Electronic Supplementary Material (ESI) for New Journal of Chemistry.

Triphenylamine/Tetrazine based π-Conjugated Systems as Molecular Donors for Organic Solar Cells

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Supporting information

Spectroscopy

Theoretical calculations

Photovoltaics

List of figures and tables:

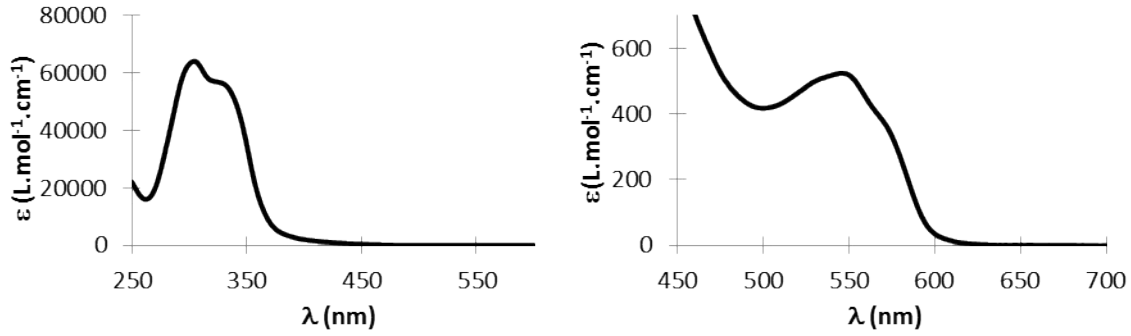

Figure S 1. Molar absorption coefficient of compound 1 in dichloromethane

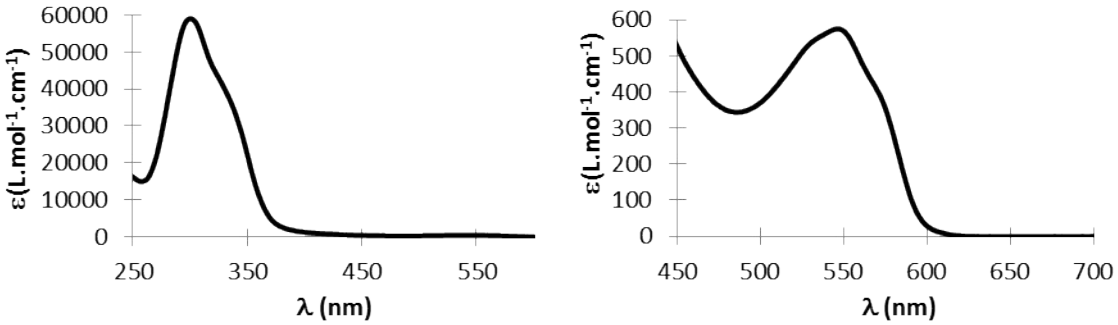

Figure S 2. Molar absorption coefficient of compound 2 in dichloromethane

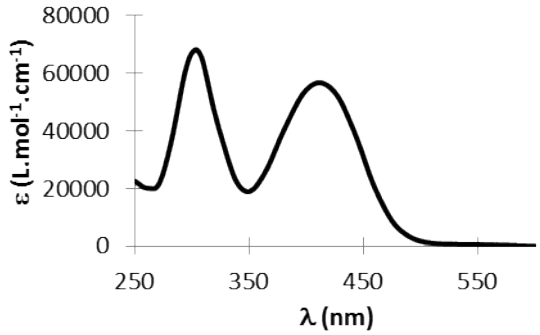

Figure S 3. Molar absorption coefficient of compound 3 in dichloromethane

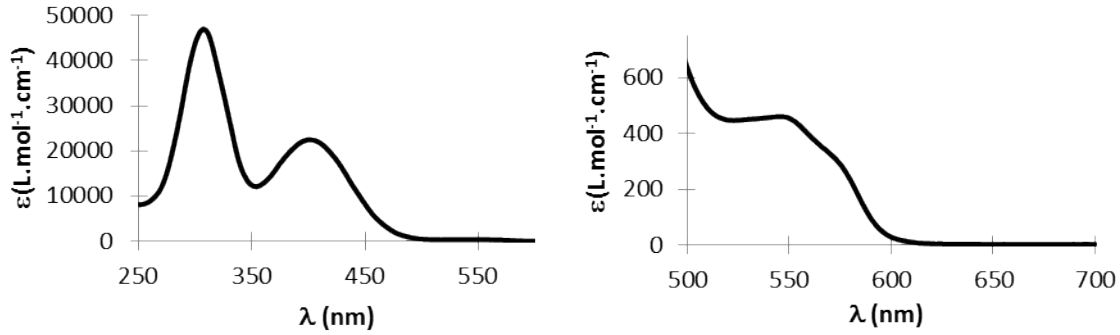

Figure S 4. Molar absorption coefficient of compound 4 in dichloromethane

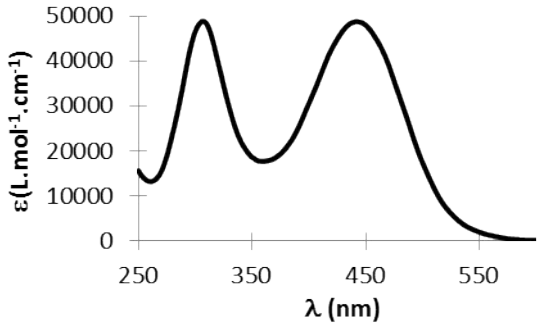

Figure S 5. Molar absorption coefficient of compound 5 in dichloromethane

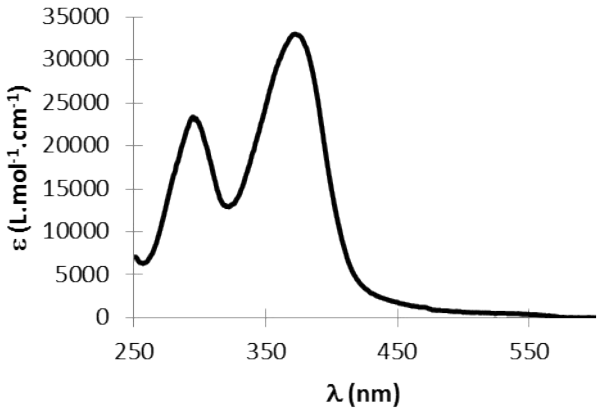

Figure S 6. Molar absorption coefficient of compound 7 in dichloromethane

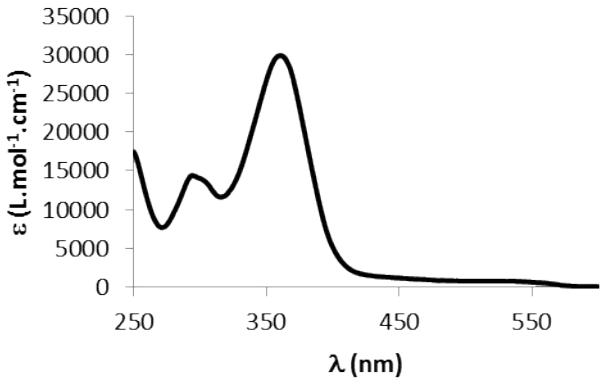

Figure S 7. Molar absorption coefficient of compound 9 in dichloromethane

Table S 1. Results of TD-DFT calculations

Compound	Energy (cm^{-1})	Energy (nm)	Oscillator strength	Major contributing molecular orbitals
4	17531	570	0.003	H-2→LUMO (84%)
	21203	472	0.51	HOMO→L+1 (95%)
	29409	340	1.14	H-1→L+1 (55%), HOMO→L+2 (22%)

3	17481	572	0.003	H-3→LUMO (80%)
	21628	462	1.18	HOMO→L+1 (94%)
	29626	338	1.46	H-2→L+1 (59%), H-1→L+2 (22%)
2	17550	570	0.003	H-2→LUMO (85%)
	31355	341	0.23	H-1→L+1 (80%)
1	17506	571	0.003	H-4→LUMO (47%), H-3→LUMO (38%)
	29111	344	1.72	H-2→L+1 (10%), H-1→L+2 (43%), HOMO→L+3 (32%)
5	18441	542	0.004	H-3→LUMO (86%)
	20675	484	0.64	HOMO→L+1 (93%)
	26134	383	0.74	H-2→LUMO (12%), H-1→L+1 (70%)
6	18394	544	0.003	H-4→LUMO (85%)
	20661	484	1.25	HOMO→L+1 (91%)
	26818	373	0.48	H-3→LUMO (31%), H-2→L+1 (53%)
	28399	352	0.32	H-5→LUMO (87%)
	29593	338	0.21	HOMO→L+2 (81%)
7	18058	554	0.004	H-2→LUMO (82%)
	25857	387	1.33	HOMO→L+1 (88%)
	33793	296	0.29	H-9→LUMO (10%), H-8→LUMO (27%), H-1→L+1 (54%)
8	17537	570	0.003	H-5→LUMO (74%)
	20220	495	0.02	HOMO→L+1 (94%)
	29891	335	0.05	H-1→L+3 (18%), HOMO→L+2 (60%), HOMO→L+3 (12%)
10	17735	564	0.003	H-2→LUMO (80%)
	27169	368	0.89	HOMO→L+1 (88%)
	32208	310	0.16	HOMO→L+3 (86%)
9	18027	555	0.004	H-1→LUMO (84%)
	26886	372	0.68	HOMO→L+1 (87%)
	32805	305	0.16	HOMO→L+3 (87%)

