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

SUPPORTING INFORMATION

Unraveling the photophysical and semiconducting properties of color converter luminogens with aggregation induced emission characteristics

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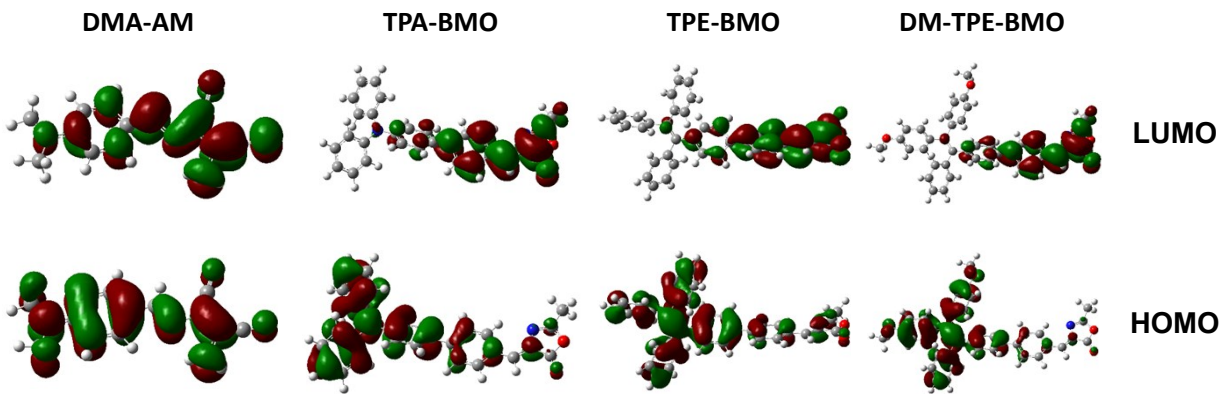

Figure S1. Shapes of HOMO and LUMO of the studied compounds calculated at the PBE0/6-31G** level in THF solution (isocontour plots, 0.02 au).

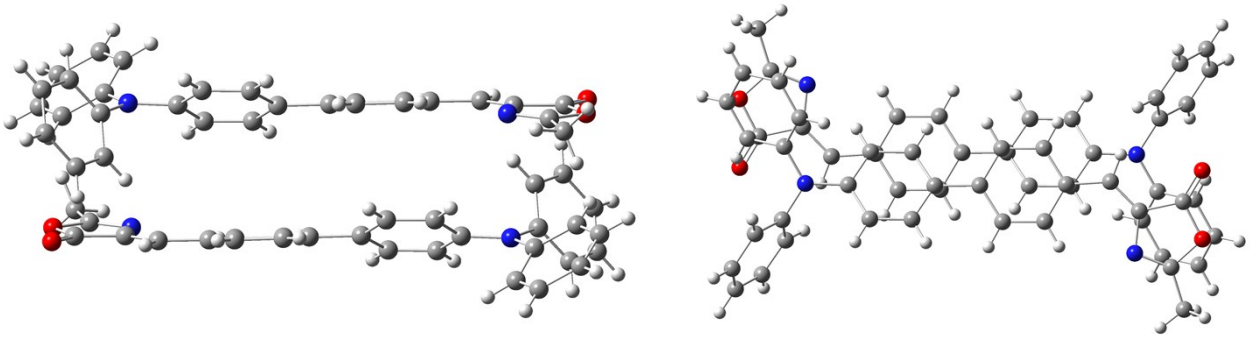

Figure S2. π-stacking arrangement in the TPA-BMO crystal.

