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

Supporting Information

for the paper

1,5-, 2,6- and 9,10-Distyrylanthracenes as Luminescent Organic Semiconductors

Afshin Dadvand, Wei-Hsin Sun, Andrey G. Moiseev, Francine Bélanger, Hong Meng, Federico Rosei, and Dmitrii F. Perepichka

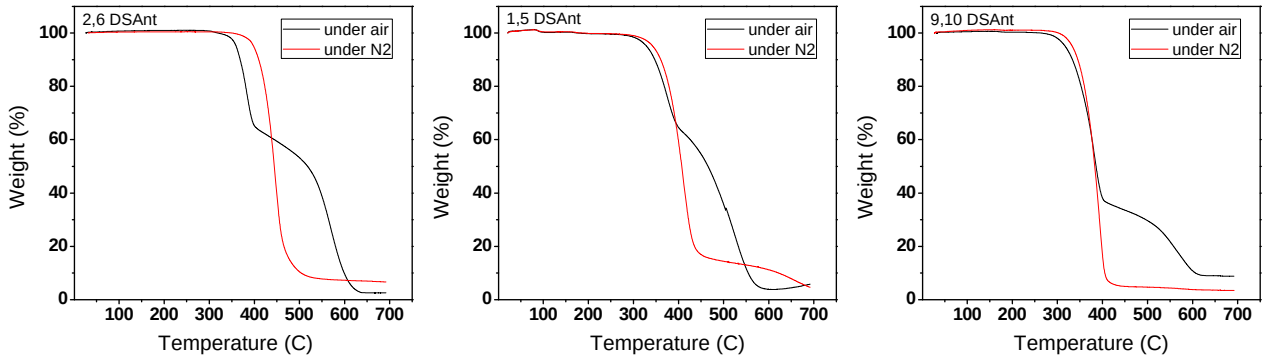


Figure SI-1: Thermogravimetric analysis (TGA) of **2,6-DPSAnt** (left), **1,5-DPSAnt** (middle) and **9,10-DPSAnt** (right).

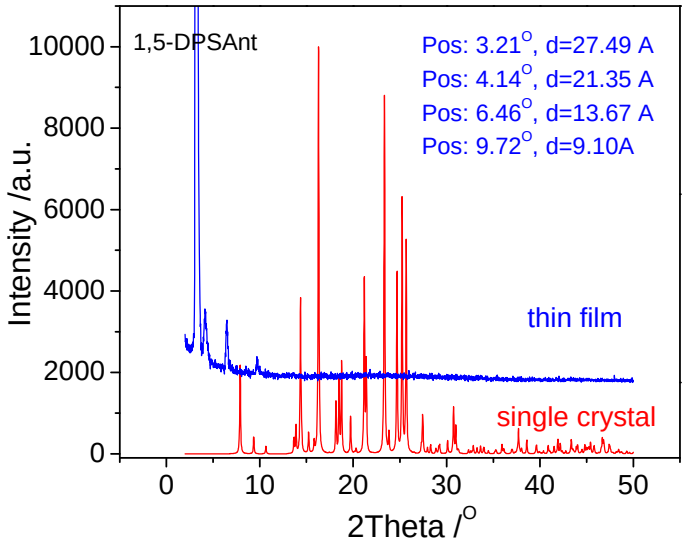


Figure SI-2: X-ray diffraction analysis of the vacuum-deposited films (blue) and the 1D diffraction pattern simulated from the single crystal X-ray data for **1,5-DSAnt**.

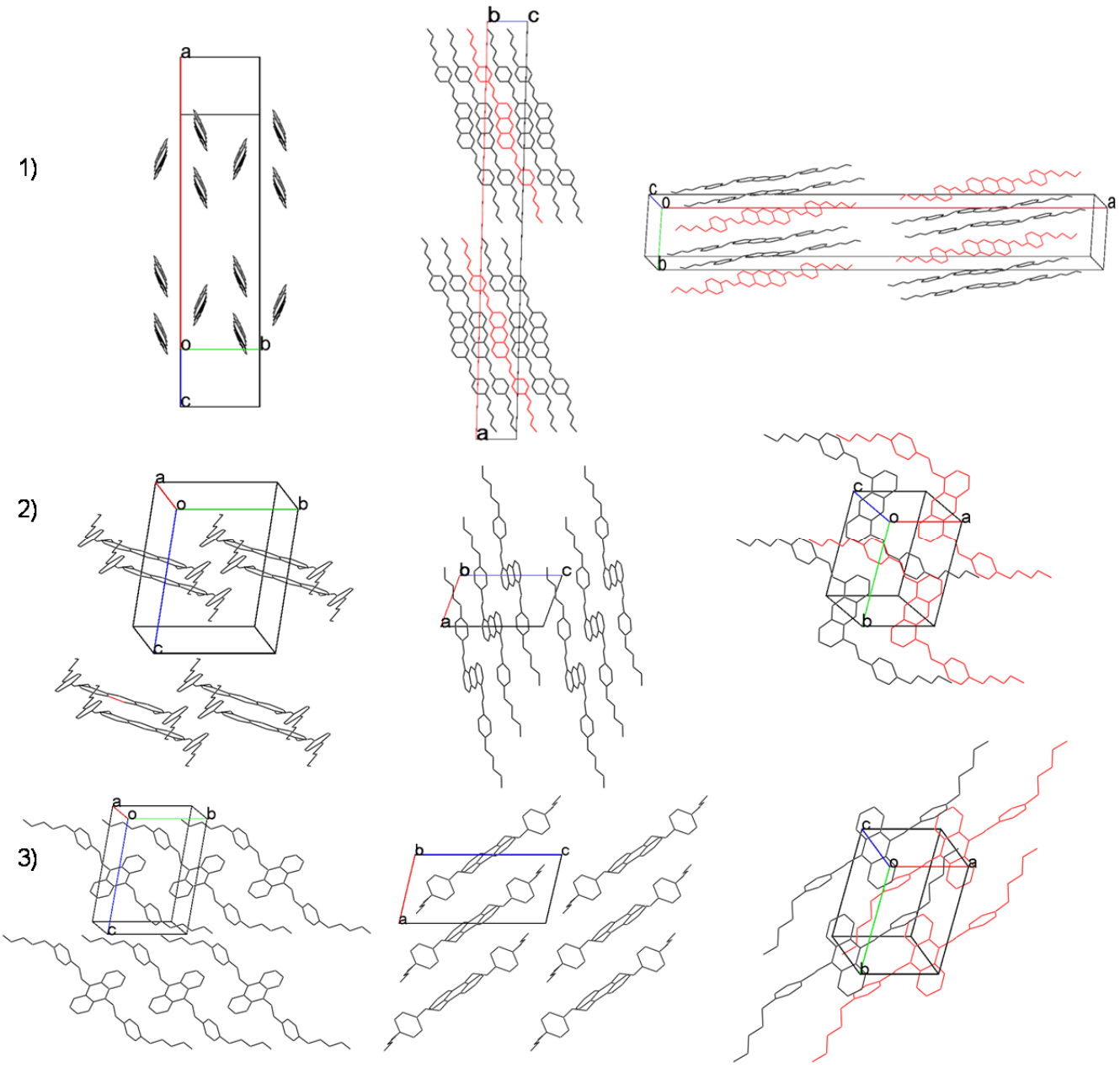


Figure SI-3. Crystal structure views of (1) **2,6-DSAnt** (2) **1,5-DSAnt** and (3) **9,10-DSAnt** in a, b, and c directions.