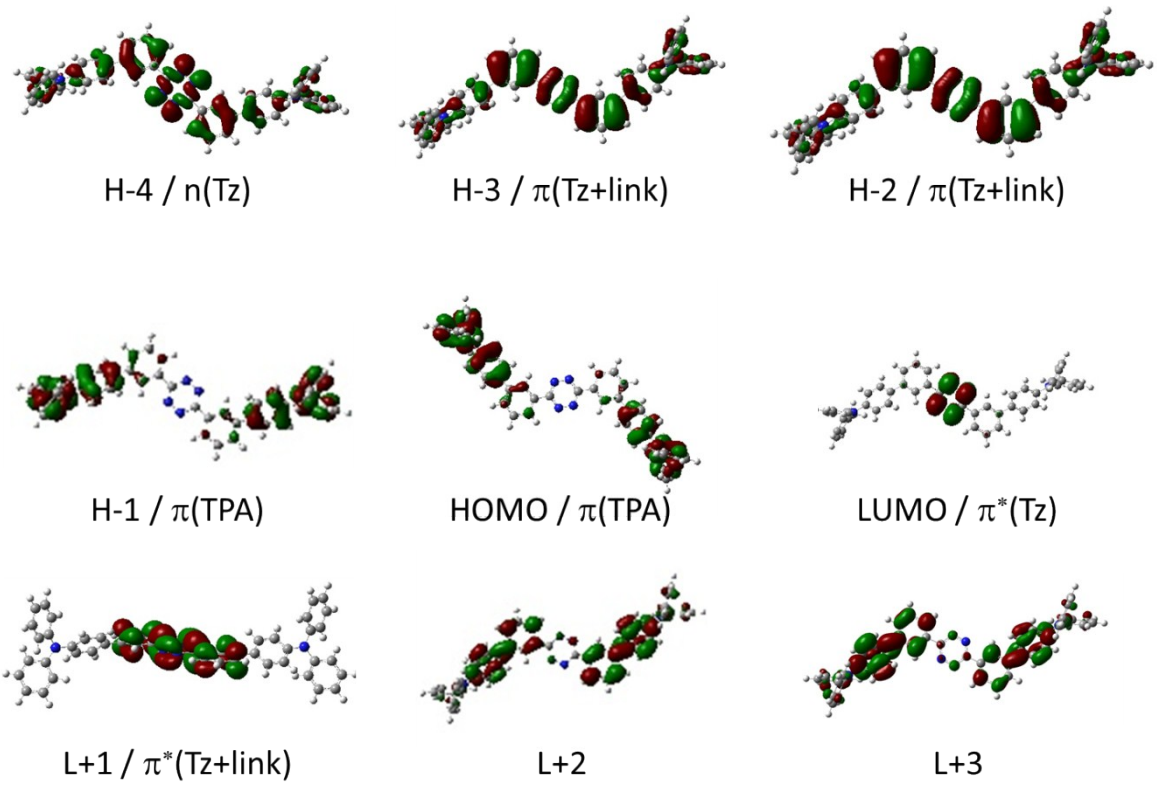

Figure S 8. Representation of the main molecular orbitals involved in the electronic transitions of 1

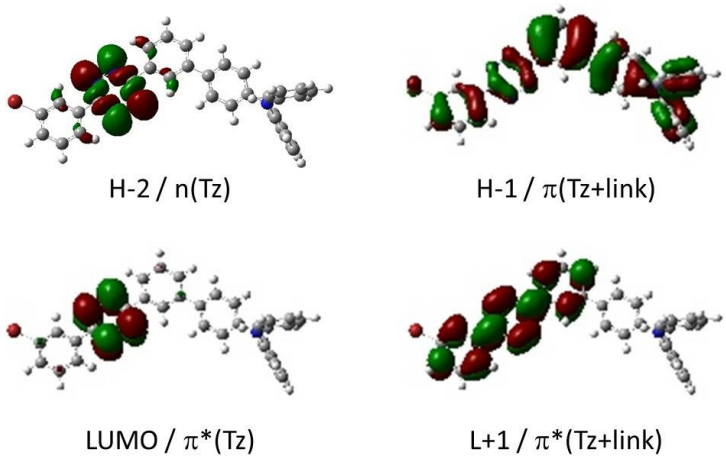

Figure S 9. Representation of the main molecular orbitals involved in the electronic transitions of 2

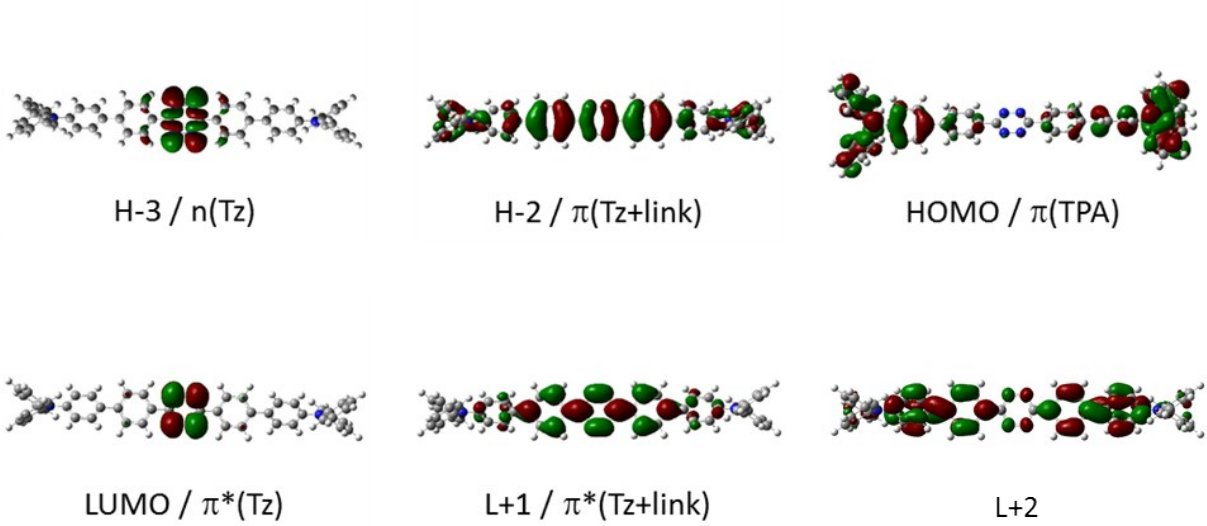

Figure S 10. Representation of the main molecular orbitals involved in the electronic transitions of 3

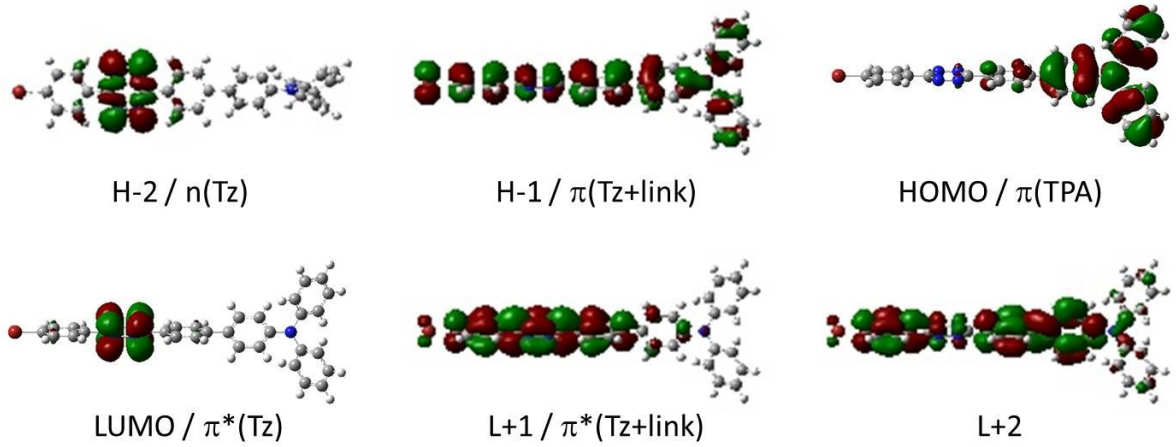

Figure S 11. Representation of the main molecular orbitals involved in the electronic transitions of 4

