Electronic Supplementary Material (ESI) for Energy & Environmental Science

Supplementary Informations

Investigation of the Photoinduced Electron Injection Processes for p-type Triphenylamine-Sensitised Solar Cells

Julien Preat, Anders Hagfeldt, and Eric A. Perpète

Optimized ICT B3LYP geometry

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.002239	5.342665	0.021778
2	6	0	0.757248	4.643573	-0.929014
3	6	0	0.761517	3.254157	-0.937881
4	6	0	-0.001951	2.551228	0.008812
5	6	0	-0.766270	3.244516	0.962628
6	6	0	-0.760390	4.632427	0.964515
7	1	0	1.336388	5.188091	-1.670198
8	1	0	1.331843	2.709344	-1.687468
9	7	0	-0.001524	1.127253	0.002310
10	1	0	-1.336356	2.692574	1.707151
11	1	0	-1.335571	5.181366	1.706401
12	6	0	1.209246	0.436388	-0.149949
13	6	0	2.397712	0.938427	0.429543
14	6	0	3.583925	0.248780	0.288881
15	6	0	3.654903	-0.968652	-0.440931

16	6	0	2.451757	-1.451608	-1.026062
17	6	0	1.259800	-0.773961	-0.882499
18	1	0	2.368157	1.853263	1.017549
19	1	0	4.475215	0.649780	0.769563
20	1	0	2.465124	-2.362610	-1.619894
21	1	0	0.360374	-1.149731	-1.365510
22	6	0	-1.212346	0.435348	0.150508
23	6	0	-2.400674	0.941371	-0.425685
24	6	0	-3.587495	0.252287	-0.287573
25	6	0	-3.659264	-0.968444	0.436615
26	6	0	-2.456039	-1.455869	1.017848
27	6	0	-1.263420	-0.778840	0.876590
28	1	0	-2.370651	1.859326	-1.008808
29	1	0	-4.478788	0.656836	-0.765264
30	1	0	-2.469862	-2.369869	1.607054
31	1	0	-0.364005	-1.157993	1.356969
32	6	0	-0.032533	6.834276	0.068261
33	8	0	-0.676474	7.469482	0.891060
34	8	0	0.715442	7.407148	-0.880717
35	1	0	0.636969	8.410329	-0.774006
36	6	0	-4.895199	-1.693018	0.589056
37	6	0	-5.103740	-2.919644	1.234509
38	6	0	-6.424077	-3.357044	1.205602
39	6	0	-7.304985	-2.486381	0.533970
40	16	0	-6.414717	-1.082861	-0.066112
41	1	0	-4.302080	-3.478770	1.710376
42	1	0	-6.771189	-4.286333	1.652778

43	6	0	4.889763	-1.694775	-0.594615
44	6	0	5.096500	-2.920243	-1.242838
45	6	0	6.415889	-3.360452	-1.213532
46	6	0	7.297883	-2.493194	-0.538921
47	16	0	6.409861	-1.089212	0.063473
48	1	0	4.294143	-3.476750	-1.720597
49	1	0	6.761529	-4.289489	-1.662365
50	6	0	8.673540	-2.736400	-0.384665
51	6	0	9.663036	-1.979158	0.251185
52	1	0	9.020125	-3.671331	-0.838336
53	6	0	-8.681361	-2.726241	0.380811
54	6	0	-9.669884	-1.965706	-0.252575
55	1	0	-9.029521	-3.661204	0.833214
56	6	0	-9.446874	-0.724889	-0.904633
57	7	0	-9.288023	0.297611	-1.447962
58	6	0	-11.011782	-2.433952	-0.268139
59	7	0	-12.114950	-2.817609	-0.281504
60	6	0	11.003811	-2.450556	0.267734
61	7	0	12.106059	-2.836828	0.281907
62	6	0	9.442095	-0.738732	0.904669
63	7	0	9.284937	0.283457	1.449087

Optimized ICT PBE0 geometry

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

1	6	0	-0.000600	5.306589	0.019440
2	6	0	0.764718	4.610865	-0.922754
3	6	0	0.767935	3.224657	-0.931228
4	6	0	-0.001653	2.527371	0.008330
5	6	0	-0.771502	3.216965	0.954029
6	6	0	-0.765245	4.601742	0.954455
7	1	0	1.350112	5.157059	-1.659464
8	1	0	1.343282	2.676055	-1.676071
9	7	0	-0.001645	1.111192	0.002759
10	1	0	-1.347145	2.662816	1.694509
11	1	0	-1.345774	5.154544	1.690902
12	6	0	1.200724	0.425391	-0.149398
13	6	0	2.390161	0.937234	0.411562
14	6	0	3.571965	0.247879	0.271084
15	6	0	3.635387	-0.976246	-0.441364
16	6	0	2.432260	-1.468154	-1.009323
17	6	0	1.244319	-0.791692	-0.864719
18	1	0	2.362946	1.861211	0.987644
19	1	0	4.468397	0.655846	0.739028
20	1	0	2.442658	-2.387329	-1.592458
21	1	0	0.339481	-1.172340	-1.336710
22	6	0	-1.204310	0.425039	0.151404
23	6	0	-2.393544	0.941136	-0.405992
24	6	0	-3.576101	0.252604	-0.267960
25	6	0	-3.640523	-0.974809	0.438661
26	6	0	-2.437472	-1.471304	1.002711
27	6	0	-1.248729	-0.795727	0.860336

28	1	0	-2.365695	1.868180	-0.977110
29	1	0	-4.472469	0.664323	-0.732733
30	1	0	-2.448515	-2.393433	1.581161
31	1	0	-0.343979	-1.179928	1.329603
32	6	0	-0.030595	6.794142	0.065153
33	8	0	-0.680218	7.423751	0.881469
34	8	0	0.720552	7.360652	-0.871610
35	1	0	0.643137	8.359965	-0.767322
36	6	0	-4.871418	-1.696270	0.590682
37	6	0	-5.076905	-2.924609	1.230724
38	6	0	-6.394599	-3.354705	1.200565
39	6	0	-7.265522	-2.474464	0.533597
40	16	0	-6.376335	-1.084914	-0.052852
41	1	0	-4.273731	-3.486389	1.702922
42	1	0	-6.750019	-4.284430	1.642099
43	6	0	4.865143	-1.699224	-0.594927
44	6	0	5.068767	-2.926358	-1.237912
45	6	0	6.385560	-3.359116	-1.207855
46	6	0	7.257802	-2.482183	-0.538149
47	16	0	6.370847	-1.092302	0.051074
48	1	0	4.264785	-3.485566	-1.711789
49	1	0	6.739442	-4.288533	-1.651262
50	6	0	8.631534	-2.715017	-0.381209
51	6	0	9.604550	-1.945200	0.254512
52	1	0	8.988660	-3.649331	-0.830722
53	6	0	-8.639880	-2.704244	0.377135
54	6	0	-9.611710	-1.931422	-0.256527

55	1	0	-8.998559	-3.638676	0.825189
56	6	0	-9.365658	-0.695149	-0.901345
57	7	0	-9.185096	0.324634	-1.438910
58	6	0	-10.956373	-2.379461	-0.281896
59	7	0	-12.062632	-2.747705	-0.302934
60	6	0	10.948226	-2.396064	0.280208
61	7	0	12.053712	-2.766654	0.301490
62	6	0	9.360660	-0.709359	0.900897
63	7	0	9.181931	0.310124	1.439682
