10.1071/CH22149
Australian Journal of Chemistry

Supplementary Material

Quantum chemical and photovoltaic modeling of D-π-A organic dyes based on substituted arylamine electron donors in dye sensitized solar cells

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Supplementary data

Table1: The Cartesian coordinates of optimized geometry of Dye-1

ATOM	X	Y	Z
C1	-11.068	3.782	1.155
C2	-9.839	1.468	1.179
C3	-7.492	1.128	0.014
C4	-6.425	3.243	-1.159
C5	-7.641	5.567	-1.177
C6	-9.995	5.888	-0.024
N7	-11.217	8.198	-0.049
H8	-12.906	8.401	0.781
N9	-6.254	-1.296	0.037
C10	-7.766	-3.561	0.043
C11	-3.591	-1.468	0.021
C12	-10.101	-3.661	-1.189
C13	-11.551	-5.842	-1.215
C14	-10.722	-8.044	-0.015
C15	-8.397	-7.951	1.237
C16	-6.959	-5.761	1.266
C17	-2.063	0.414	1.119
C18	0.539	0.236	1.094
C19	1.753	-1.842	-0.024
C20	0.235	-3.722	-1.125
C21	-2.363	-3.542	-1.106
N22	-12.149	-10.232	-0.059
C23	4.408	-2.066	-0.058
C24	6.663	-2.334	-0.123
C25	9.261	-2.737	-0.235
S26	11.450	-0.445	0.636
C27	13.980	-2.478	-0.006
C28	13.078	-4.798	-0.894
C29	10.458	-4.952	-1.020
C30	16.576	-1.954	0.331
C31	17.746	0.193	1.193
C32	20.519	0.182	1.414
O33	21.814	-1.608	0.874
O34	21.639	2.345	2.258
C35	16.426	2.417	1.900
N36	15.382	4.249	2.341
H37	-12.882	3.955	2.093
H38	-10.715	-0.071	2.192
H39	-4.646	3.088	-2.147
H40	-6.745	7.149	-2.122
H41	-10.788	-2.039	-2.219
H42	-13.344	-5.836	-2.207
H43	-7.703	-9.609	2.222
H44	-5.213	-5.770	2.323
H45	-2.922	2.006	2.061

H46	1.657	1.707	1.972
H47	1.125	-5.330	-2.023
H48	-3.449	-4.989	-2.047
H49	-11.533	-11.801	0.801
H50	14.335	-6.327	-1.407
H51	9.422	-6.597	-1.640
H52	17.865	-3.474	-0.140
H53	20.378	3.444	3.010
H54	-10.426	9.699	-0.891
H55	-13.817	-10.276	-0.954

Table2: The Cartesian coordinates of optimized geometry of Dye-2

ATOM	X	Y	Z
C1	-5.681	2.005	1.125
C2	-4.976	0.828	0.919
C3	-3.980	0.735	-0.053
C4	-3.722	1.867	-0.829
C5	-4.401	3.058	-0.607
C6	-5.402	3.164	0.379
N7	-6.078	4.363	0.617
N8	-3.317	-0.513	-0.287
C9	-4.148	-1.683	-0.240
C10	-1.932	-0.649	-0.351
C11	-5.093	-1.917	-1.235
C12	-5.958	-2.999	-1.160
C13	-5.915	-3.891	-0.070
C14	-4.926	-3.664	0.909
C15	-4.072	-2.574	0.826
C16	-1.053	0.369	0.067
C17	0.315	0.188	0.032
C18	0.882	-1.017	-0.418
C19	0.002	-2.024	-0.858
C20	-1.364	-1.848	-0.832
N21	-6.820	-4.939	0.042
C22	2.277	-1.225	-0.411
C23	3.478	-1.427	-0.372
C24	4.851	-1.664	-0.291
S25	5.954	-0.383	0.112
C26	7.321	-1.475	0.081
C27	6.902	-2.758	-0.263
C28	5.528	-2.869	-0.471
C29	8.657	-1.121	0.387
C30	9.191	0.085	0.745
C31	10.657	0.162	1.015
O32	11.400	-0.788	0.939
O33	11.145	1.381	1.358
C34	8.433	1.277	0.859
N35	7.894	2.298	0.983