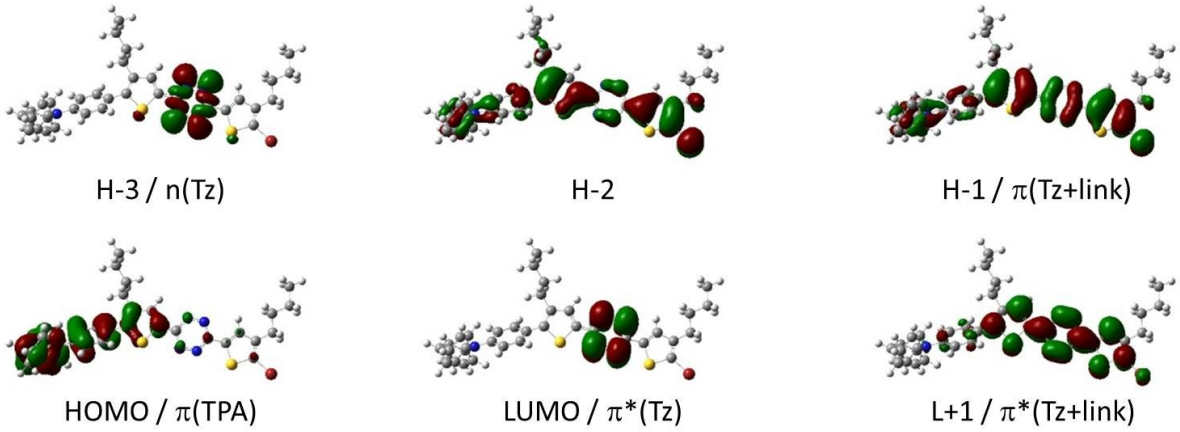

Figure S 12. Representation of the main molecular orbitals involved in the electronic transitions of 5

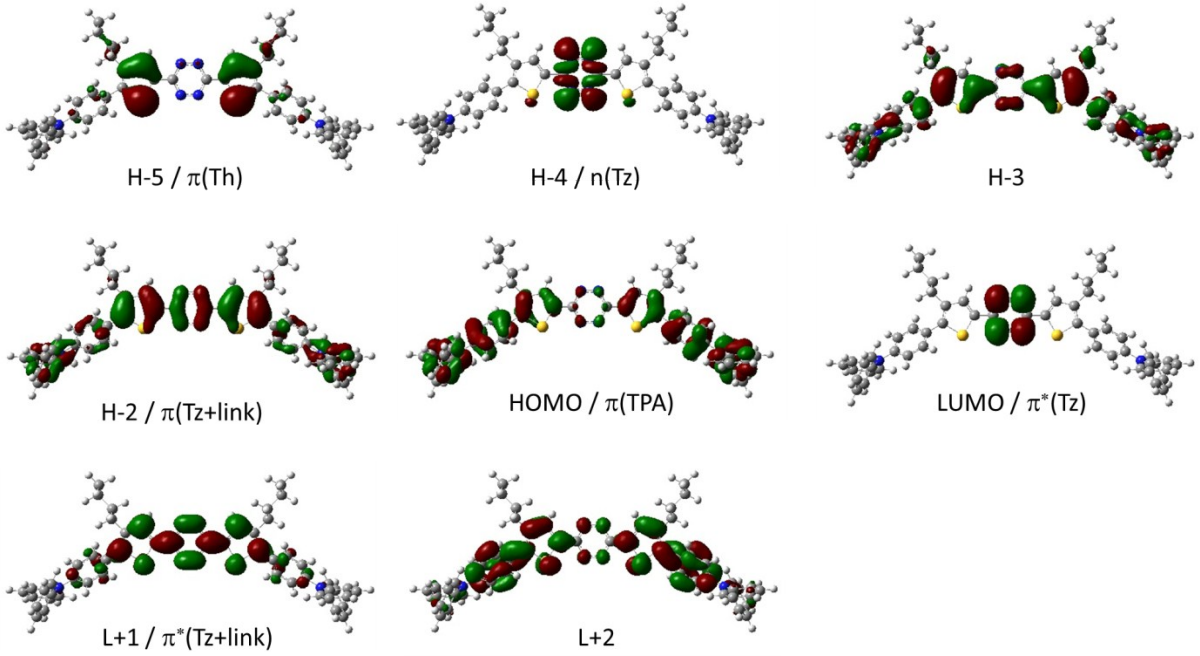

Figure S 13. Representation of the main molecular orbitals involved in the electronic transitions of 6

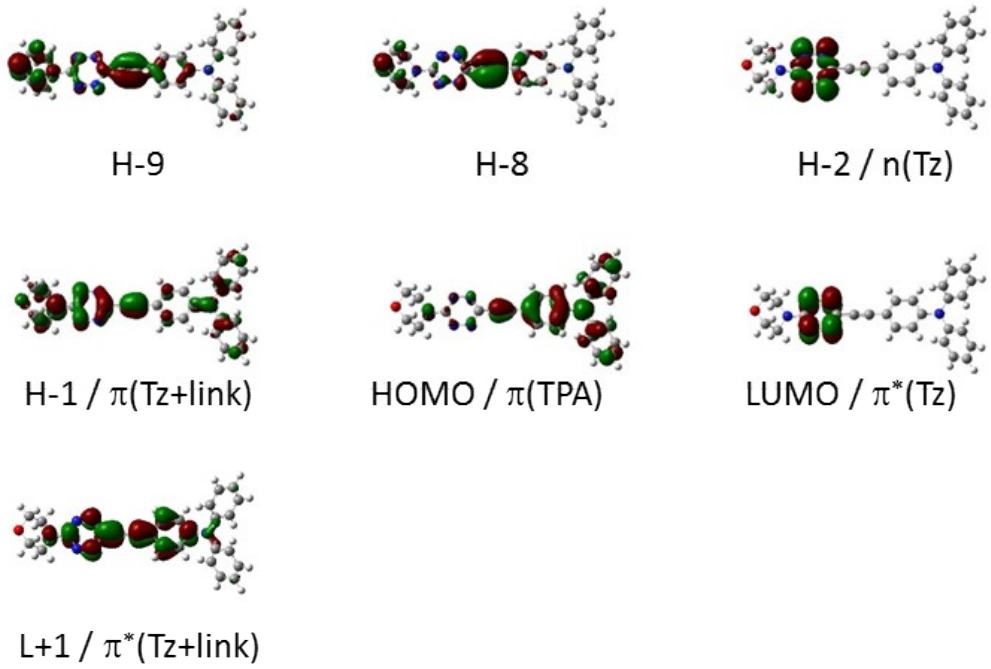

Figure S 14. Representation of the main molecular orbitals involved in the electronic transitions of 7

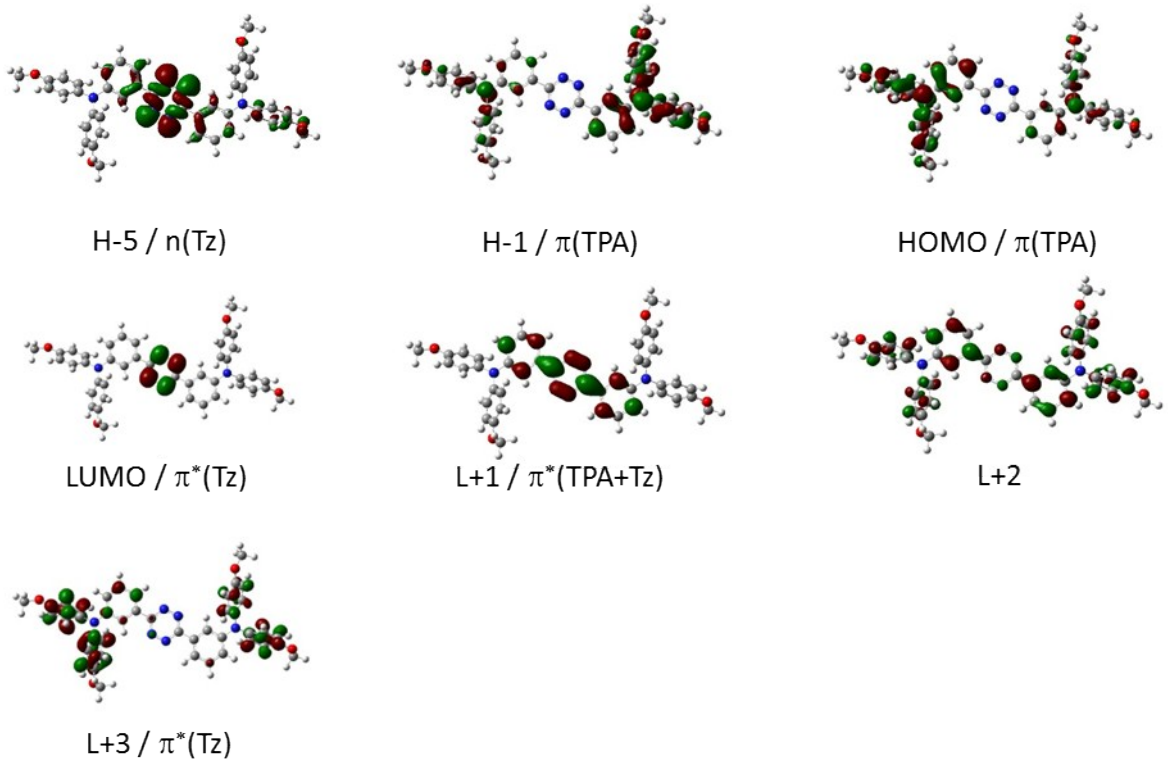

Figure S 15. Representation of the main molecular orbitals involved in the electronic transitions of 8