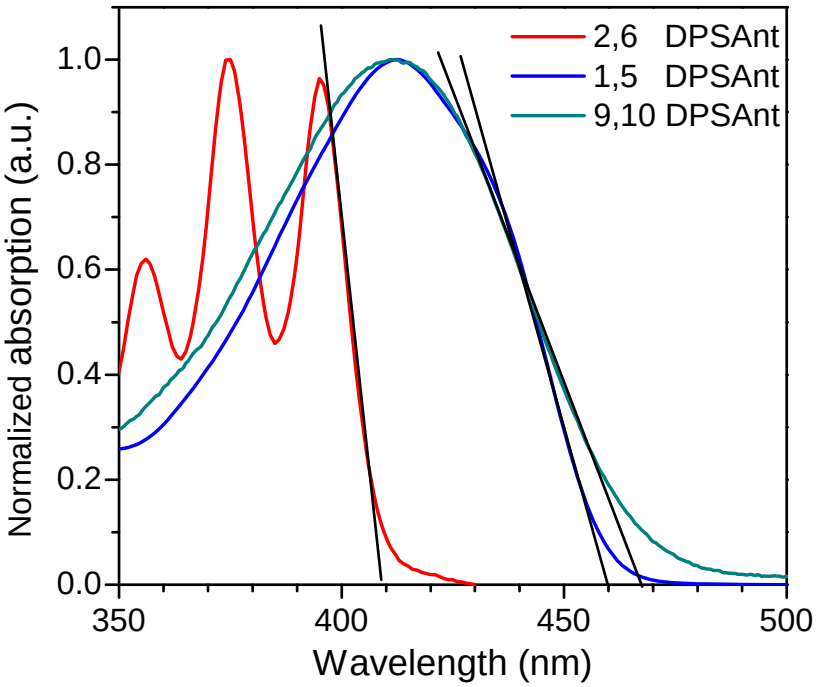


Figure SI-4. Absorption of **2,6-, 1,5-** and **9,10-DPSAnt** in degassed toluene solution (~10^{-5} M) showing the estimation of optical gap of the isomers.

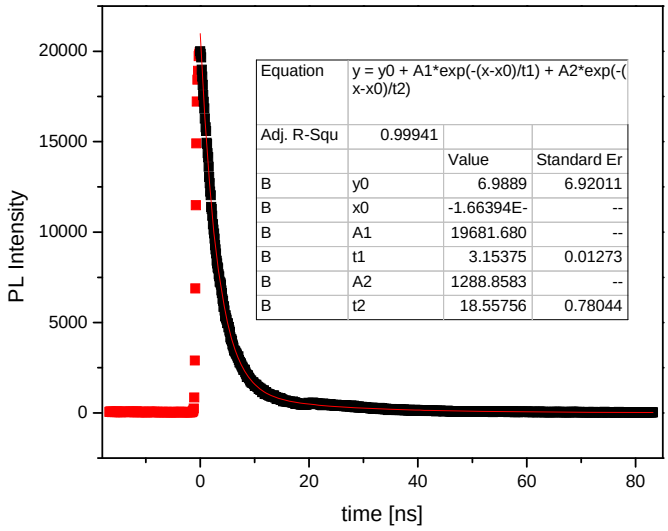


Figure SI-5. Fluorescence decay of **2,6-DPSAnt** in degassed toluene. Monitoring of fluorescence decay at 450 nm shows biexponential decay with the lifetimes τ_1 ~ 3.1 ns (94 %) and τ_2 ~ 18.5 ns (6 %).

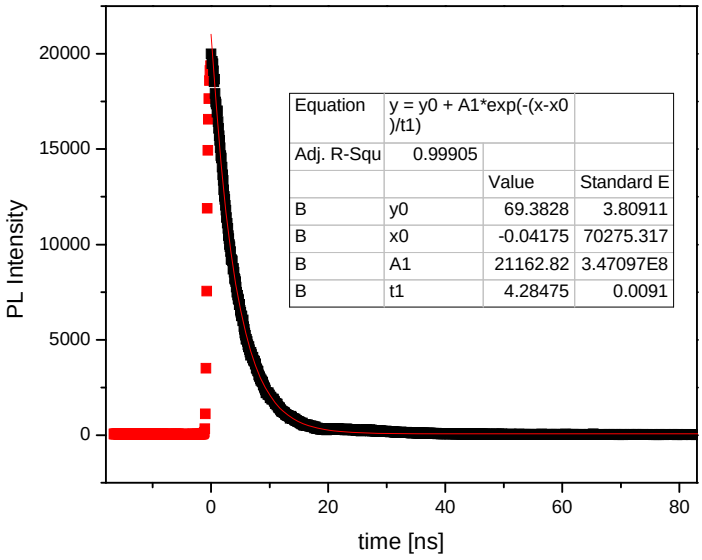


Figure SI-6. Fluorescence decay of **9,10-DPSAnt** in degassed toluene. Monitoring of fluorescence decay at 500 nm shows monoexponential decay with the lifetimes $\tau \sim 4.28$ ns.

