule A3T-W2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.269605	-1.937591	0.030451

2	6	0	-0.707637	-0.668216	0.011455
3	6	0	0.707808	-0.668224	-0.010571
4	6	0	1.269753	-1.937600	-0.030345
5	16	0	0.000063	-3.135428	-0.000313
6	8	0	1.469376	0.446644	-0.017498
7	8	0	-1.469191	0.446657	0.019023
8	6	0	0.974683	1.535055	0.775597
9	6	0	-0.974436	1.535576	-0.773339
10	6	0	0.000121	2.428039	0.001432
11	6	0	-0.751528	3.294772	1.014213
12	6	0	0.751771	3.295445	-1.010772
13	1	0	-1.396975	2.684309	1.651244
14	1	0	-1.378160	4.029870	0.502107
15	1	0	-0.055883	3.843230	1.656480
16	1	0	0.056133	3.844349	-1.652664
17	1	0	1.397205	2.685400	-1.648218
18	1	0	1.378422	4.030185	-0.498173
19	6	0	5.162156	-2.147005	-0.015090
20	6	0	4.650261	-3.445891	-0.019099
21	6	0	3.260294	-3.542411	-0.029432
22	6	0	2.665863	-2.268235	-0.030482
23	16	0	3.856121	-0.993495	-0.025079
24	1	0	5.303046	-4.311928	-0.016472
25	6	0	-2.665724	-2.268193	0.030354
26	6	0	-3.260208	-3.542347	0.028639
27	6	0	-4.650167	-3.445764	0.018261
28	6	0	-5.162014	-2.146852	0.014877
29	16	0	-3.855933	-0.993408	0.025499

30	1	0	-5.302986	-4.311774	0.015166
31	6	0	2.549397	-4.861316	-0.041822
32	6	0	-2.549376	-4.861294	0.040415
33	1	0	1.928681	-5.000876	0.848354
34	1	0	3.275232	-5.675704	-0.067636
35	1	0	1.902409	-4.970057	-0.917187
36	1	0	-3.275252	-5.675656	0.065891
37	1	0	-1.902358	-4.970458	0.915705
38	1	0	-1.928705	-5.000491	-0.849849
39	6	0	-6.563260	-1.939353	0.011852
40	6	0	6.563403	-1.939517	-0.012068
41	6	0	-7.361122	-0.819994	0.004616
42	6	0	-8.822106	-0.792960	0.008229
43	6	0	-9.237616	0.626862	-0.003156
44	6	0	-8.078195	1.435104	-0.015845
45	6	0	-6.881416	0.575914	-0.012792
46	6	0	-9.693708	-1.863265	0.021574
47	6	0	-11.110832	-1.717026	0.024147
48	6	0	-9.286330	-3.228212	0.034427
49	7	0	-8.992048	-4.353463	0.044913
50	7	0	-12.271017	-1.640309	0.026502
51	8	0	-5.723409	0.963858	-0.025552
52	1	0	-7.083482	-2.890474	0.017314
53	6	0	-10.490918	1.221178	-0.002474
54	6	0	-10.562268	2.624061	-0.014511
55	6	0	-9.375860	3.403827	-0.027233
56	6	0	-8.112872	2.812578	-0.027996
57	1	0	-11.407087	0.647301	0.007331