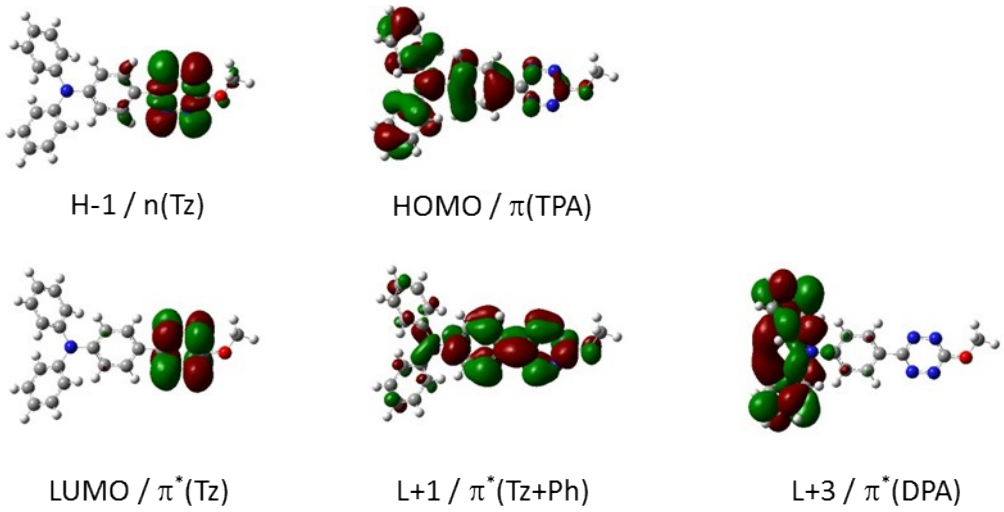

Figure S 16. Representation of the main molecular orbitals involved in the electronic transitions of 9

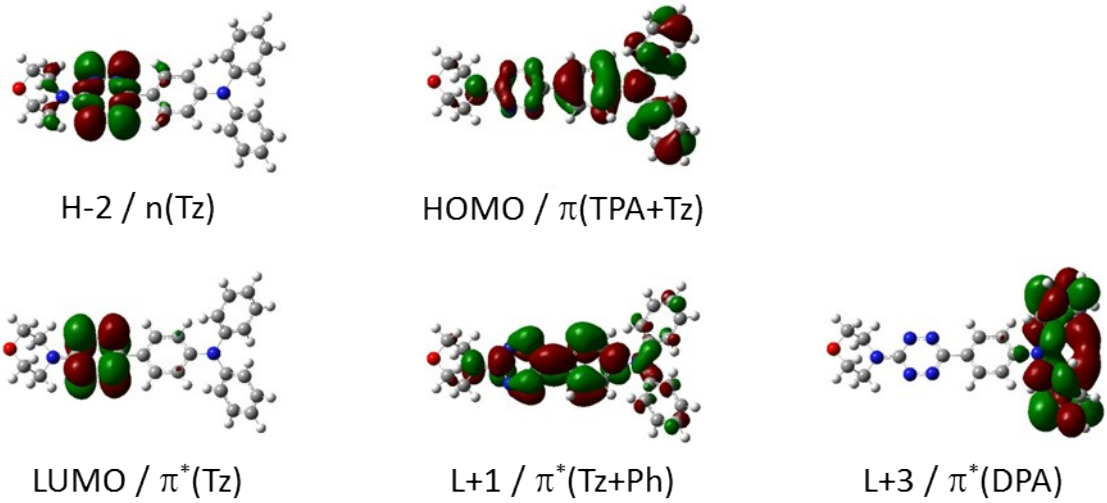

Figure S 17. Representation of the main molecular orbitals involved in the electronic transitions of 10

Table S 2. Atomic coordinates of compound 1 after geometry optimization

Number	Atomic number	X	Y	Z
1	6	1.032935	-0.314396	0.747203
2	6	-1.039865	0.107116	-0.812768
3	7	-0.20792	-0.460006	1.283818
4	7	-1.276146	-0.2418	0.480095
5	7	1.269236	0.03482	-0.545331
6	7	0.200625	0.250915	-1.349906
7	6	2.189533	-0.544198	1.621313
8	6	3.487163	-0.397212	1.114312
9	6	1.992783	-0.916388	2.959851
10	6	4.604343	-0.609732	1.93307
11	1	3.609	-0.136004	0.071519
12	6	3.098426	-1.133838	3.77727
13	1	0.983267	-1.024926	3.332105

14	6	4.391015	-0.979591	3.274481
15	1	2.954685	-1.411457	4.814791
16	1	5.243566	-1.118806	3.928768
17	6	-2.197428	0.347776	-1.682666
18	6	-3.494597	0.220419	-1.168654
19	6	-2.00309	0.69836	-3.0274
20	6	-4.611282	0.447444	-1.983116
21	1	-3.617616	-0.074847	-0.135074
22	6	-3.109471	0.920776	-3.842709
23	1	-0.994003	0.79112	-3.405189
24	6	-4.401687	0.800879	-3.328988
25	1	-2.966462	1.200647	-4.879719
26	1	-5.257101	1.003894	-3.96277
27	6	5.981042	-0.438301	1.401107
28	6	7.028148	-1.284851	1.803251
29	6	6.280034	0.58011	0.479606
30	6	8.320463	-1.114333	1.320195
31	1	6.824215	-2.096641	2.491889
32	6	7.566475	0.747037	-0.019368
33	1	5.496441	1.257272	0.160196
34	6	8.613128	-0.09367	0.398489
35	1	9.111551	-1.777715	1.643848
36	1	7.773687	1.538393	-0.727538
37	7	9.934259	0.081885	-0.099455
38	6	10.773167	-1.054389	-0.329396
39	6	10.437764	1.393102	-0.36812
40	6	10.260044	-2.208337	-0.943345
41	6	12.123846	-1.029172	0.053249
42	6	10.163624	2.458125	0.505907
43	6	11.221005	1.633788	-1.50867
44	6	11.080349	-3.314401	-1.158684
45	1	9.220593	-2.23006	-1.24443
46	6	12.942492	-2.132345	-0.18196
47	1	12.521571	-0.142108	0.529086
48	6	10.651891	3.734888	0.234866
49	1	9.566672	2.277171	1.390417
50	6	11.720481	2.90969	-1.76329
51	1	11.433246	0.816645	-2.185807
52	6	12.426139	-3.282605	-0.784135
53	1	10.669424	-4.197856	-1.633705
54	1	13.98334	-2.097245	0.118742
55	6	11.435681	3.968988	-0.897806
56	1	10.430393	4.545899	0.919166
57	1	12.322785	3.078756	-2.648541
58	1	13.062991	-4.141285	-0.95933
59	1	11.819061	4.961297	-1.10248
60	6	-5.987384	0.325136	-1.435697
61	6	-7.014006	-0.280227	-2.179624
62	6	-6.303033	0.817181	-0.15806
63	6	-8.30592	-0.380325	-1.675073

64	1	-6.793713	-0.686214	-3.160321
65	6	-7.589178	0.707005	0.358408
66	1	-5.532552	1.299676	0.43222
67	6	-8.615156	0.110394	-0.394794
68	1	-9.083225	-0.850206	-2.263205
69	1	-7.811918	1.092487	1.344661
70	7	-9.936654	0.006234	0.125796
71	6	-10.724385	-1.156404	-0.143206
72	6	-10.482353	1.065215	0.91628
73	6	-10.146237	-2.435862	-0.102665
74	6	-12.090252	-1.036562	-0.447544
75	6	-10.256402	2.406682	0.566427
76	6	-11.254728	0.78005	2.05423
77	6	-10.916951	-3.565585	-0.370876
78	1	-9.095452	-2.534697	0.137306
79	6	-12.858166	-2.172437	-0.697168
80	1	-12.540066	-0.052766	-0.482709
81	6	-10.782437	3.435746	1.345024
82	1	-9.665984	2.631883	-0.312219
83	6	-11.792192	1.814733	2.817556
84	1	-11.429451	-0.25185	2.329905
85	6	-12.277306	-3.442789	-0.66529
86	1	-10.455138	-4.545633	-0.33521
87	1	-13.911015	-2.062445	-0.930611
88	6	-11.556514	3.147939	2.47213
89	1	-10.597838	4.465593	1.061474
90	1	-12.385377	1.57729	3.693242
91	1	-12.875453	-4.323343	-0.866319
92	1	-11.969655	3.949978	3.071787

Number of imaginary frequencies: 0

Table S 3. Atomic coordinates of compound 2 after geometry optimization

Number	Atomic number	X	Y	Z
1	6	-4.8032	-0.197053	0.07026
2	6	-2.618077	1.164227	-0.448011
3	7	-3.609601	-0.811875	0.275239
4	7	-2.481797	-0.110383	0.007047
5	7	-4.941305	1.07218	-0.393507
6	7	-3.814758	1.775458	-0.660343
7	6	-6.024261	-0.955768	0.368459
8	6	-7.277485	-0.360337	0.16427
9	6	-5.939994	-2.267948	0.855306
10	6	-8.428415	-1.076812	0.446365
11	1	-7.327862	0.65127	-0.211287
12	6	-7.10781	-2.972742	1.134004
13	1	-4.964069	-2.70865	1.005544
14	6	-8.356098	-2.379573	0.9303
15	1	-7.053116	-3.98675	1.510857