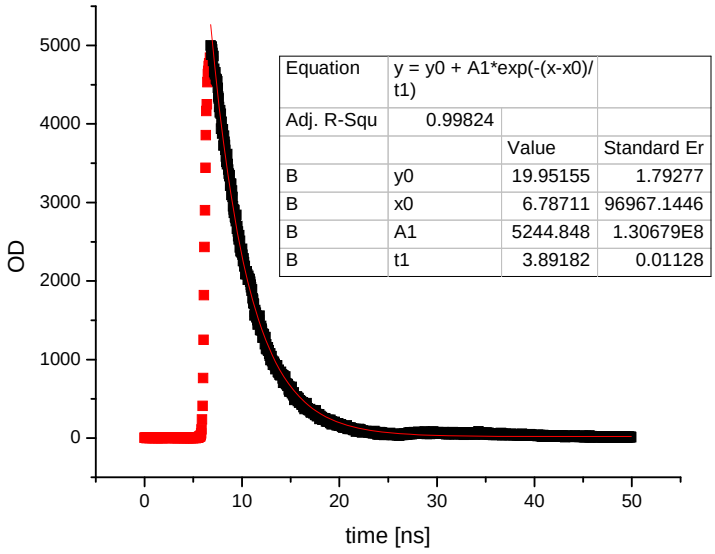


Figure SI-7. Fluorescence decay of **1,5-DPSAnt** in degassed toluene. Monitoring of fluorescence decay at 500 nm shows monoexponential decay with the lifetimes $\tau \sim 3.89$ ns.

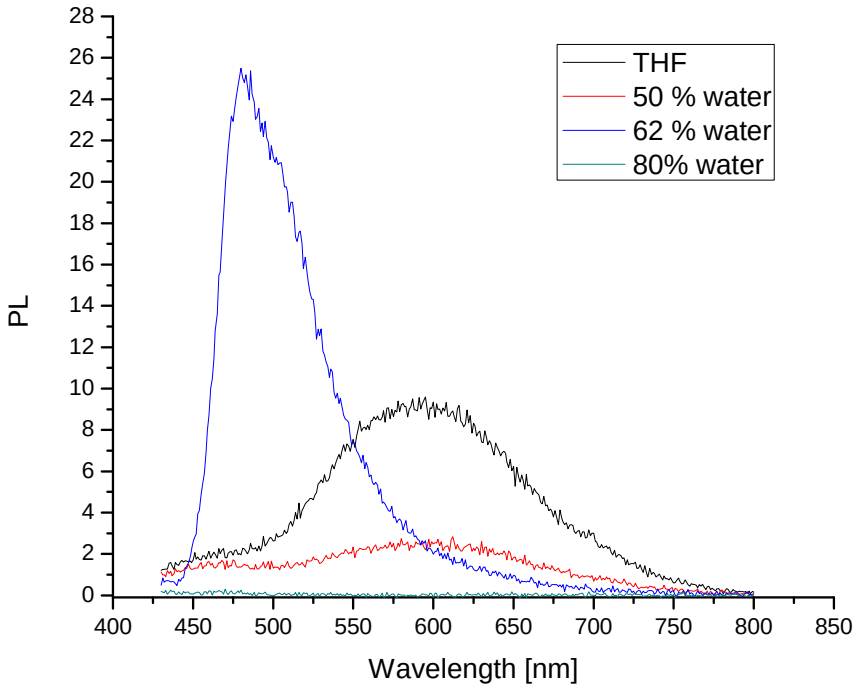
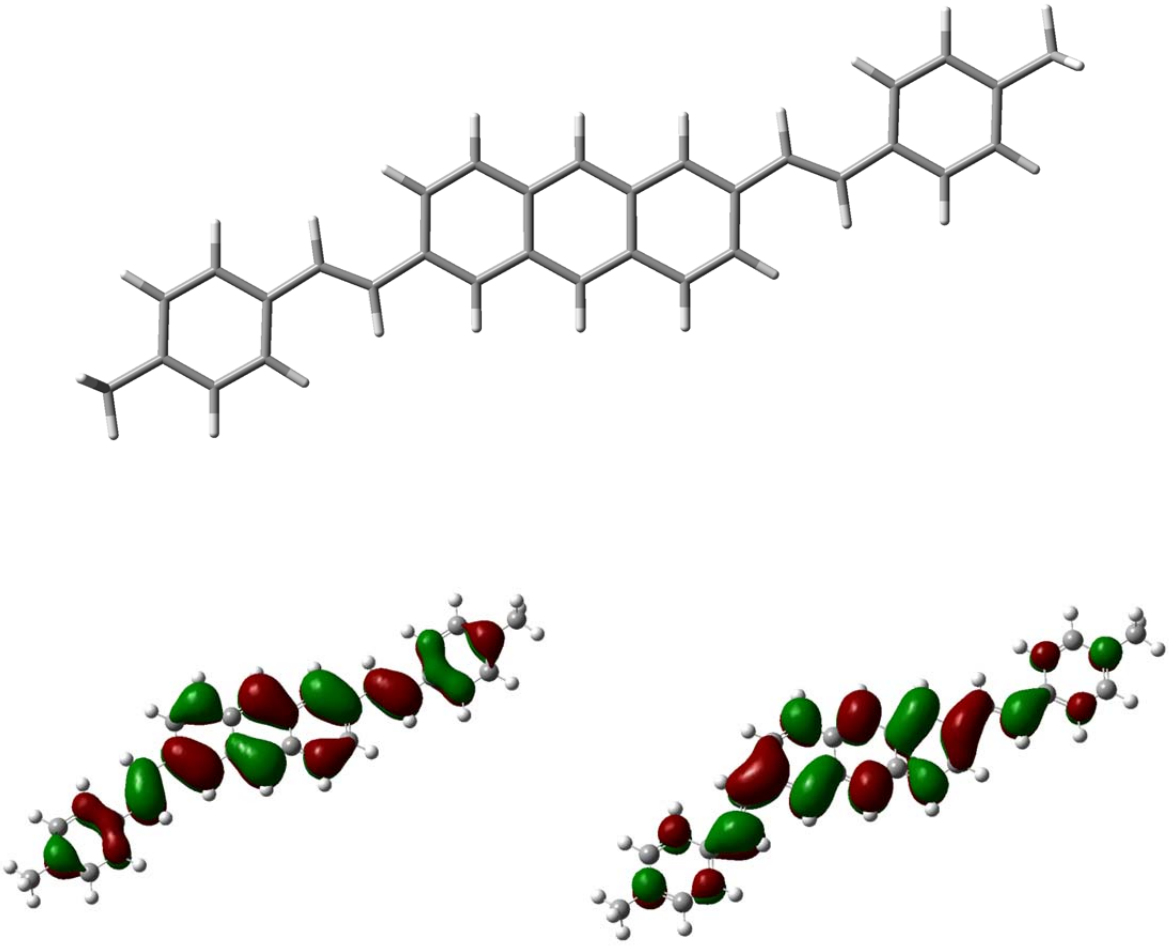