58	1	0	-7.191851	3.384042	-0.037064
59	6	0	7.361192	-0.820110	-0.004372
60	6	0	8.822172	-0.792931	-0.008084
61	6	0	9.237535	0.626934	0.003135
62	6	0	8.078034	1.435050	0.016232
63	6	0	6.881349	0.575735	0.013745
64	6	0	9.693881	-1.863149	-0.021492
65	6	0	11.110989	-1.716764	-0.024212
66	6	0	9.286633	-3.228133	-0.034258
67	7	0	8.992464	-4.353414	-0.044635
68	7	0	12.271167	-1.639949	-0.026667
69	8	0	5.723292	0.963565	0.025596
70	6	0	10.490774	1.221383	0.001936
71	6	0	10.561980	2.624272	0.013982
72	6	0	9.375492	3.403912	0.027030
73	6	0	8.112568	2.812530	0.028223
74	1	0	11.406999	0.647602	-0.008197
75	1	0	7.191490	3.383897	0.037502
76	1	0	7.083649	-2.890622	-0.018010
77	1	0	-0.499986	1.131972	-1.673307
78	1	0	-1.858935	2.101202	-1.072878
79	1	0	0.500254	1.130874	1.675318
80	1	0	1.859206	2.100464	1.075476
81	6	0	-11.736622	3.446926	-0.015154
82	6	0	11.736246	3.447262	0.014272
83	6	0	-11.446365	4.771011	-0.029958
84	6	0	11.445847	4.771336	0.027037
85	1	0	12.744138	3.053245	-0.000455

86	1	0	-12.744534	3.052710	-0.010697
87	16	0	-9.742058	5.102390	-0.040808
88	16	0	9.741517	5.102518	0.039985
89	1	0	-12.142348	5.597702	-0.035924
90	1	0	12.141714	5.598146	0.027545

Cartesian coordinates of Designed Molecule A3T-W3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.281147	-1.852008	0.066345
2	6	0	-0.726764	-0.549213	0.024239
3	6	0	0.724909	-0.549457	-0.022891
4	6	0	1.278871	-1.852343	-0.065654
5	16	0	-0.001313	-3.073828	0.000063
6	8	0	1.591249	0.602293	-0.008010
7	8	0	-1.592611	0.602927	0.009909
8	6	0	0.993173	1.596976	0.801850
9	6	0	-0.994041	1.597848	-0.799316
10	6	0	-0.000244	2.457296	0.001519
11	6	0	-0.755414	3.343249	1.010414
12	6	0	0.755330	3.343476	-1.006883
13	1	0	-1.285595	2.723790	1.702907
14	1	0	-1.448724	3.968417	0.487631
15	1	0	-0.055201	3.954022	1.541858
16	1	0	0.055392	3.954850	-1.537993

17	1	0	1.285244	2.724164	-1.699715
18	1	0	1.448914	3.968048	-0.483751
19	6	0	5.217863	-2.212922	-0.060995
20	6	0	4.629153	-3.466260	-0.023504
21	6	0	3.225907	-3.449148	-0.076898
22	6	0	2.669706	-2.144831	-0.121268
23	16	0	3.985456	-0.948320	-0.255469
24	1	0	5.202406	-4.365336	0.046119
25	6	0	-2.672031	-2.144251	0.121435
26	6	0	-3.228435	-3.448508	0.077029
27	6	0	-4.631622	-3.465604	0.023781
28	6	0	-5.219918	-2.212238	0.061198
29	16	0	-3.987622	-0.947715	0.255826
30	1	0	-5.204982	-4.364462	-0.046652
31	6	0	2.430999	-4.758994	-0.073600
32	6	0	-2.433886	-4.758426	0.073474
33	1	0	2.183523	-5.023844	0.932427
34	1	0	3.031381	-5.533505	-0.508618
35	1	0	1.537177	-4.637797	-0.642867
36	1	0	-3.034532	-5.532836	0.508609
37	1	0	-1.540160	-4.637489	0.643131
38	1	0	-2.186378	-5.023238	-0.932291
39	6	0	-6.608335	-2.098390	-0.040501
40	6	0	6.606430	-2.099671	0.040022
41	6	0	-7.275032	-0.946836	-0.037446
42	6	0	-8.814196	-0.843347	-0.015697
43	6	0	-9.124294	0.631733	-0.058743
44	6	0	-8.000865	1.333483	-0.071728