16	1	-9.267	-2.921922	1.144638
17	6	-1.397762	1.928236	-0.729376
18	6	-0.143055	1.340801	-0.51906
19	6	-1.489691	3.249128	-1.194457
20	6	1.033016	2.058276	-0.772218
21	1	-0.099154	0.32961	-0.136768
22	6	-0.323956	3.967482	-1.445732
23	1	-2.467202	3.685001	-1.34938
24	6	0.925874	3.381214	-1.23991
25	1	-0.387086	4.984876	-1.813123
26	1	1.828106	3.938637	-1.463043
27	6	2.36359	1.435081	-0.550447
28	6	3.414869	2.160634	0.034676
29	6	2.608515	0.100627	-0.915539
30	6	4.661641	1.581369	0.242292
31	1	3.247813	3.186237	0.343394
32	6	3.849023	-0.488692	-0.6991
33	1	1.819179	-0.477515	-1.381943
34	6	4.898871	0.243344	-0.11769
35	1	5.457975	2.156191	0.696464
36	1	4.01806	-1.518014	-0.986531
37	7	6.170939	-0.355972	0.10379
38	6	6.919254	-0.038703	1.280504
39	6	6.699752	-1.290769	-0.840736
40	6	6.276836	0.082356	2.523734
41	6	8.308847	0.151989	1.211038
42	6	6.579242	-1.056346	-2.220322
43	6	7.35068	-2.455309	-0.402319
44	6	7.008956	0.398568	3.666532
45	1	5.207028	-0.07035	2.583958
46	6	9.036677	0.449798	2.36172
47	1	8.80775	0.062388	0.254761
48	6	7.088812	-1.973786	-3.137255
49	1	6.083613	-0.157225	-2.562946
50	6	7.872995	-3.359365	-1.325461
51	1	7.443991	-2.640417	0.65989
52	6	8.392479	0.580146	3.594786
53	1	6.497986	0.488463	4.618295
54	1	10.108737	0.593806	2.2912
55	6	7.741804	-3.128043	-2.697151
56	1	6.987124	-1.778569	-4.198654
57	1	8.372131	-4.253913	-0.970984
58	1	8.959977	0.81878	4.486169
59	1	8.142674	-3.836175	-3.412291
60	35	-10.154645	-0.261823	0.165412

Number of imaginary frequencies: 0

Table S 4. Atomic coordinates of compound 3 after geometry optimization

Number	Atomic number	X	Y	Z

1	6	-2.931521	-0.000079	-0.000011
2	6	-5.560709	0.000055	0.000018
3	7	-3.569275	0.297177	-1.164958
4	7	-4.922952	0.29462	-1.165609
5	7	-3.569278	-0.297212	1.164964
6	7	-4.922958	-0.294559	1.165634
7	6	-1.467714	-0.000069	-0.000007
8	6	-0.759534	-0.324357	1.168129
9	6	-0.759533	0.324225	-1.168139
10	6	0.629288	-0.325005	1.164694
11	1	-1.315956	-0.562092	2.065023
12	6	0.629289	0.324883	-1.164701
13	1	-1.315955	0.561952	-2.065037
14	6	1.350806	-0.000056	-0.000002
15	1	1.168781	-0.550777	2.076789
16	1	1.168783	0.550653	-2.076797
17	6	-7.024516	0.000036	0.000011
18	6	-7.732694	0.272318	-1.181331
19	6	-7.7327	-0.272263	1.181345
20	6	-9.121517	0.270093	-1.178627
21	1	-7.176272	0.491286	-2.08299
22	6	-9.121522	-0.270062	1.17863
23	1	-7.176281	-0.491217	2.083009
24	6	-9.843036	0.000009	-0.000001
25	1	-9.661007	0.506812	-2.087945
26	1	-9.661016	-0.506794	2.087943
27	6	2.833518	-0.000044	0.000001
28	6	3.559062	0.999037	-0.672192
29	6	3.559083	-0.999109	0.672197
30	6	4.948956	0.999748	-0.677299
31	1	3.025485	1.79159	-1.18407
32	6	4.948976	-0.999788	0.677309
33	1	3.025521	-1.791677	1.184072
34	6	5.669112	-0.000012	0.000006
35	1	5.488776	1.779797	-1.197862
36	1	5.488813	-1.779826	1.19787
37	7	7.092223	0.000005	0.000007
38	6	7.810263	1.234769	0.072721
39	6	7.810304	-1.234732	-0.072715
40	6	7.377334	2.261833	0.927423
41	6	8.9618	1.436799	-0.705494
42	6	7.377362	-2.26184	-0.927359
43	6	8.961897	-1.436694	0.705434
44	6	8.076331	3.465668	0.991541
45	1	6.493809	2.108891	1.533587
46	6	9.665609	2.636808	-0.622153
47	1	9.297916	0.649012	-1.367119
48	6	8.076403	-3.465649	-0.991484
49	1	6.493794	-2.108955	-1.533474
50	6	9.665749	-2.636676	0.622084

51	1	9.298025	-0.648873	1.367014
52	6	9.226227	3.659941	0.221891
53	1	7.72882	4.248437	1.656003
54	1	10.552575	2.777047	-1.229306
55	6	9.226357	-3.659854	-0.221902
56	1	7.728882	-4.248452	-1.6559
57	1	10.552758	-2.776861	1.229186
58	1	9.771585	4.594196	0.279208
59	1	9.771748	-4.594088	-0.279223
60	35	-11.753036	0.000004	-0.00001

Number of imaginary frequencies: 0

Table S 5. Atomic coordinates of compound 4 after geometry optimization

Number	Atomic number	X	Y	Z
1	6	-1.314592	-0.000084	-0.000019
2	6	1.314596	0.000052	-0.000018
3	7	-0.676837	0.001361	1.202253
4	7	0.676841	-0.001279	1.202253
5	7	-0.676837	-0.001403	-1.20229
6	7	0.676842	0.001333	-1.202289
7	6	-2.778399	-0.000072	-0.000018
8	6	-3.486581	-0.026933	-1.212032
9	6	-3.486578	0.026796	1.211997
10	6	-4.875403	-0.028405	-1.20886
11	1	-2.93016	-0.03665	-2.139849
12	6	-4.8754	0.028281	1.208829
13	1	-2.930155	0.036504	2.139814
14	6	-5.596919	-0.000057	-0.000015
15	1	-5.414898	-0.022785	-2.148466
16	1	-5.414893	0.02266	2.148436
17	6	2.778403	0.000031	-0.000018
18	6	3.486583	-0.026765	1.211999
19	6	3.486585	0.026807	-1.212034
20	6	4.875406	-0.028258	1.208829
21	1	2.930162	-0.036411	2.139816
22	6	4.875407	0.028271	-1.208863
23	1	2.930164	0.036467	-2.139851
24	6	5.596923	0	-0.000017
25	1	5.414897	-0.022584	2.148436
26	1	5.4149	0.022583	-2.14847
27	6	-7.079631	-0.000043	-0.000013
28	6	-7.805173	0.802903	0.897366
29	6	-7.805198	-0.802972	-0.897387
30	6	-9.195067	0.802336	0.902493
31	1	-7.271594	1.445122	1.588534
32	6	-9.195091	-0.802371	-0.902507
33	1	-7.271638	-1.445206	-1.588557
34	6	-9.915225	-0.000009	-0.000005
35	1	-9.734886	1.430298	1.599003

36	1	-9.734929	-1.430322	-1.599011
37	7	-11.338336	0.000009	0
38	6	-12.056375	1.214697	0.233375
39	6	-12.056418	-1.214655	-0.233356
40	6	-11.623446	2.420503	-0.342306
41	6	-13.20791	1.219012	1.037377
42	6	-11.623476	-2.420489	0.342255
43	6	-13.208013	-1.218918	-1.037274
44	6	-12.322442	3.603098	-0.108211
45	1	-10.739922	2.421429	-0.967467
46	6	-13.911719	2.402629	1.251897
47	1	-13.544027	0.292637	1.484798
48	6	-12.322519	-3.60306	0.108176
49	1	-10.739907	-2.421459	0.967352
50	6	-13.911866	-2.40251	-1.251778
51	1	-13.54414	-0.292521	-1.484643
52	6	-13.472337	3.602003	0.685581
53	1	-11.974931	4.525307	-0.559617
54	1	-14.798683	2.389148	1.874892
55	6	-13.472473	-3.601913	-0.68553
56	1	-11.974997	-4.525291	0.559528
57	1	-14.798876	-2.388988	-1.874707
58	1	-14.017694	4.521634	0.859928
59	1	-14.017866	-4.521525	-0.859866
60	6	7.079636	-0.000007	-0.000014
61	6	7.805187	-0.802913	0.897393
62	6	7.805192	0.802898	-0.897419
63	6	9.195081	-0.802325	0.902522
64	1	7.271617	-1.445117	1.588581
65	6	9.195086	0.802314	-0.902537
66	1	7.271625	1.445097	-1.588615
67	6	9.915228	-0.000003	-0.000003
68	1	9.734908	-1.430257	1.599053
69	1	9.734917	1.430244	-1.599067
70	7	11.338342	0.000001	0.000005
71	6	12.0564	-1.214672	0.233382
72	6	12.056394	1.21468	-0.233362
73	6	11.623449	-2.420503	-0.342229
74	6	13.207979	-1.218951	1.037324
75	6	11.623437	2.420504	0.342262
76	6	13.207971	1.218974	-1.037305
77	6	12.322465	-3.603085	-0.108126
78	1	10.739893	-2.421461	-0.967344
79	6	13.911806	-2.402555	1.251852
80	1	13.544114	-0.292558	1.484694
81	6	12.322447	3.603091	0.108172
82	1	10.739881	2.42145	0.967378
83	6	13.911793	2.402585	-1.25182
84	1	13.544112	0.292588	-1.484686
85	6	13.472401	-3.601954	0.685605