H36	-6.454	2.005	1.876
H37	-5.223	-0.038	1.516
H38	-2.987	1.815	-1.621
H39	-4.168	3.898	-1.243
H40	-5.157	-1.239	-2.076
H41	-6.673	-3.141	-1.955
H42	-4.826	-4.328	1.754
H43	-3.338	-2.410	1.604
H44	-1.455	1.298	0.443
H45	0.964	0.982	0.378
H46	0.414	-2.953	-1.230
H47	-2.009	-2.641	-1.181
H48	7.595	-3.585	-0.335
H49	5.017	-3.786	-0.721
H50	9.381	-1.927	0.331
H51	10.445	2.051	1.373
C52	-6.010	5.417	-0.382
C53	-6.612	-5.953	1.061
C54	-7.302	4.327	1.407
C55	-7.612	-5.326	-1.113
H56	-6.504	5.144	-1.325
H57	-4.974	5.679	-0.599
H58	-6.491	6.310	0.013
H59	-5.691	-6.532	0.905
H60	-7.456	-6.639	1.054
H61	-6.566	-5.502	2.054
H62	-7.117	3.909	2.396
H63	-8.100	3.743	0.926
H64	-7.661	5.346	1.543
H65	-8.277	-6.136	-0.825
H66	-6.994	-5.667	-1.954
H67	-8.234	-4.498	-1.456

Table3: The Cartesian coordinates of optimized geometry of Dye-3

ATOM	X	Y	Z
C1	-5.140	2.115	1.649
C2	-4.547	0.871	1.515
C3	-3.922	0.509	0.320
C4	-3.926	1.413	-0.735
C5	-4.523	2.660	-0.614
C6	-5.128	3.045	0.593
N7	-5.683	4.299	0.774
H8	-6.280	4.403	1.576
N9	-3.297	-0.776	0.182
C10	-4.170	-1.901	0.032
C11	-1.915	-0.894	0.145
C12	-5.104	-1.933	-1.004
C13	-5.987	-2.992	-1.129
C14	-5.965	-4.064	-0.222
C15	-5.016	-4.031	0.811

C16	-4.145	-2.958	0.940
C17	-1.086	0.176	0.544
C18	0.287	0.073	0.492
C19	0.912	-1.104	0.040
C20	0.084	-2.176	-0.341
C21	-1.291	-2.080	-0.295
N22	-6.899	-5.085	-0.342
C23	2.315	-1.210	-0.034
C24	3.525	-1.319	-0.112
C25	4.903	-1.511	-0.204
S26	6.042	-0.268	0.229
C27	7.399	-1.321	-0.106
C28	6.946	-2.556	-0.565
C29	5.559	-2.669	-0.616
C30	8.762	-1.023	0.130
C31	9.372	0.067	0.684
C32	10.857	0.023	0.856
O33	11.539	-0.903	0.486
O34	11.430	1.085	1.476
C35	8.702	1.235	1.123
N36	8.265	2.243	1.501
H37	-5.615	2.383	2.586
H38	-4.565	0.173	2.342
H39	-3.444	1.139	-1.665
H40	-4.507	3.331	-1.459
H41	-5.142	-1.116	-1.713
H42	-6.707	-2.995	-1.940
H43	-4.965	-4.833	1.533
H44	-3.433	-2.943	1.755
H45	-1.537	1.091	0.898
H46	0.897	0.908	0.808
H47	0.541	-3.092	-0.693
H48	-1.894	-2.917	-0.610
H49	-7.395	-5.074	-1.221
H50	7.628	-3.355	-0.823
H51	5.022	-3.552	-0.926
H52	9.456	-1.810	-0.147
H53	10.769	1.749	1.726
C54	-5.848	5.272	-0.293
C55	-4.563	6.025	-0.637
C56	6.681	-6.424	0.191
C57	-5.654	-7.265	-0.568
H58	-6.609	5.980	0.035
H59	-6.247	4.785	-1.193
H60	-3.762	5.342	-0.921
H61	-4.216	6.599	0.223
H62	-4.731	6.711	-1.470
H63	-7.651	-6.927	0.183
H64	-6.404	-6.339	1.242
H65	-5.961	-7.412	-1.606
H66	-5.546	-8.249	-0.106
H67	-4.674	-6.783	-0.571