45	6	0	-6.738298	0.483833	-0.060770
46	6	0	-9.704224	-1.853082	0.018941
47	6	0	-11.075750	-1.598710	0.026511
48	6	0	-9.255530	-3.167681	0.046798
49	7	0	-8.897573	-4.249053	0.069830
50	7	0	-12.204562	-1.400018	0.032983
51	8	0	-5.542498	0.880394	-0.070569
52	1	0	-7.180010	-2.994744	-0.118612
53	6	0	-9.559268	3.075082	-0.012983
54	6	0	-8.261317	2.789316	-0.088475
55	6	0	7.274964	-0.949426	0.037782
56	6	0	8.816756	-0.848300	0.016150
57	6	0	9.125888	0.627154	0.058382
58	6	0	8.003105	1.330895	0.071235
59	6	0	6.739414	0.482789	0.060660
60	6	0	9.703290	-1.856358	-0.020931
61	6	0	11.077544	-1.597759	-0.028511
62	6	0	9.249757	-3.170814	-0.047881
63	7	0	8.877740	-4.247978	-0.069962
64	7	0	12.203143	-1.393105	-0.034896
65	8	0	5.543913	0.881047	0.070706
66	6	0	9.563999	3.070891	0.012307
67	6	0	8.265644	2.787163	0.088302
68	1	0	7.177570	-2.996102	0.118651
69	1	0	-0.488243	1.101512	-1.600688
70	1	0	-1.743685	2.251823	-1.193702
71	1	0	0.487187	1.100402	1.602955
72	1	0	1.743124	2.250389	1.196595

73	16	0	10.603495	1.621534	0.104880
74	16	0	-10.601031	1.627294	-0.105330
75	6	0	9.803910	4.569116	-0.150457
76	6	0	-9.796363	4.574120	0.148776
77	16	0	-7.202172	4.162302	-0.174573
78	16	0	7.208989	4.162432	0.173628
79	6	0	-8.579134	5.246508	0.165059
80	6	0	8.588077	5.243753	-0.166903
81	1	0	-10.763532	5.028779	0.243906
82	1	0	-8.457583	6.281064	0.359476
83	1	0	8.468697	6.278436	-0.361398
84	1	0	10.772051	5.021625	-0.245403

Cartesian coordinates of Designed Molecule A3T-W4

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.269391	-2.731057	0.035336
2	6	0	-0.707596	-1.461444	0.013672
3	6	0	0.707692	-1.461436	-0.013410
4	6	0	1.269485	-2.731044	-0.035610
5	16	0	0.000046	-3.928819	-0.000377
6	8	0	1.469603	-0.347040	-0.022941
7	8	0	-1.469512	-0.347054	0.023584
8	6	0	0.977700	0.742018	0.771291
9	6	0	-0.977625	0.742234	-0.770337
10	6	0	0.000034	1.634586	0.000607

11	6	0	-0.747552	2.501279	1.016477
12	6	0	0.747603	2.501593	-1.015010
13	1	0	-1.390331	1.890607	1.656021
14	1	0	-1.376049	3.236624	0.507061
15	1	0	-0.049349	3.049590	1.656089
16	1	0	0.049387	3.050101	-1.654438
17	1	0	1.390371	1.891121	-1.654755
18	1	0	1.376104	3.236784	-0.505379
19	6	0	5.161880	-2.940937	-0.031718
20	6	0	4.649720	-4.239932	-0.038431
21	6	0	3.259986	-4.336173	-0.045512
22	6	0	2.665599	-3.061576	-0.040673
23	16	0	3.855937	-1.787133	-0.034291
24	1	0	5.302394	-5.106050	-0.040576
25	6	0	-2.665513	-3.061568	0.040223
26	6	0	-3.259947	-4.336148	0.044521
27	6	0	-4.649675	-4.239847	0.037443
28	6	0	-5.161787	-2.940825	0.031280
29	16	0	-3.855799	-1.787079	0.034341
30	1	0	-5.302383	-5.105940	0.039215
31	6	0	2.548722	-5.654792	-0.059957
32	6	0	-2.548743	-5.654805	0.058420
33	1	0	1.931782	-5.797709	0.832284
34	1	0	3.274169	-6.469255	-0.091790
35	1	0	1.898064	-5.759623	-0.933131
36	1	0	-3.274225	-6.469249	0.089939
37	1	0	-1.898066	-5.760014	0.931534
38	1	0	-1.931833	-5.797391	-0.833895