86	1	11.974934	-4.525312	-0.559478
87	1	14.798802	-2.389045	1.8748
88	6	13.472383	3.601974	-0.685559
89	1	11.974913	4.525312	0.559536
90	1	14.798789	2.389085	-1.874769
91	1	14.017774	-4.521575	0.859959
92	1	14.017751	4.5216	-0.859903

Number of imaginary frequencies: 0

Table S 6. Atomic coordinates of compound 5 after geometry optimization

Number	Atomic number	X	Y	Z
1	6	4.473433	-0.207088	-0.044977
2	6	1.935054	0.416092	-0.18245
3	7	4.156434	1.092521	-0.317679
4	7	2.845927	1.414985	-0.389278
5	7	3.565232	-1.200385	0.168176
6	7	2.255955	-0.8808	0.097528
7	6	5.860029	-0.555103	0.023701
8	6	6.946875	0.255009	-0.149572
9	16	6.336227	-2.261699	0.376725
10	6	8.210552	-0.407952	-0.017222
11	1	6.834468	1.306405	-0.36839
12	6	8.054721	-1.736754	0.259281
13	6	0.547925	0.753204	-0.266107
14	6	-0.008149	1.974955	-0.527162
15	16	-0.711962	-0.513243	-0.021735
16	6	-1.438697	1.989436	-0.544044
17	1	0.606081	2.849229	-0.693856
18	6	-1.994232	0.751148	-0.300749
19	6	-3.400408	0.349775	-0.232418
20	6	-4.306212	0.691738	-1.254401
21	6	-3.881724	-0.419216	0.844019
22	6	-5.640584	0.31075	-1.187704
23	1	-3.95164	1.2462	-2.114629
24	6	-5.211176	-0.814911	0.906834
25	1	-3.199186	-0.704405	1.636122
26	6	-6.119096	-0.450401	-0.105037
27	1	-6.321097	0.585985	-1.982296
28	1	-5.5601	-1.407052	1.742215
29	7	-7.479774	-0.847541	-0.040258
30	6	-8.202769	-1.146581	-1.240361
31	6	-8.146919	-0.955223	1.221605
32	6	-7.615678	-1.922168	-2.252692
33	6	-9.512401	-0.672908	-1.415058
34	6	-9.00795	-2.033898	1.478201
35	6	-7.961059	0.020065	2.214696
36	6	-8.322624	-2.20519	-3.420214
37	1	-6.608372	-2.29494	-2.117829

38	6	-10.219363	-0.974591	-2.577811
39	1	-9.966865	-0.074392	-0.636128
40	6	-9.670159	-2.129752	2.700846
41	1	-9.153315	-2.787601	0.715171
42	6	-8.612922	-0.092222	3.441478
43	1	-7.304573	0.85816	2.018897
44	6	-9.628372	-1.73714	-3.588519
45	1	-7.856498	-2.805021	-4.193353
46	1	-11.230006	-0.602081	-2.69909
47	6	-9.473814	-1.163985	3.691246
48	1	-10.331218	-2.968964	2.884111
49	1	-8.458364	0.668151	4.198372
50	1	-10.177996	-1.96464	-4.493912
51	1	-9.984362	-1.245047	4.64322
52	6	9.563811	0.259644	-0.162395
53	6	9.506843	1.76912	-0.481872
54	1	10.124479	-0.252343	-0.956069
55	1	10.129111	0.113289	0.767937
56	6	10.920587	2.376218	-0.615346
57	1	8.957725	1.928444	-1.419105
58	1	8.964436	2.29527	0.31461
59	6	10.876187	3.886327	-0.931634
60	1	11.471783	2.211874	0.320014
61	1	11.464852	1.849343	-1.410238
62	1	11.887175	4.298571	-1.020231
63	1	10.348559	4.067249	-1.875303
64	1	10.352305	4.430942	-0.137547
65	6	-2.222559	3.276197	-0.706282
66	6	-2.008326	4.23309	0.497241
67	1	-3.289106	3.0508	-0.789987
68	1	-1.912598	3.784321	-1.629544
69	6	-2.797448	5.551195	0.342418
70	1	-2.323306	3.720517	1.414579
71	1	-0.939016	4.458894	0.599973
72	6	-2.587621	6.495546	1.545589
73	1	-2.481961	6.055426	-0.58089
74	1	-3.865911	5.320433	0.237539
75	1	-3.155491	7.424146	1.42128
76	1	-2.916267	6.013661	2.473738
77	1	-1.527484	6.753416	1.652198
78	35	9.44413	-3.006948	0.514011

Number of imaginary frequencies: 0

Table S 7. Atomic coordinates of compound 6 after geometry optimization

Number	Atomic number	X	Y	Z
1	6	1.309168	1.647066	0.030112
2	6	-1.309143	1.647067	-0.029982
3	7	0.675304	2.858293	0.015978

4	7	-0.675275	2.858294	-0.016039
5	7	0.675055	0.439747	0.015613
6	7	-0.67504	0.439747	-0.015207
7	6	2.739763	1.645778	0.06305
8	6	3.583642	2.721019	0.081012
9	16	3.646052	0.08735	0.088475
10	6	4.9756	2.388579	0.108079
11	1	3.204786	3.733708	0.063363
12	6	5.206016	1.029524	0.121055
13	6	-2.739733	1.64578	-0.063011
14	6	-3.583619	2.72101	-0.081112
15	16	-3.646019	0.087335	-0.088248
16	6	-4.975576	2.388559	-0.108246
17	1	-3.204775	3.733705	-0.063541
18	6	-5.20598	1.029501	-0.121096
19	6	6.470602	0.291983	0.142355
20	6	7.478666	0.598696	1.07579
21	6	6.704606	-0.767127	-0.7551
22	6	8.680727	-0.098245	1.08903
23	1	7.306225	1.380225	1.805568
24	6	7.898009	-1.476827	-0.73422
25	1	5.93723	-1.028901	-1.474257
26	6	8.91348	-1.149522	0.1834
27	1	9.444195	0.155248	1.81236
28	1	8.056616	-2.288286	-1.431877
29	7	10.138514	-1.86725	0.201358
30	6	10.820983	-2.098954	1.438871
31	6	10.705438	-2.3649	-1.01479
32	6	10.109334	-2.495269	2.582469
33	6	12.213186	-1.940049	1.522073
34	6	11.278525	-3.645794	-1.058604
35	6	10.705026	-1.577952	-2.177942
36	6	10.77794	-2.713703	3.785737
37	1	9.036705	-2.626551	2.519815
38	6	12.877085	-2.177351	2.724434
39	1	12.764185	-1.634649	0.641933
40	6	11.842064	-4.123954	-2.240255
41	1	11.279075	-4.255462	-0.164358
42	6	11.254012	-2.070298	-3.360522
43	1	10.271475	-0.586673	-2.147075
44	6	12.164587	-2.560008	3.863808
45	1	10.21499	-3.01884	4.660299
46	1	13.952446	-2.050442	2.773501
47	6	11.829043	-3.343101	-3.398894
48	1	12.280042	-5.115285	-2.258447
49	1	11.24497	-1.451267	-4.250283
50	1	12.682441	-2.737302	4.798667
51	1	12.260926	-3.720668	-4.317832
52	6	-6.470561	0.291955	-0.142377
53	6	-7.478542	0.598498	-1.075964

