

Table 1. Percentage contribution of donor, linker and acceptor groups towards HOMO and LUMO are given.

Molecules	Orbitals	Donor	Linker	Acceptor
1a	HOMO	89	9	2
	LUMO	2	35	63
1b	HOMO	85	12	3
	LUMO	2	25	73
1c	HOMO	83	14	3
	LUMO	2	17	81
1d	HOMO	87	10	3
	LUMO	2	18	80
1e	HOMO	86	11	3
	LUMO	3	18	79
2a	HOMO	95	4	1
	LUMO	1	4	95
2b	HOMO	95	4	1
	LUMO	1	3	96
2c	HOMO	96	3	1
	LUMO	0	0	100
2d	HOMO	96	3	1
	LUMO	0	0	100
2e	HOMO	96	3	1
	LUMO	0	0	100

Table2: Absorption , fluorescence energies and their corresponding oscillator strengths in gas Phase.

System	Absorption		Emission	
	Absorption (eV)	Oscillator strength	Fluorescence (eV)	Oscillator strength
1a	3.14	0.0942	2.51	0.0005
1b	2.79	0.1847	2.25	0.0000
1c	2.47	0.1929	1.94	0.0003
1d	2.22	0.2023	1.40	0.0007
1e	2.08	0.2227	1.29	0.0006
2a	3.58	0.0707	3.14	0.0439
2b	2.75	0.0453	2.14	0.0144
2c	2.23	0.0006	1.64	0.0003
2d	1.91	0.0007	1.11	0.0007
2e	1.69	0.0005	1.00	0.0002

Table3. HOMO, LUMO Energies

System	In Gas		In Cyclohexane		In Methanol	
	HOMO (eV)	LUMO (eV)	HOMO (eV)	LUMO (eV)	HOMO (eV)	LUMO (eV)
1a	-5.92	2.28	-5.93	-2.25	-5.96	-2.20
1b	-6.00	-2.77	-5.95	-2.68	-5.95	2.56
1c	-5.99	-3.12	-5.94	-3.01	-5.96	-2.82
1d	-5.65	-3.07	-5.61	-2.99	-5.64	-2.82
1e	-5.45	-3.02	-5.41	-2.95	-5.44	-2.80
2a	-5.78	-1.76	-5.75	-1.71	-5.75	-1.65
2b	-5.76	-2.55	-5.75	-2.42	-5.79	-2.22
2c	-5.77	-3.08	-5.77	-2.89	-5.82	-2.60
2d	-5.40	-3.06	-5.41	-2.88	-5.49	-2.59
2e	-5.16	-3.04	-5.18	-2.86	-5.29	-2.59

Table 4. Ionization potentials and electron affinities (Bothe vertical and adiabatic)

System	in Gas				in Cyclohexane				in Methanol			
	IP (A)	IP (V)	EA (A)	EA (V)	IP (A)	IP (V)	EA (A)	EA (V)	IP (A)	IP (V)	EA (A)	EA (V)
1a	7.274	7.006	-0.829	-1.081	6.254	6.566	-1.800	-1.567	5.544	5.851	-2.522	-2.297
1b	7.333	7.201	-1.343	-1.593	6.425	6.562	-2.259	-2.015	5.687	5.829	-2.891	-2.657
1c	7.328	7.238	-1.714	-1.918	6.459	6.556	-2.556	-2.352	5.736	5.848	-3.138	-2.914
1d	6.973	6.849	-1.687	-1.831	6.095	6.225	-2.466	-2.083	5.404	5.547	-3.129	-2.92
1e	6.708	6.580	-1.657	-1.738	5.871	5.990	-2.372	-2.316	5.236	5.341	-3.117	-2.907
2a	7.283	7.237	-0.252	-0.277	6.400	6.446	-1.062	-0.945	5.607	5.655	-1.864	-1.688
2b	7.270	7.188	-0.908	-1.067	6.384	6.453	-1.781	-1.620	5.639	5.691	-2.448	-2.290
2c	7.273	7.191	-1.450	-1.626	6.406	6.469	-2.268	-2.100	5.628	5.731	-2.827	-2.664
2d	6.865	6.705	-1.454	-1.555	5.961	6.106	-2.191	-2.092	5.283	5.418	-2.821	-2.658
2e	6.562	6.410	-1.424	-1.490	5.716	5.845	-2.190	-2.083	5.098	5.027	-2.819	-2.656