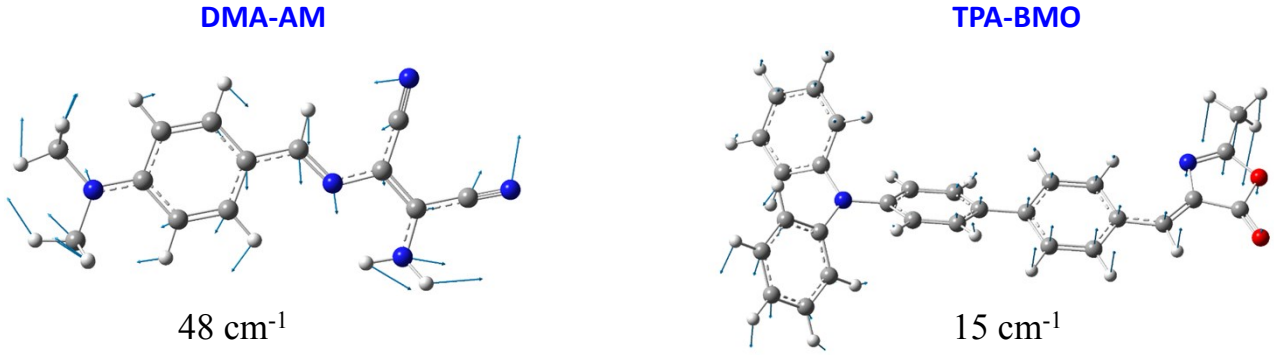

Figure S3. Atomic displacements of some selected normal modes (corresponding to high HR factor values) calculated for DMA-AM and TPA-BMO in THF solution at the PBE0/6-31G** level of theory.