54	6	-6.704648	-0.766988	0.755248
55	6	-8.680601	-0.098444	-1.089184
56	1	-7.306032	1.379888	-1.805874
57	6	-7.898053	-1.476687	0.734396
58	1	-5.937341	-1.02863	1.474528
59	6	-8.91344	-1.149549	-0.183373
60	1	-9.444006	0.154917	-1.812627
61	1	-8.056726	-2.288014	1.432192
62	7	-10.138475	-1.867275	-0.201299
63	6	-10.820866	-2.099176	-1.438818
64	6	-10.705487	-2.364723	1.014894
65	6	-10.109144	-2.495669	-2.582309
66	6	-12.213063	-1.94028	-1.522134
67	6	-11.278527	-3.64563	1.058889
68	6	-10.705209	-1.577562	2.177901
69	6	-10.777674	-2.714295	-3.785584
70	1	-9.036519	-2.626941	-2.519566
71	6	-12.876886	-2.177776	-2.7245
72	1	-12.764119	-1.634738	-0.64208
73	6	-11.842155	-4.123597	2.240577
74	1	-11.278974	-4.255461	0.164755
75	6	-11.254282	-2.069714	3.360522
76	1	-10.271691	-0.586273	2.146893
77	6	-12.164317	-2.560615	-3.863766
78	1	-10.214669	-3.019571	-4.660062
79	1	-13.952245	-2.050874	-2.773654
80	6	-11.829268	-3.342532	3.399074
81	1	-12.280095	-5.114942	2.258911
82	1	-11.245344	-1.450521	4.25017
83	1	-12.682111	-2.738059	-4.79863
84	1	-12.261218	-3.719949	4.318042
85	6	6.053252	3.45101	0.026585
86	6	5.996821	4.229746	-1.315112
87	1	7.037634	2.984354	0.120274
88	1	5.937415	4.159908	0.858005
89	6	7.092492	5.313635	-1.406306
90	1	6.113225	3.51739	-2.141227
91	1	5.010863	4.699346	-1.425589
92	6	7.034428	6.084079	-2.742991
93	1	6.975876	6.017183	-0.570932
94	1	8.077273	4.840261	-1.296774
95	1	7.815851	6.850502	-2.790407
96	1	7.17348	5.399306	-3.587636
97	1	6.062384	6.577119	-2.860407
98	6	-6.053223	3.451011	-0.026915
99	6	-5.996999	4.229733	1.314806
100	1	-7.037597	2.984375	-0.12076
101	1	-5.937242	4.159917	-0.858308
102	6	-7.092649	5.313655	1.405821
103	1	-6.113569	3.517369	2.140889

104	1	-5.011045	4.699298	1.42546
105	6	-7.034812	6.084074	2.742531
106	1	-6.975859	6.017213	0.570481
107	1	-8.077426	4.840314	1.2961
108	1	-7.816185	6.850557	2.789791
109	1	-7.174098	5.399299	3.587136
110	1	-6.062755	6.577037	2.860162

Number of imaginary frequencies: 0

Table S 8. Atomic coordinates of compound 7 after geometry optimization

Number	Atomic number	X	Y	Z
1	7	4.773196	0.016489	0.028789
2	6	3.358638	0.003066	-0.01254
3	6	2.629965	-1.067801	0.543441
4	6	2.643101	1.060022	-0.610604
5	6	1.244611	-1.084228	0.497999
6	1	3.164143	-1.883322	1.011757
7	6	1.257304	1.049678	-0.646341
8	1	3.187798	1.886002	-1.047444
9	6	0.526547	-0.024309	-0.095434
10	1	0.698402	-1.911128	0.934546
11	1	0.721786	1.866133	-1.114651
12	6	5.51614	-1.209184	-0.000823
13	6	5.173585	-2.231608	-0.899462
14	6	6.606611	-1.394007	0.862853
15	6	5.900889	-3.420679	-0.920002
16	1	4.337895	-2.088088	-1.572282
17	6	7.339892	-2.578774	0.824509
18	1	6.872051	-0.605926	1.555659
19	6	6.989052	-3.600063	-0.062014
20	1	5.624765	-4.202487	-1.618066
21	1	8.179314	-2.708464	1.497792
22	1	7.556428	-4.522634	-0.084911
23	6	5.489846	1.255876	0.100549
24	6	5.075229	2.271733	0.976011
25	6	6.625972	1.46127	-0.697046
26	6	5.777053	3.474514	1.037729
27	1	4.204232	2.11246	1.598678
28	6	7.332915	2.659907	-0.617115
29	1	6.94684	0.677888	-1.371461
30	6	6.91053	3.674612	0.245493
31	1	5.445159	4.251039	1.717168
32	1	8.208184	2.80537	-1.239599
33	1	7.45768	4.607959	0.300714
34	6	-0.889596	-0.039419	-0.136428
35	6	-2.101574	-0.055457	-0.170132
36	6	-3.50998	-0.079957	-0.208009

37	6	-6.133208	-0.139906	-0.300758
38	7	-4.152013	1.00666	-0.734375
39	7	-5.499068	0.979621	-0.782293
40	7	-4.138481	-1.186562	0.293466
41	7	-5.484938	-1.219946	0.248339
42	6	-8.281917	0.943909	-0.896334
43	6	-8.26395	-1.321027	0.154249
44	6	-9.270328	1.388262	0.193425
45	1	-8.842085	0.592906	-1.77082
46	1	-7.600324	1.745463	-1.179568
47	6	-9.251516	-0.789228	1.204035
48	1	-8.824089	-1.76848	-0.675071
49	1	-7.570206	-2.046326	0.578387
50	1	-9.965034	2.135895	-0.195794
51	1	-8.709308	1.80762	1.041166
52	1	-9.93311	-1.578418	1.529003
53	1	-8.689122	-0.404728	2.067256
54	7	-7.480097	-0.180487	-0.367168
55	8	-10.097058	0.259704	0.628339

Number of imaginary frequencies: 0

Table S 9. Atomic coordinates of compound 8 after geometry optimization

Number	Atomic number	X	Y	Z
1	7	-6.095796	0.24162	-0.086969
2	6	-4.917794	1.028194	-0.061804
3	6	-4.995239	2.435413	-0.036179
4	6	-3.64971	0.42751	-0.062175
5	6	-3.837062	3.209708	-0.020656
6	1	-5.967511	2.909573	-0.030721
7	6	-2.492576	1.213258	-0.030752
8	1	-3.552306	-0.648292	-0.084877
9	6	-2.578465	2.61387	-0.013585
10	1	-3.921878	4.289973	-0.000185
11	6	-7.286909	0.739529	-0.708927
12	6	-7.239871	1.331463	-1.984576
13	6	-8.526531	0.629472	-0.070334
14	6	-8.394219	1.810149	-2.584214
15	1	-6.2894	1.414373	-2.496095
16	6	-9.69287	1.091258	-0.68198
17	1	-8.576658	0.171159	0.909094
18	6	-9.636397	1.692709	-1.94207
19	1	-8.369935	2.269058	-3.56373
20	1	-10.634426	0.98491	-0.160385
21	6	-6.124043	-1.058342	0.515714
22	6	-5.580934	-1.278496	1.786243
23	6	-6.718459	-2.141535	-0.155805
24	6	-5.608607	-2.546235	2.368432
25	1	-5.124414	-0.454156	2.319313
26	6	-6.766984	-3.396459	0.430906
27	1	-7.142846	-1.985225	-1.139111

28	6	-6.206525	-3.616667	1.698095
29	1	-5.170025	-2.680554	3.347872
30	1	-7.221176	-4.236789	-0.077189
31	8	-10.72634	2.195478	-2.63583
32	8	-6.298019	-4.911068	2.186105
33	6	-12.039345	2.096071	-2.008586
34	1	-12.079019	2.649437	-1.062165
35	1	-12.72876	2.544399	-2.724367
36	1	-12.3235	1.052164	-1.826993
37	6	-5.706331	-5.190879	3.489596
38	1	-6.185147	-4.607362	4.28577
39	1	-5.88307	-6.253536	3.657521
40	1	-4.627908	-4.990415	3.495335
41	1	-1.670161	3.199194	0.006247
42	6	-1.175939	0.562932	-0.030737
43	6	1.183955	-0.595246	-0.019253
44	7	-1.133466	-0.795806	-0.050523
45	7	0.083547	-1.392889	-0.046214
46	7	-0.075099	1.360696	-0.01132
47	7	1.14144	0.763741	-0.003887
48	6	2.50116	-1.244394	-0.006423
49	6	2.590008	-2.644198	-0.03966
50	6	3.656909	-0.456368	0.023463
51	6	3.850297	-3.237245	-0.035468
52	1	1.683127	-3.23146	-0.066974
53	6	4.926279	-1.054262	0.036
54	1	3.55701	0.619318	0.039414
55	6	5.006553	-2.46153	0.009179
56	1	3.937227	-4.317431	-0.0531
57	1	5.979302	-2.934538	0.024067
58	7	6.099705	-0.262849	0.081189
59	6	7.318201	-0.723102	-0.515649
60	6	7.331346	-1.28031	-1.799304
61	6	8.536865	-0.606723	0.176841
62	6	8.521325	-1.728777	-2.374859
63	1	6.402665	-1.368848	-2.348865
64	6	9.722368	-1.031866	-0.401948
65	1	8.540713	-0.173699	1.168754
66	6	9.729001	-1.604126	-1.68302
67	1	8.49283	-2.159175	-3.366703
68	1	10.665745	-0.945522	0.120777
69	6	6.09018	1.021101	0.719886
70	6	5.527904	1.186298	1.998538
71	6	6.664228	2.132182	0.09429
72	6	5.531517	2.427001	2.616242
73	1	5.083649	0.334366	2.497123
74	6	6.687504	3.37741	0.723518
75	1	7.101284	2.017507	-0.889488
76	6	6.115627	3.537657	1.98835
77	1	5.09782	2.567584	3.597367