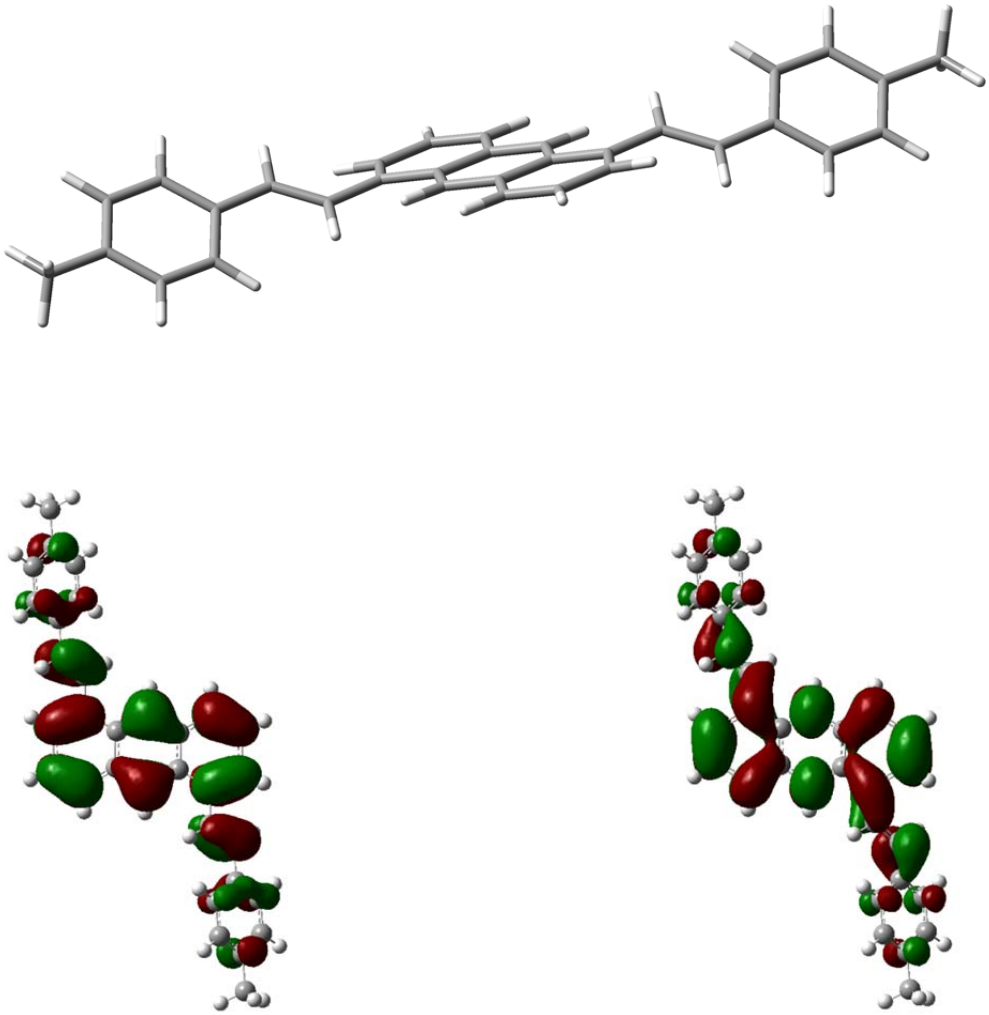
Figure SI-8. Photoluminescence (PL) of **9,10-DPSAnt** in THF–water solution. The addition of water first leads to decrease of PL intensity (50% water; as a result of increased solvent polarity and concentration decrease during dilution), then to significant increase (2x increase of the integrated PL intensity, accounting for the dilution effect) and blue shift of the PL band. The disappearance of PL in 80% H_2O/THF system is due to precipitation of the compound out of solution.

DFT calculated structures of the model di(2-(4-methylphenyl)vinyl))anthracene derivatives



HOMO **LUMO**

Figure SI-9. The optimized molecular geometry and frontier HOMO and LUMO of **2,6-DMSAnt** calculated at B3LYP/6-31G(d) level.



HOMO **LUMO**

Figure SI-10. The optimized molecular geometry and frontier HOMO and LUMO of **1,5-DMSAnt** calculated at B3LYP/6-31G(d) level.