39	6	0	-6.562586	-2.733784	0.031542
40	6	0	6.562683	-2.733923	-0.031908
41	6	0	-7.360940	-1.614282	0.022242
42	6	0	-8.821382	-1.588141	0.028803
43	6	0	-9.237904	-0.167852	0.011862
44	6	0	-8.079582	0.639755	-0.006317
45	6	0	-6.881909	-0.218885	-0.001896
46	6	0	-9.693239	-2.657619	0.049535
47	6	0	-11.110295	-2.510387	0.054310
48	6	0	-9.285780	-4.022553	0.068993
49	7	0	-8.990260	-5.147343	0.085015
50	7	0	-12.270274	-2.431334	0.058487
51	8	0	-5.724777	0.171232	-0.016354
52	1	0	-7.082831	-3.684850	0.041964
53	6	0	-10.491866	0.425509	0.011827
54	6	0	-10.562954	1.828175	-0.006460
55	6	0	-9.376278	2.607781	-0.024280
56	6	0	-8.114148	2.017941	-0.024380
57	1	0	-11.408133	-0.147934	0.025377
58	1	0	-7.193006	2.589069	-0.037467
59	6	0	7.361015	-1.614411	-0.022066
60	6	0	8.821473	-1.588161	-0.028628
61	6	0	9.237881	-0.167865	-0.010590
62	6	0	8.079511	0.639654	0.008079
63	6	0	6.881896	-0.219057	0.002837
64	6	0	9.693517	-2.657473	-0.050201
65	6	0	11.110537	-2.509895	-0.054886
66	6	0	9.286387	-4.022488	-0.070737

67	7	0	8.991340	-5.147390	-0.087639
68	7	0	12.270491	-2.430490	-0.059029
69	8	0	5.724742	0.170963	0.018234
70	6	0	10.491813	0.425552	-0.009963
71	6	0	10.562825	1.828206	0.009466
72	6	0	9.376101	2.607733	0.027810
73	6	0	8.114000	2.017827	0.027207
74	1	0	11.408108	-0.147844	-0.023817
75	1	0	7.192825	2.588895	0.040586
76	1	0	7.082914	-3.684984	-0.042771
77	1	0	-0.507166	0.339009	-1.672616
78	1	0	-1.863304	1.308095	-1.065897
79	1	0	0.507244	0.338530	1.673455
80	1	0	1.863374	1.307799	1.067016
81	6	0	-11.741984	2.642609	-0.009316
82	6	0	11.741812	2.642697	0.013317
83	6	0	-11.443629	3.964691	-0.029833
84	6	0	11.443382	3.964755	0.034325
85	1	0	12.751609	2.256163	0.001555
86	1	0	-12.751754	2.256025	0.003109
87	16	0	-9.736248	4.310260	-0.044702
88	16	0	9.735981	4.310217	0.049482
89	35	0	-12.652245	5.380535	-0.047054
90	35	0	12.651850	5.380807	0.041517