78	1	7.143286	4.214029	0.211553
79	8	6.074725	4.726385	2.699877
80	8	10.967149	-2.005446	-2.161118
81	6	11.024848	-2.599153	-3.492109
82	1	10.685323	-1.897256	-4.263814
83	1	12.077187	-2.836444	-3.649974
84	1	10.426881	-3.516956	-3.552675
85	6	6.650186	5.913865	2.078308
86	1	6.14204	6.165177	1.139231
87	1	6.497794	6.713701	2.80332
88	1	7.723119	5.79052	1.885275

Number of imaginary frequencies: 0

Table S 10. Atomic coordinates of compound 9 after geometry optimization

Number	Atomic number	X	Y	Z
1	6	0	0	0
2	6	0	0	2.605723
3	7	1.200328	0	0.625539
4	7	1.197983	0.002142	1.992562
5	7	-1.208886	-0.004672	0.645273
6	7	-1.217223	-0.006765	1.992857
7	6	-0.0184	0.004277	-1.460846
8	6	-1.235304	-0.011503	-2.161616
9	6	1.181712	0.025086	-2.190199
10	6	-1.253513	-0.010866	-3.547656
11	1	-2.159324	-0.03814	-1.59956
12	6	1.167709	0.034374	-3.575741
13	1	2.119029	0.047749	-1.650039
14	6	-0.051607	0.014443	-4.284491
15	1	-2.197092	-0.033911	-4.075565
16	1	2.098389	0.060861	-4.125814
17	7	-0.066186	0.018363	-5.698343
18	6	-1.153584	0.611532	-6.420283
19	6	1.006941	-0.577363	-6.44055
20	6	-1.672553	1.85788	-6.036434
21	6	-1.700569	-0.04402	-7.533785
22	6	1.556098	0.09023	-7.545602
23	6	1.509087	-1.837967	-6.08232
24	6	-2.729458	2.426427	-6.745649
25	1	-1.246996	2.369399	-5.18271
26	6	-2.745779	0.538703	-8.248487
27	1	-1.299814	-1.004318	-7.831532
28	6	2.587255	-0.495519	-8.27824
29	1	1.168023	1.061941	-7.82261
30	6	2.552093	-2.409958	-6.809137
31	1	1.080866	-2.357847	-5.234951
32	6	-3.269599	1.773136	-7.856422
33	1	-3.121852	3.388535	-6.437234

34	1	-3.159342	0.020698	-9.106028
35	6	3.094237	-1.74488	-7.911918
36	1	3.003093	0.031185	-9.129337
37	1	2.93166	-3.383508	-6.521277
38	1	-4.086668	2.220587	-8.409365
39	1	3.900087	-2.194996	-8.479025
40	8	-0.049837	0.004205	3.952423
41	6	1.246775	0.013579	4.664552
42	1	0.968719	0.018165	5.716776
43	1	1.830244	-0.873929	4.410872
44	1	1.822731	0.903073	4.40095

Number of imaginary frequencies: 0

Table S 11. Atomic coordinates of compound 10 after geometry optimization

Number	Atomic number	X	Y	Z
1	6	-2.048414	-0.10979	-0.211929
2	6	-4.674925	-0.174156	-0.320729
3	7	-2.69041	0.941886	-0.787533
4	7	-4.036886	0.920414	-0.84986
5	7	-2.684198	-1.188969	0.318461
6	7	-4.030019	-1.232862	0.270379
7	6	-6.82307	0.895767	-0.948431
8	6	-6.81068	-1.324125	0.191231
9	6	-7.794248	1.392577	0.134257
10	1	-7.396867	0.516335	-1.802073
11	1	-6.138751	1.679894	-1.271261
12	6	-7.77953	-0.742701	1.232037
13	1	-7.386025	-1.799796	-0.611656
14	1	-6.118023	-2.03837	0.635444
15	1	-8.488382	2.129404	-0.276192
16	1	-7.218971	1.841686	0.956936
17	1	-8.463512	-1.511771	1.597874
18	1	-7.20203	-0.328635	2.071371
19	7	-6.024395	-0.212861	-0.384561
20	8	-8.624286	0.290007	0.626183
21	6	-0.586657	-0.076643	-0.153893
22	6	0.127977	-1.119551	0.456459
23	6	0.127388	0.99854	-0.706061
24	6	1.513056	-1.08689	0.519694
25	1	-0.423219	-1.943445	0.890141
26	6	1.51315	1.028476	-0.655888
27	1	-0.423212	1.797869	-1.184271
28	6	2.234091	-0.012822	-0.038525
29	1	2.051536	-1.890867	1.002983
30	1	2.052398	1.856919	-1.094991
31	7	3.650403	0.020248	0.020228
32	6	4.410185	-1.193693	-0.001309
33	6	4.345915	1.269722	0.105028

34	6	4.081538	-2.229017	-0.890806
35	6	5.504632	-1.357387	0.862339
36	6	5.49309	1.494536	-0.671856
37	6	3.899542	2.279349	0.97239
38	6	4.825645	-3.407652	-0.902849
39	1	3.242299	-2.103513	-1.562674
40	6	6.254596	-2.531758	0.832367
41	1	5.75998	-0.560668	1.548987
42	6	6.179397	2.704085	-0.578774
43	1	5.838505	0.717004	-1.340892
44	6	4.580874	3.492982	1.047126
45	1	3.019283	2.106416	1.578054
46	6	5.917601	-3.565205	-0.045368
47	1	4.559157	-4.198944	-1.594025
48	1	7.096386	-2.643987	1.505947
49	6	5.725609	3.711685	0.27622
50	1	7.063239	2.863723	-1.185576
51	1	4.223867	4.263974	1.720193
52	1	6.497861	-4.479899	-0.061534
53	1	6.256729	4.653632	0.341564

Number of imaginary frequencies: 0

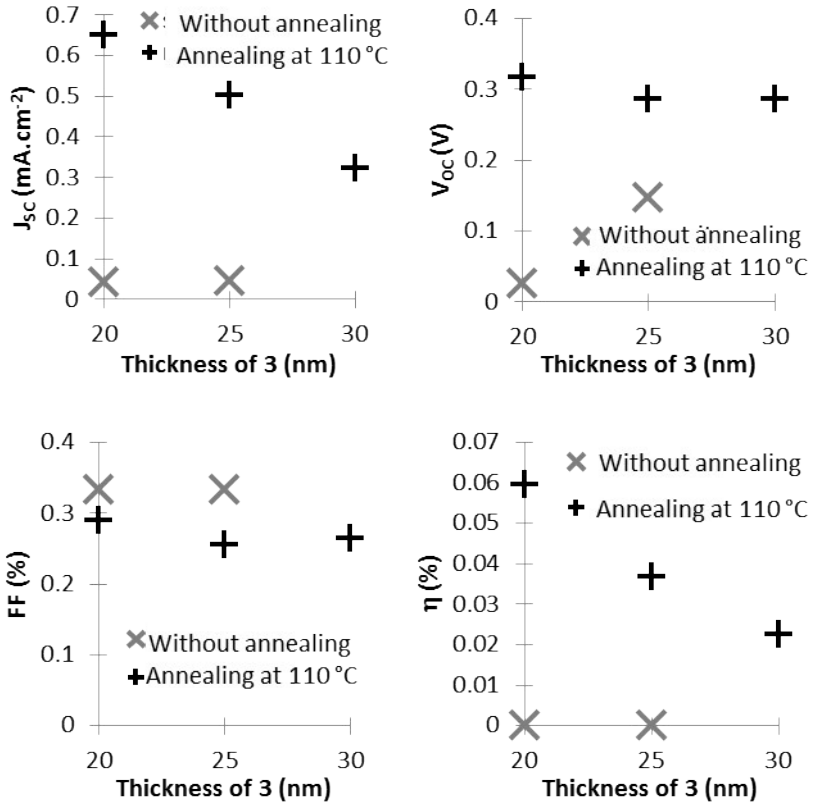

Figure S 18. Optimization of the thickness of the donor 3 (thickness of C60 is 25 nm)

Table S 12. Optimisation of annealing temperature and thickness of C60 (thickness of 3 is fixed to 20 nm)

thickness C60(nm)	Annealing temperature	Jsc (mA/cm²)	Voc (V)	FF (%)	PCE (%)	Rs (ohms)	Rsh (ohms)
25	110 °C	0.651	0.317	29.0	0.06	622.406	533.743
		0.554	0.266	27.3	0.04	1034.288	570.244
30	110 °C	1.635	0.206	37.9	0.128	49.96	271.146
		0.905	0.236	31.3	0.067	252.855	430.79
40	150 °C	2.003	0.256	41.5	0.213	34.794	284.891
		1.409	0.377	31.6	0.168	528.97	407.176
		1.37	0.206	40.7	0.115	54.707	338.993