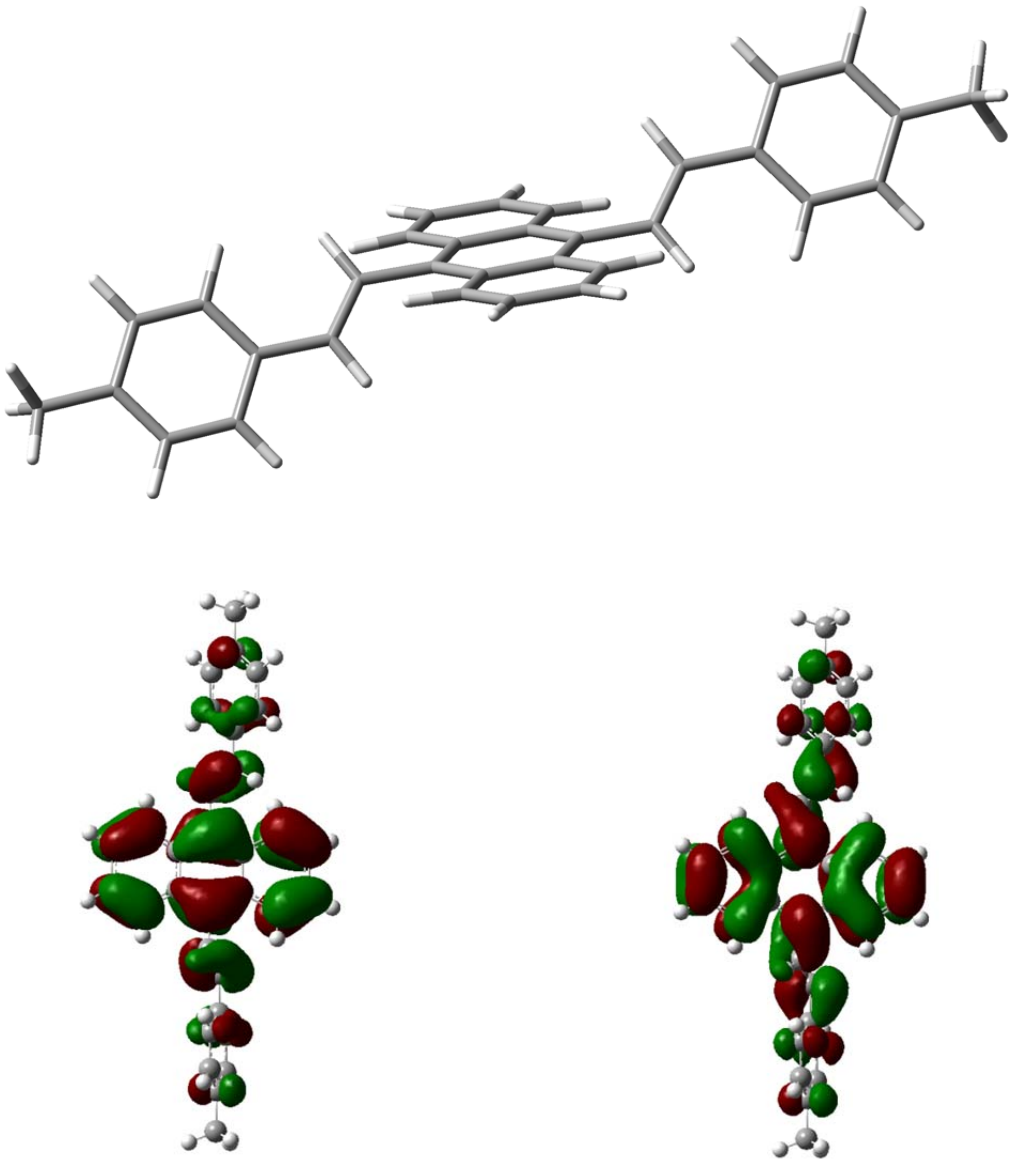


Figure SI-11. The optimized molecular geometry and frontier HOMO and LUMO of **9,10-DMSAnt** at B3LYP/6-31G(d) level.

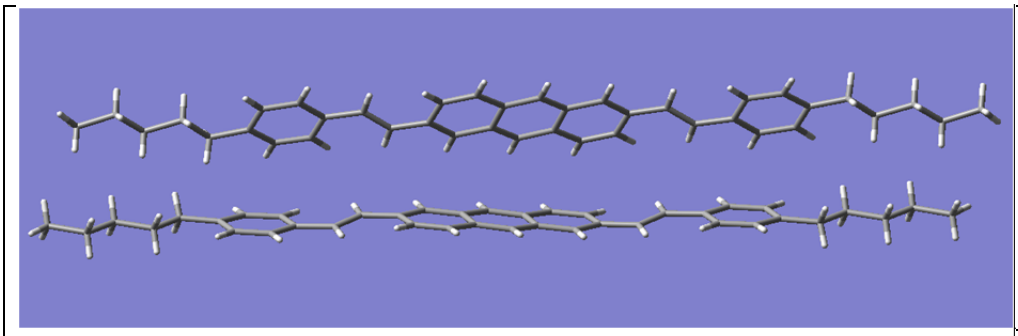
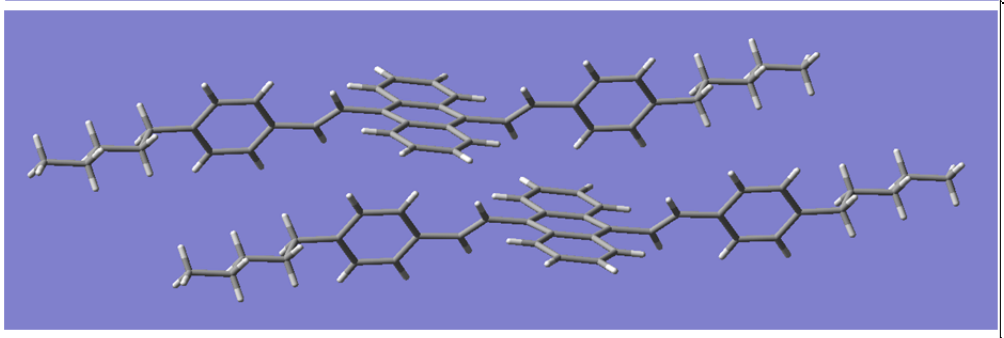
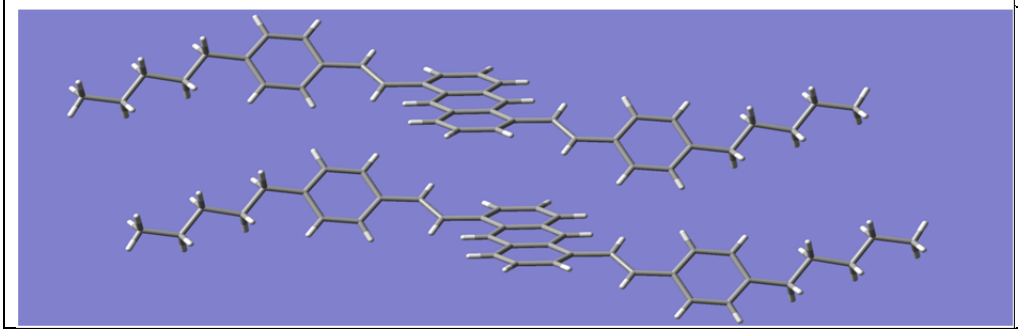
	HOMO – HOMO-1 = 0.41 eV
	HOMO – HOMO-1 = 0.11 eV
	HOMO – HOMO-1 = 0.03 eV

Figure SI-12. Structure of the closest contact dimers observed in the crystals of **2,6-**, **1,5-** and **9,10-DPSAnt** by X-ray analysis and used in calculated HOMO splitting (Table 2 in the article). Analysis of other observed dimeric interactions in the crystal revealed smaller orbital splitting.