Cartesian coordinates of Designed Molecule A3T-W5

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.278667	-1.850959	0.034857
2	6	0	-0.716165	-0.581760	0.013309
3	6	0	0.699358	-0.583001	-0.011994
4	6	0	1.259613	-1.853176	-0.034269
5	16	0	-0.010584	-3.050241	-0.000093
6	8	0	1.462120	0.530426	-0.020531
7	8	0	-1.476972	0.533007	0.022524
8	6	0	0.969878	1.620171	0.773720
9	6	0	-0.982846	1.622321	-0.771089
10	6	0	-0.005674	2.513638	0.001539
11	6	0	-0.753950	3.380924	1.016422
12	6	0	0.744230	3.380054	-1.012889
13	1	0	-1.398259	2.770888	1.655049
14	1	0	-1.380757	4.117060	0.506123
15	1	0	-0.056227	3.928431	1.657164
16	1	0	0.047556	3.929171	-1.653391
17	1	0	1.387426	2.769130	-1.651791
18	1	0	1.372382	4.114772	-0.502198
19	6	0	5.151589	-2.064563	-0.026282
20	6	0	4.639345	-3.363454	-0.037044
21	6	0	3.249551	-3.459329	-0.045602
22	6	0	2.655486	-2.184611	-0.037897
23	16	0	3.845775	-0.910526	-0.028100
24	1	0	5.291611	-4.229854	-0.040456
25	6	0	-2.675129	-2.179944	0.038236

26	6	0	-3.271451	-3.453614	0.045655
27	6	0	-4.661075	-3.355286	0.036764
28	6	0	-5.171026	-2.055495	0.026038
29	16	0	-3.863175	-0.903769	0.028333
30	1	0	-5.314868	-4.220535	0.039947
31	6	0	2.537565	-4.777494	-0.064474
32	6	0	-2.561825	-4.773048	0.064592
33	1	0	1.918274	-4.921896	0.825819
34	1	0	3.262456	-5.592388	-0.096034
35	1	0	1.889202	-4.879722	-0.939713
36	1	0	-3.288172	-5.586628	0.096607
37	1	0	-1.913331	-4.876228	0.939615
38	1	0	-1.943119	-4.918783	-0.825897
39	6	0	-6.571046	-1.844866	0.023481
40	6	0	6.551976	-1.856396	-0.023957
41	6	0	-7.366073	-0.723126	0.011124
42	6	0	-8.826230	-0.693038	0.016631
43	6	0	-9.235728	0.729559	-0.006988
44	6	0	-8.087007	1.530030	-0.026416
45	6	0	-6.886177	0.671442	-0.016171
46	6	0	-9.705128	-1.754770	0.040622
47	6	0	-11.120940	-1.594246	0.043706
48	6	0	-9.305746	-3.122308	0.065121
49	7	0	-9.014860	-4.248011	0.085413
50	7	0	-12.279597	-1.500478	0.046807
51	8	0	-5.731928	1.066000	-0.030154
52	1	0	-7.094608	-2.794169	0.034582
53	6	0	-10.493076	1.337253	-0.011752

54	6	0	-8.131785	2.914234	-0.050486
55	1	0	-11.426962	0.792995	0.002232
56	6	0	7.348968	-0.736052	-0.011584
57	6	0	8.809172	-0.708526	-0.017326
58	6	0	9.221169	0.713352	0.006170
59	6	0	8.073856	1.515834	0.025828
60	6	0	6.871522	0.659352	0.015842
61	6	0	9.686198	-1.771802	-0.041360
62	6	0	11.102289	-1.613766	-0.044691
63	6	0	9.284400	-3.138635	-0.065653
64	7	0	8.991559	-4.263834	-0.085780
65	7	0	12.261108	-1.522034	-0.048000
66	8	0	5.717966	1.055925	0.030070
67	6	0	10.479581	1.318841	0.010657
68	6	0	8.121065	2.899959	0.049863
69	1	0	11.412509	0.772947	-0.003519
70	1	0	7.073871	-2.806613	-0.035310
71	1	0	-0.511514	1.218356	-1.672487
72	1	0	-1.867709	2.188694	-1.067823
73	1	0	0.497829	1.216524	1.674883
74	1	0	1.855748	2.184807	1.070758
75	16	0	-9.840712	2.996833	-0.044082
76	16	0	9.862748	2.977914	0.042903
77	16	0	6.636824	3.882245	0.073182
78	16	0	-6.645821	3.893918	-0.073508
79	6	0	-6.751504	5.670319	-0.113889
80	6	0	7.068446	5.608667	0.112808
81	1	0	8.002284	5.754447	-0.388784