Table4: The Cartesian coordinates of optimized geometry of Dye-4

ATOM	X	Y	Z
C1	-5.422	2.088	1.439
C2	-4.848	0.839	1.258
C3	-3.913	0.621	0.241
C4	-3.603	1.678	-0.611
C5	-4.151	2.940	-0.419
C6	-5.084	3.170	0.605
N7	-5.639	4.418	0.805
H8	-6.381	4.499	1.479
N9	-3.296	-0.662	0.072
C10	-4.140	-1.816	-0.012
C11	-1.911	-0.788	-0.030
C12	-5.204	-1.857	-0.918
C13	-5.981	-2.996	-1.051
C14	-5.697	-4.157	-0.308
C15	-4.659	-4.094	0.634
C16	-3.907	-2.934	0.786
C17	-1.040	0.218	0.437
C18	0.329	0.077	0.346
C19	0.910	-1.085	-0.194
C20	0.040	-2.082	-0.673
C21	-1.329	-1.940	-0.602
N22	-6.448	-5.306	-0.495
C23	2.308	-1.258	-0.248
C24	3.513	-1.431	-0.302
C25	4.890	-1.655	-0.285
S26	6.003	-0.367	0.066
C27	7.370	-1.459	0.015
C28	6.942	-2.747	-0.303
C29	5.564	-2.859	-0.478
C30	8.707	-1.102	0.314
C31	9.247	0.110	0.641
C32	10.705	0.182	0.943
O33	11.441	-0.775	0.924
O34	11.192	1.410	1.260
C35	8.514	1.323	0.681
N36	8.005	2.365	0.710
H37	-6.139	2.235	2.240
H38	-5.118	0.024	1.917
H39	-2.901	1.520	-1.419
H40	-3.871	3.737	-1.092
H41	-5.418	-0.988	-1.528
H42	-6.804	-3.003	-1.756
H43	-4.436	-4.947	1.258
H44	-3.103	-2.912	1.511
H45	-1.450	1.111	0.884
H46	0.969	0.862	0.726
H47	0.458	-2.975	-1.119
H48	-1.961	-2.720	-0.996
H49	-6.961	-5.347	-1.360
H50	7.631	-3.577	-0.378
H51	5.046	-3.779	-0.702
H52	9.423	-1.917	0.298

H53	10.499	2.087	1.225
C54	-5.389	5.550	-0.066
C55	-6.200	6.773	0.341
C56	-5.879	7.990	-0.527
C57	-6.059	-6.592	0.063
C58	-6.882	-7.735	-0.520
C59	-6.554	-9.084	0.124
H60	-5.626	5.292	-1.106
H61	-4.322	5.802	-0.040
H62	-5.996	7.006	1.391
H63	-7.267	6.538	0.269
H64	-6.083	7.786	-1.581
H65	-4.825	8.267	-0.441
H66	-6.475	8.856	-0.233
H67	-6.200	-6.566	1.149
H68	-4.993	-6.787	-0.113
H69	-6.703	-7.790	-1.599
H70	-7.945	-7.512	-0.385
H71	-5.498	-9.336	-0.008
H72	-7.144	-9.888	-0.318
H73	-6.759	-9.069	1.197