Table S1. Optimized ground state of **2,6-DMSAnt**. Total Energy -1235.0929565. # of imaginary frequencies: 0.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.150166	0.104884	-0.000405
2	6	0	-6.230599	-0.705695	-0.002726
3	6	0	-7.637952	-0.302716	-0.001843
4	6	0	-8.631152	-1.297908	-0.008007
5	6	0	-8.070741	1.039218	0.003003
6	6	0	-9.986378	-0.974454	-0.008781
7	6	0	-10.410877	0.358201	-0.001955
8	6	0	-9.422445	1.356598	0.002304
9	1	0	-5.303918	1.183025	0.001654
10	1	0	-6.077588	-1.783717	-0.005455
11	1	0	-8.331254	-2.343640	-0.014360
12	1	0	-7.342156	1.844708	0.005439
13	1	0	-10.726191	-1.771836	-0.015302
14	1	0	-9.722512	2.402613	0.004445
15	6	0	-3.746303	-0.298029	-0.000521
16	6	0	-2.763593	0.676043	-0.000132
17	6	0	-1.375475	0.361507	-0.000189
18	6	0	-3.331010	-1.675640	-0.000849
19	6	0	-2.009803	-2.019681	-0.000829
20	6	0	-0.978669	-1.026642	-0.000495
21	6	0	-0.380593	1.351624	0.000065
22	6	0	0.978676	1.026645	0.000091
23	6	0	0.380600	-1.351621	-0.000357
24	6	0	1.375483	-0.361503	-0.000031
25	6	0	2.009808	2.019685	0.000352
26	6	0	3.331014	1.675647	0.000457
27	6	0	2.763602	-0.676038	0.000184
28	6	0	3.746311	0.298036	0.000315
29	1	0	-3.052329	1.725428	0.000175
30	1	0	-4.082316	-2.458878	-0.000872
31	1	0	-1.718691	-3.067613	-0.000966
32	1	0	1.718694	3.067618	0.000586
33	1	0	4.082317	2.458886	0.000935
34	1	0	3.052340	-1.725422	0.000146
35	6	0	5.150177	-0.104871	0.000449
36	6	0	6.230601	0.705721	-0.001952
37	6	0	7.637958	0.302776	-0.001233
38	6	0	8.070758	-1.039193	0.005107
39	6	0	8.631125	1.297931	-0.008953
40	6	0	9.422420	-1.356573	0.004116
41	6	0	10.410878	-0.358146	-0.002048
42	6	0	9.986389	0.974454	-0.010037
43	1	0	5.303938	-1.183011	0.002428
44	1	0	6.077574	1.783741	-0.004868
45	1	0	7.342152	-1.844658	0.009249
46	1	0	8.331252	2.343665	-0.016151
47	1	0	9.722494	-2.402587	0.007639
48	1	0	10.726200	1.771823	-0.017654
49	1	0	-0.676249	2.399015	0.000244
50	1	0	0.676258	-2.399011	-0.000509
51	6	0	-11.876788	0.720186	0.013025
52	1	0	-12.507850	-0.159307	-0.149655
53	1	0	-12.169684	1.164078	0.973698
54	1	0	-12.117157	1.454936	-0.764935
55	6	0	11.876765	-0.720326	0.010869
56	1	0	12.508168	0.161769	-0.135475
57	1	0	12.167124	-1.180582	0.964514
58	1	0	12.119260	-1.441762	-0.778916

Table S2. Optimized excited state (S_1) of **2,6-DMSAnt**. Total Energy -1235.0877495.
$S_0 \rightarrow S_1$ (ground state absorption) = 446 nm (f=1.1); $S_1 \rightarrow S_0$ (excited state emission) = 499 nm (f=1.3)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.147353	0.056980	-0.000480
2	6	0	-6.253972	-0.747552	-0.003361
3	6	0	-7.638464	-0.324882	-0.002200
4	6	0	-8.657065	-1.304852	-0.009009
5	6	0	-8.053447	1.030063	0.003460
6	6	0	-10.002466	-0.957048	-0.009414
7	6	0	-10.405035	0.385776	-0.001609
8	6	0	-9.397491	1.368013	0.003146
9	1	0	-5.297669	1.135624	0.001955
10	1	0	-6.110518	-1.826871	-0.006979
11	1	0	-8.375120	-2.355429	-0.016150
12	1	0	-7.312082	1.823484	0.006255
13	1	0	-10.757149	-1.740419	-0.016377
14	1	0	-9.680730	2.418779	0.006047
15	6	0	-3.767594	-0.351155	-0.000612
16	6	0	-2.755568	0.649594	-0.000123
17	6	0	-1.390550	0.346271	-0.000235
18	6	0	-3.340700	-1.707842	-0.001024
19	6	0	-2.003884	-2.037652	-0.000950
20	6	0	-0.979640	-1.040550	-0.000534
21	6	0	-0.378831	1.351366	-0.000094
22	6	0	0.979653	1.040621	-0.000119
23	6	0	0.378844	-1.351294	-0.000320
24	6	0	1.390562	-0.346199	-0.000046
25	6	0	2.003899	2.037723	-0.000111
26	6	0	3.340715	1.707911	-0.000030
27	6	0	2.755579	-0.649524	0.000250
28	6	0	3.767606	0.351223	0.000123
29	1	0	-3.058766	1.694855	0.000171
30	1	0	-4.078974	-2.503810	-0.001064
31	1	0	-1.705529	-3.083486	-0.001096
32	1	0	1.705545	3.083556	-0.000040
33	1	0	4.078990	2.503878	0.000295
34	1	0	3.058776	-1.694786	0.000358
35	6	0	5.147364	-0.056920	0.000294
36	6	0	6.253988	0.747603	-0.002785
37	6	0	7.638477	0.324923	-0.001705
38	6	0	8.053426	-1.030057	0.005040
39	6	0	8.657083	1.304838	-0.009572
40	6	0	9.397425	-1.368050	0.004529
41	6	0	10.405024	-0.385820	-0.001630
42	6	0	10.002503	0.956972	-0.010197
43	1	0	5.297671	-1.135565	0.002783
44	1	0	6.110544	1.826923	-0.006728
45	1	0	7.312026	-1.823440	0.009108
46	1	0	8.375185	2.355422	-0.017241
47	1	0	9.680625	-2.418828	0.008456
48	1	0	10.757214	1.740302	-0.017881
49	1	0	-0.684592	2.395807	-0.000008
50	1	0	0.684604	-2.395735	-0.000410
51	6	0	-11.862826	0.772878	0.014518
52	1	0	-12.509697	-0.094647	-0.150372
53	1	0	-12.148701	1.219911	0.976472
54	1	0	-12.090759	1.515022	-0.760663
55	6	0	11.862772	-0.773169	0.012505
56	1	0	12.510067	0.096915	-0.136338
57	1	0	12.145805	-1.236307	0.967578
58	1	0	12.093031	-1.502313	-0.774361