82	1	0	6.307129	6.178010	-0.378257
83	1	0	7.155383	5.931336	1.129286
84	1	0	-5.900816	6.066635	-0.627857
85	1	0	-7.645036	5.962939	-0.624647
86	1	0	-6.772189	6.049220	0.886565

Cartesian coordinates of Designed Molecule A3T-W6

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.287350	-2.518989	0.035502
2	6	0	-0.722603	-1.250765	0.015267
3	6	0	0.692862	-1.254507	-0.012887
4	6	0	1.250778	-2.525644	-0.038736
5	16	0	-0.021507	-3.720483	-0.004310
6	8	0	1.457613	-0.142442	-0.020814
7	8	0	-1.481377	-0.134650	0.028161
8	6	0	0.968936	0.946654	0.776524
9	6	0	-0.986881	0.955301	-0.764345
10	6	0	-0.006551	1.843365	0.008030
11	6	0	-0.751220	2.710036	1.026086
12	6	0	0.742876	2.710385	-1.006234
13	1	0	-1.395345	2.099931	1.664833
14	1	0	-1.377722	3.448284	0.518469
15	1	0	-0.051225	3.255049	1.666476
16	1	0	0.045908	3.261990	-1.644273

17	1	0	1.383683	2.099538	-1.647605
18	1	0	1.373378	3.442983	-0.495394
19	6	0	5.142373	-2.744055	-0.038990
20	6	0	4.627766	-4.041999	-0.051223
21	6	0	3.237787	-4.135354	-0.057168
22	6	0	2.646040	-2.859584	-0.045812
23	16	0	3.838644	-1.587667	-0.035956
24	1	0	5.278459	-4.909564	-0.057616
25	6	0	-2.684395	-2.845465	0.041058
26	6	0	-3.282999	-4.118070	0.047224
27	6	0	-4.672457	-4.017222	0.041319
28	6	0	-5.180082	-2.716497	0.034123
29	16	0	-3.870152	-1.567135	0.036005
30	1	0	-5.327804	-4.881297	0.044151
31	6	0	2.523386	-5.452196	-0.077147
32	6	0	-2.575718	-5.438814	0.062191
33	1	0	1.905625	-5.597199	0.814111
34	1	0	3.246740	-6.268331	-0.111735
35	1	0	1.873082	-5.551566	-0.951274
36	1	0	-3.303466	-6.251145	0.094101
37	1	0	-1.925655	-5.544851	0.935707
38	1	0	-1.959066	-5.583944	-0.829820
39	6	0	-6.579722	-2.503342	0.034790
40	6	0	6.543136	-2.538416	-0.039082
41	6	0	-7.372746	-1.380150	0.026194
42	6	0	-8.832833	-1.347443	0.034698
43	6	0	-9.239809	0.075932	0.014644
44	6	0	-8.089686	0.874369	-0.005554

45	6	0	-6.890390	0.013601	0.000619
46	6	0	-9.713595	-2.407635	0.058412
47	6	0	-11.129107	-2.244567	0.064655
48	6	0	-9.316635	-3.775935	0.079473
49	7	0	-9.027740	-4.902196	0.097011
50	7	0	-12.287584	-2.148719	0.070269
51	8	0	-5.735461	0.406106	-0.014926
52	1	0	-7.104973	-3.451721	0.045116
53	6	0	-10.496065	0.685898	0.013581
54	6	0	-10.540752	2.069969	-0.007849
55	6	0	-9.380517	2.852323	-0.027760
56	6	0	-8.132015	2.258695	-0.026868
57	1	0	-11.430902	0.143297	0.028396
58	1	0	-7.226738	2.853245	-0.041549
59	6	0	7.342172	-1.419535	-0.026155
60	6	0	8.802409	-1.394628	-0.034783
61	6	0	9.217018	0.026458	-0.009377
62	6	0	8.071197	0.830966	0.014136
63	6	0	6.867301	-0.023329	0.004919
64	6	0	9.677464	-2.459433	-0.062630
65	6	0	11.093828	-2.303942	-0.068507
66	6	0	9.273152	-3.825491	-0.088747
67	7	0	8.978241	-4.950119	-0.110452
68	7	0	12.252802	-2.214291	-0.073971
69	8	0	5.714494	0.375293	0.022233
70	6	0	10.476527	0.629670	-0.006257
71	6	0	10.528639	2.013389	0.020460
72	6	0	9.372621	2.801871	0.043628

73	6	0	8.120952	2.214954	0.040742
74	1	0	11.408438	0.082125	-0.023362
75	1	0	7.063291	-3.489547	-0.053316
76	1	0	-0.518091	0.552229	-1.667466
77	1	0	-1.871315	1.523839	-1.058206
78	1	0	0.497970	0.542118	1.677856
79	1	0	1.856419	1.509119	1.072865
80	6	0	-11.911943	2.770991	-0.009834
81	6	0	-9.495602	4.387843	-0.050865
82	6	0	9.495943	4.336652	0.072588
83	6	0	11.903570	2.707037	0.024816
84	1	0	7.228401	2.804821	0.058317
85	8	0	-11.976088	4.027718	-0.019381
86	8	0	-10.629378	4.933821	-0.056323
87	8	0	10.632632	4.876515	0.080117
88	8	0	11.974454	3.963363	0.038637
89	8	0	13.099741	1.923495	0.013155
90	8	0	8.318764	5.148326	0.090923
91	8	0	-8.314085	5.193252	-0.066116
92	8	0	-13.112299	1.993840	-0.000827
93	6	0	-14.385548	2.644788	-0.002669
94	6	0	-7.918932	6.556286	-0.241878
95	6	0	8.691813	6.528575	0.116330
96	6	0	14.237270	2.790029	0.020019
97	1	0	-14.306691	3.581106	-0.514519
98	1	0	-15.102069	2.025393	-0.500511
99	1	0	-14.700594	2.814938	1.005643
100	1	0	15.049170	2.316864	-0.491678

101	1	0	13.990336	3.706688	-0.473600
102	1	0	14.523463	2.994920	1.030471
103	1	0	9.627029	6.654615	-0.388036
104	1	0	7.940235	7.110280	-0.375250
105	1	0	8.787309	6.853605	1.131286
106	1	0	-6.982158	6.592387	-0.757678
107	1	0	-8.661418	7.071904	-0.814376
108	1	0	-7.817548	7.024461	0.714905

Cartesian coordinates of Designed Molecule A3T-W7

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.271799	-1.894353	0.035295
2	6	0	-0.709575	-0.625034	0.013540
3	6	0	0.705942	-0.625974	-0.012180
4	6	0	1.266461	-1.896030	-0.034579
5	16	0	-0.003470	-3.093365	0.000010
6	8	0	1.468463	0.487615	-0.020978
7	8	0	-1.470617	0.489571	0.022943
8	6	0	0.976223	1.577282	0.773383
9	6	0	-0.976958	1.578964	-0.770851
10	6	0	0.000252	2.470515	0.001460
11	6	0	-0.747910	3.337673	1.016536
12	6	0	0.749672	3.337058	-1.013217
13	1	0	-1.391900	2.727521	1.655373