Table S3. Optimized ground state of **1,5-DMSAnt**. Total Energy -1235.0831071. # of imaginary frequencies: 0.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.239777	3.496158	-0.344168
2	6	0	-0.046654	2.831188	-0.237671
3	6	0	-0.017265	1.408330	-0.128197
4	6	0	-1.261354	0.673710	-0.130759
5	6	0	-2.463577	2.779097	-0.368627
6	6	0	-2.509110	1.401065	-0.263635
7	6	0	1.197330	0.717236	-0.009816
8	6	0	1.261277	-0.673663	0.130287
9	6	0	-1.197411	-0.717192	0.009309
10	6	0	0.017186	-1.408285	0.127700
11	6	0	0.046573	-2.831139	0.237201
12	6	0	1.239693	-3.496100	0.343790
13	6	0	2.509033	-1.401010	0.263264
14	6	0	2.463489	-2.779040	0.368312
15	1	0	-1.258304	4.578965	-0.433899
16	1	0	0.895488	3.373899	-0.236553
17	1	0	-3.389995	3.327135	-0.512833
18	6	0	-3.789950	0.685458	-0.320397
19	1	0	2.112826	1.299732	-0.040326
20	1	0	-2.112914	-1.299678	0.039808
21	1	0	-0.895567	-3.373854	0.236047
22	1	0	1.258218	-4.578905	0.433558
23	6	0	3.789845	-0.685361	0.320120
24	1	0	3.389889	-3.327082	0.512613
25	6	0	-4.960746	1.154003	0.159923
26	6	0	-6.272606	0.506572	0.076333
27	6	0	4.960794	-1.153992	-0.159746
28	6	0	6.272630	-0.506529	-0.076110
29	6	0	6.534843	0.620780	0.727956
30	6	0	7.341864	-1.026527	-0.825507
31	6	0	7.796538	1.200637	0.760060
32	6	0	8.859342	0.684752	0.000195
33	6	0	8.606364	-0.442293	-0.788934
34	6	0	-7.341254	1.025144	0.827599
35	6	0	-6.535418	-0.619209	-0.729619
36	6	0	-8.605701	0.440860	0.791074
37	6	0	-8.859244	-0.684830	0.000133
38	6	0	-7.797119	-1.199134	-0.761690
39	1	0	-3.772896	-0.295446	-0.790591
40	1	0	3.772608	0.295651	0.790068
41	1	0	-4.952457	2.102064	0.697249
42	1	0	4.952713	-2.102301	-0.696637
43	1	0	5.746287	1.037667	1.348019
44	1	0	7.174405	-1.901789	-1.449376
45	1	0	7.967399	2.067685	1.395022
46	1	0	9.410586	-0.870946	-1.382822
47	1	0	-7.173346	1.899361	1.452811
48	1	0	-5.747423	-1.034668	-1.351354
49	1	0	-9.409479	0.868419	1.386356
50	1	0	-7.968522	-2.064899	-1.398245
51	6	0	-10.222125	-1.334309	-0.033747
52	1	0	-10.217645	-2.300544	0.488106
53	1	0	-10.977640	-0.704550	0.446739
54	1	0	-10.549562	-1.527873	-1.062202
55	6	0	10.222415	1.333791	0.034826
56	1	0	10.216178	2.304613	-0.478344
57	1	0	10.553633	1.518207	1.063806
58	1	0	10.976100	0.708125	-0.453780

Table S4. Optimized excited state (S_1) of **1,5-DMSAnt**. Total Energy -1235.0746287.
$S_0 \rightarrow S_1$ (ground state absorption) = 455 nm (f=0.5); $S_1 \rightarrow S_0$ (excited state emission) = 559 nm (f=0.6)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.319187	3.501621	-0.187037
2	6	0	-0.094969	2.818756	-0.167598
3	6	0	-0.055735	1.416005	-0.095289
4	6	0	-1.292598	0.665431	-0.040054
5	6	0	-2.514150	2.801175	-0.146110
6	6	0	-2.552896	1.381032	-0.083833
7	6	0	1.182619	0.724836	-0.068048
8	6	0	1.292571	-0.665392	0.039597
9	6	0	-1.182642	-0.724801	0.067552
10	6	0	0.055711	-1.415968	0.094792
11	6	0	0.094947	-2.818721	0.167063
12	6	0	1.319165	-3.501584	0.186522
13	6	0	2.552867	-1.380985	0.083444
14	6	0	2.514127	-2.801130	0.145670
15	1	0	-1.330944	4.586223	-0.249775
16	1	0	0.839826	3.372198	-0.206161
17	1	0	-3.447070	3.351015	-0.205803
18	6	0	-3.809320	0.678442	-0.095359
19	1	0	2.075699	1.336209	-0.147164
20	1	0	-2.075717	-1.336185	0.146634
21	1	0	-0.839847	-3.372168	0.205584
22	1	0	1.330925	-4.586188	0.249225
23	6	0	3.809282	-0.678375	0.095112
24	1	0	3.447044	-3.350970	0.205392
25	6	0	-5.052334	1.222484	0.082799
26	6	0	-6.321988	0.524587	0.035438
27	6	0	5.052314	-1.222411	-0.082922
28	6	0	6.321988	-0.524566	-0.035390
29	6	0	6.463177	0.842987	0.302581
30	6	0	7.506128	-1.233552	-0.335952
31	6	0	7.708973	1.451377	0.325892
32	6	0	8.882277	0.739909	0.017650
33	6	0	8.751383	-0.616551	-0.309817
34	6	0	-7.506092	1.233420	0.336630
35	6	0	-6.463222	-0.842805	-0.303050
36	6	0	-8.751298	0.616378	0.310711
37	6	0	-8.882219	-0.740027	-0.017136
38	6	0	-7.709024	-1.451261	-0.326157
39	1	0	-3.758304	-0.392696	-0.264221
40	1	0	3.758223	0.392752	0.264038
41	1	0	-5.130986	2.283805	0.310295
42	1	0	5.130980	-2.283740	-0.310371
43	1	0	5.587148	1.430673	0.560475
44	1	0	7.436298	-2.287991	-0.593897
45	1	0	7.780829	2.503586	0.594092
46	1	0	9.640334	-1.196978	-0.546942
47	1	0	-7.436228	2.287795	0.594830
48	1	0	-5.587279	-1.430302	-0.561661
49	1	0	-9.640207	1.196703	0.548262
50	1	0	-7.780942	-2.503333	-0.594862
51	6	0	-10.227561	-1.422715	-0.025593
52	1	0	-10.349687	-2.077932	0.847903
53	1	0	-11.045849	-0.695744	-0.006420
54	1	0	-10.354572	-2.050958	-0.915360
55	6	0	10.227687	1.422457	0.027195
56	1	0	10.346336	2.086088	-0.840365
57	1	0	10.358321	2.042158	0.922474
58	1	0	11.045800	0.695651	-0.002031