14	1	0	-1.375025	4.073659	0.506398
15	1	0	-0.050115	3.885351	1.657055
16	1	0	0.052692	3.886005	-1.653531
17	1	0	1.392810	2.726251	-1.652288
18	1	0	1.377818	4.071927	-0.502734
19	6	0	5.158484	-2.106586	-0.027732
20	6	0	4.646515	-3.405587	-0.038302
21	6	0	3.256739	-3.501759	-0.046446
22	6	0	2.662404	-2.227167	-0.038607
23	16	0	3.852423	-0.952828	-0.029202
24	1	0	5.298965	-4.271847	-0.041877
25	6	0	-2.668190	-2.223636	0.039097
26	6	0	-3.264238	-3.497433	0.046733
27	6	0	-4.653885	-3.399402	0.038248
28	6	0	-5.164117	-2.099721	0.027630
29	16	0	-3.856511	-0.947715	0.029503
30	1	0	-5.307492	-4.264791	0.041651
31	6	0	2.545029	-4.820077	-0.065066
32	6	0	-2.554324	-4.816715	0.065503
33	1	0	1.926031	-4.964581	0.825414
34	1	0	3.270085	-5.634817	-0.096813
35	1	0	1.896430	-4.922471	-0.940110
36	1	0	-3.280488	-5.630449	0.097759
37	1	0	-1.905550	-4.919728	0.940339
38	1	0	-1.935849	-4.962346	-0.825163
39	6	0	-6.564182	-1.889391	0.025479
40	6	0	6.558827	-1.898120	-0.025827
41	6	0	-7.359452	-0.767820	0.013320

42	6	0	-8.819615	-0.738044	0.019257
43	6	0	-9.229423	0.684465	-0.004287
44	6	0	-8.080879	1.485180	-0.024080
45	6	0	-6.879863	0.626849	-0.014162
46	6	0	-9.698278	-1.799963	0.043541
47	6	0	-11.114124	-1.639741	0.047037
48	6	0	-9.298597	-3.167415	0.067966
49	7	0	-9.007465	-4.293055	0.088209
50	7	0	-12.272799	-1.546221	0.050477
51	8	0	-5.725702	1.021653	-0.028498
52	1	0	-7.087538	-2.838805	0.036765
53	6	0	-10.486901	1.291890	-0.008701
54	6	0	-10.534341	2.675824	-0.032923
55	6	0	-9.375653	3.460477	-0.052379
56	6	0	-8.125960	2.869374	-0.048182
57	1	0	-11.420668	0.747433	0.005577
58	1	0	-7.221859	3.465720	-0.062477
59	6	0	7.355583	-0.777605	-0.013725
60	6	0	8.815780	-0.749767	-0.019898
61	6	0	9.227480	0.672200	0.003430
62	6	0	8.080002	1.474437	0.023401
63	6	0	6.877848	0.617697	0.013796
64	6	0	9.693026	-1.812857	-0.044156
65	6	0	11.109082	-1.654519	-0.047910
66	6	0	9.291513	-3.179776	-0.068286
67	7	0	8.998906	-4.305038	-0.088291
68	7	0	12.267881	-1.562540	-0.051563
69	8	0	5.724211	1.014025	0.028351

70	6	0	10.485764	1.277957	0.007526
71	6	0	10.535042	2.661829	0.031618
72	6	0	9.377398	3.448019	0.051257
73	6	0	8.126922	2.858573	0.047377
74	1	0	11.418804	0.732262	-0.006907
75	1	0	7.223615	3.456117	0.061814
76	1	0	7.080922	-2.848226	-0.037303
77	1	0	-0.505804	1.175070	-1.672374
78	1	0	-1.862029	2.145139	-1.067342
79	1	0	0.504525	1.173562	1.674698
80	1	0	1.862059	2.142116	1.070141
81	6	0	-11.753777	3.321847	-0.038182
82	6	0	-9.512563	4.833472	-0.075619
83	6	0	9.516134	4.820833	0.074352
84	6	0	11.755335	3.306236	0.036561
85	6	0	-11.865653	4.669329	-0.049500
86	6	0	-10.718067	5.447084	-0.086334
87	6	0	10.770265	5.504542	0.084955
88	6	0	11.917854	4.725303	0.049428
89	1	0	8.624751	5.412628	0.085029
90	1	0	12.638760	2.702563	0.030341
91	1	0	12.890158	5.171655	0.032277
92	1	0	10.822582	6.572724	0.118869
93	1	0	-8.629236	5.437240	-0.085568
94	1	0	-12.646901	2.732607	-0.033099
95	1	0	-12.830625	5.131234	-0.030215
96	1	0	-10.785041	6.514370	-0.122613