Table S5. Optimized ground state of **9,10-DMSAnt**. Total Energy -1235.0710912. # of imaginary frequencies: 0.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.690091	-3.396363	-0.172086
2	6	0	1.364271	-2.212087	-0.302366
3	6	0	0.716379	-0.946906	-0.113524
4	6	0	-0.687112	-3.396884	0.175834
5	6	0	-1.362329	-2.213136	0.305550
6	6	0	-0.715544	-0.947478	0.116099
7	6	0	1.428457	0.278261	-0.174204
8	6	0	0.716439	1.502584	-0.070985
9	6	0	-1.428702	0.277096	0.176140
10	6	0	-0.717744	1.501994	0.072494
11	6	0	1.392207	2.763973	-0.093427
12	6	0	0.706710	3.950000	-0.039794
13	6	0	-1.394605	2.762803	0.094528
14	6	0	-0.710133	3.949404	0.040521
15	6	0	2.890657	0.328613	-0.374171
16	6	0	3.812137	-0.332087	0.355425
17	6	0	5.269005	-0.289371	0.186230
18	6	0	6.088260	-0.847267	1.182151
19	6	0	5.907356	0.285898	-0.930179
20	6	0	7.477619	-0.819195	1.078825
21	6	0	8.108589	-0.239689	-0.027085
22	6	0	7.292768	0.311878	-1.028586
23	6	0	-2.890989	0.326199	0.375796
24	6	0	-3.811609	-0.335857	-0.353647
25	6	0	-5.268602	-0.293543	-0.185344
26	6	0	-6.087027	-0.855545	-1.180032
27	6	0	-5.907760	0.279241	0.931525
28	6	0	-7.476086	-0.832163	-1.075596
29	6	0	-8.108270	-0.249765	0.028524
30	6	0	-7.293492	0.300683	1.031011
31	1	0	1.210738	-4.337663	-0.327180
32	1	0	2.414225	-2.219234	-0.566600
33	1	0	-1.206936	-4.338562	0.331392
34	1	0	-2.412272	-2.221077	0.569806
35	1	0	2.475535	2.776865	-0.137229
36	1	0	1.247420	4.892436	-0.059960
37	1	0	-2.477941	2.774759	0.138381
38	1	0	-1.251647	4.891384	0.060426
39	1	0	3.234538	1.003834	-1.157065
40	1	0	3.465904	-0.947524	1.184965
41	1	0	5.625165	-1.301707	2.055225
42	1	0	5.312658	0.707244	-1.735825
43	1	0	8.081322	-1.255889	1.871324
44	1	0	7.755253	0.763585	-1.903901
45	1	0	-3.235793	1.001538	1.158193
46	1	0	-3.464526	-0.951516	-1.182661
47	1	0	-5.622911	-1.314936	-2.049969
48	1	0	-5.313777	0.696562	1.739779
49	1	0	-8.078780	-1.276490	-1.864665
50	1	0	-7.756736	0.745561	1.909344
51	6	0	9.613010	-0.224406	-0.157769
52	1	0	10.098810	-0.503023	0.782776
53	1	0	9.955001	-0.929387	-0.927159
54	1	0	9.981246	0.767287	-0.446280
55	6	0	-9.613630	-0.200110	0.137663
56	1	0	-9.999953	0.795315	-0.120059
57	1	0	-10.088197	-0.919602	-0.537422
58	1	0	-9.950259	-0.420398	1.157239

Table S6. Optimized excited state (S_1) of **9,10-DMSAnt**. Total Energy -1235.06191690.
$S_0 \rightarrow S_1$ (ground state absorption) = 458 nm (f=0.6); $S_1 \rightarrow S_0$ (excited state emission) = 574 nm (f=0.8)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.349733	3.757980	0.211039
2	6	0	-1.132857	2.628977	-0.012812
3	6	0	-0.592875	1.320412	-0.048291
4	6	0	1.012832	3.608509	0.469858
5	6	0	1.574183	2.333984	0.467814
6	6	0	0.826473	1.173175	0.158700
7	6	0	-1.438087	0.152059	-0.183128
8	6	0	-0.828178	-1.159734	-0.201233
9	6	0	1.434858	-0.139258	0.150270
10	6	0	0.590809	-1.306811	0.005426
11	6	0	-1.574629	-2.318838	-0.519178
12	6	0	-1.011601	-3.592688	-0.530971
13	6	0	1.132872	-2.614260	-0.040443
14	6	0	0.351159	-3.742454	-0.273306
15	6	0	-2.864334	0.338429	-0.266709
16	6	0	-3.855045	-0.450469	0.258435
17	6	0	-5.282253	-0.226141	0.144001
18	6	0	-6.165604	-0.979079	0.950018
19	6	0	-5.864018	0.712115	-0.743033
20	6	0	-7.541501	-0.792889	0.889666
21	6	0	-8.109723	0.149195	0.020402
22	6	0	-7.238032	0.892023	-0.795985
23	6	0	2.859671	-0.329464	0.254799
24	6	0	3.861011	0.449206	-0.264740
25	6	0	5.285509	0.220037	-0.125994
26	6	0	6.184346	0.954127	-0.932562
27	6	0	5.849352	-0.704281	0.786329
28	6	0	7.557965	0.762171	-0.849053
29	6	0	8.108772	-0.167409	0.045120
30	6	0	7.221865	-0.889977	0.862567
31	1	0	-0.811972	4.741133	0.219020
32	1	0	-2.199170	2.772206	-0.134713
33	1	0	1.632452	4.470722	0.699974
34	1	0	2.612304	2.224703	0.753224
35	1	0	-2.612848	-2.208272	-0.803943
36	1	0	-1.629945	-4.453840	-0.768389
37	1	0	2.199723	-2.756068	0.078834
38	1	0	0.814687	-4.724899	-0.289548
39	1	0	-3.190194	1.257537	-0.747454
40	1	0	-3.570122	-1.294693	0.882538
41	1	0	-5.753040	-1.715888	1.635690
42	1	0	-5.229999	1.289094	-1.409973
43	1	0	-8.190282	-1.389438	1.527354
44	1	0	-7.652447	1.618420	-1.492382
45	1	0	3.174250	-1.244700	0.750703
46	1	0	3.589052	1.286561	-0.903732
47	1	0	5.785530	1.681097	-1.636637
48	1	0	5.202924	-1.264811	1.455380
49	1	0	8.219012	1.344335	-1.487498
50	1	0	7.622425	-1.604751	1.578761
51	6	0	-9.601050	0.370099	-0.036261
52	1	0	-10.144125	-0.426138	0.482937
53	1	0	-9.883678	1.321901	0.434455
54	1	0	-9.963630	0.407028	-1.070718
55	6	0	9.597735	-0.398113	0.120766
56	1	0	9.889995	-1.309017	-0.420356
57	1	0	10.155542	0.434952	-0.319502
58	1	0	9.934217	-0.520978	1.156908