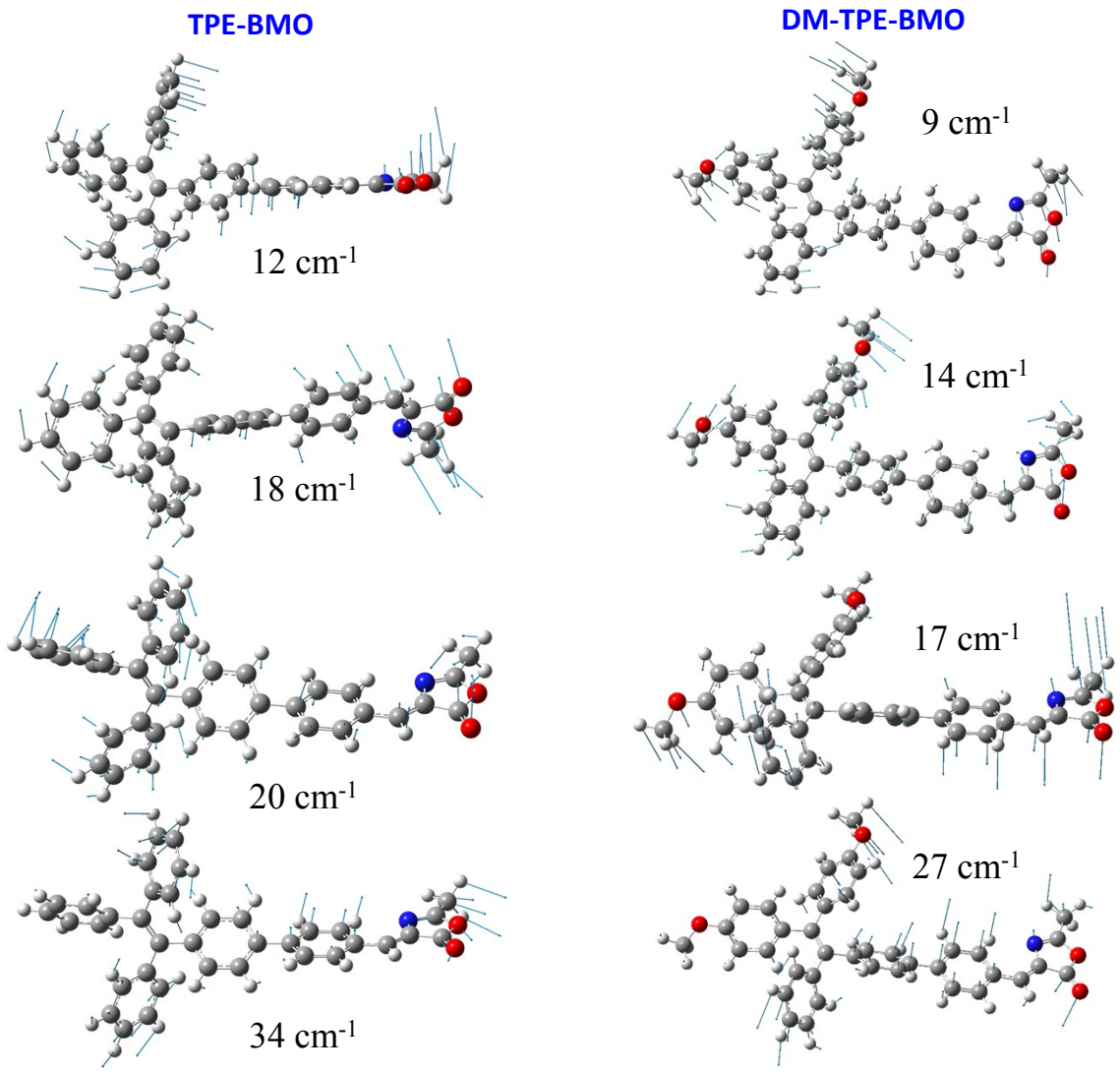

Figure S4. Atomic displacements of some selected normal modes (corresponding to high HR factor values) calculated for TPE-BMO and DM-TPE-BMO in THF solution at the PBE0/6-31G** level of theory.

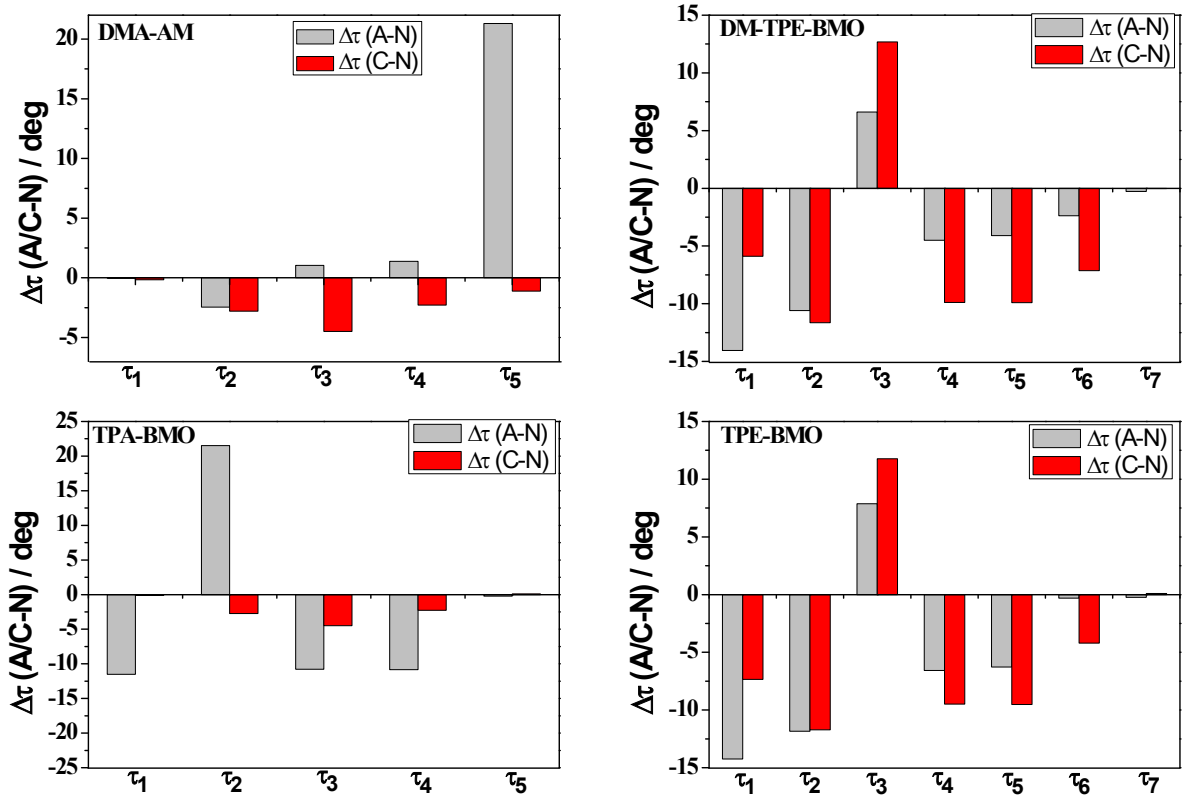

Figure S5. Variation of selected dihedral angles from neutral form (N) to anionic state (A) or cationic state (C) calculated at the B3LYP/6-31G** level of theory in the gas phase.

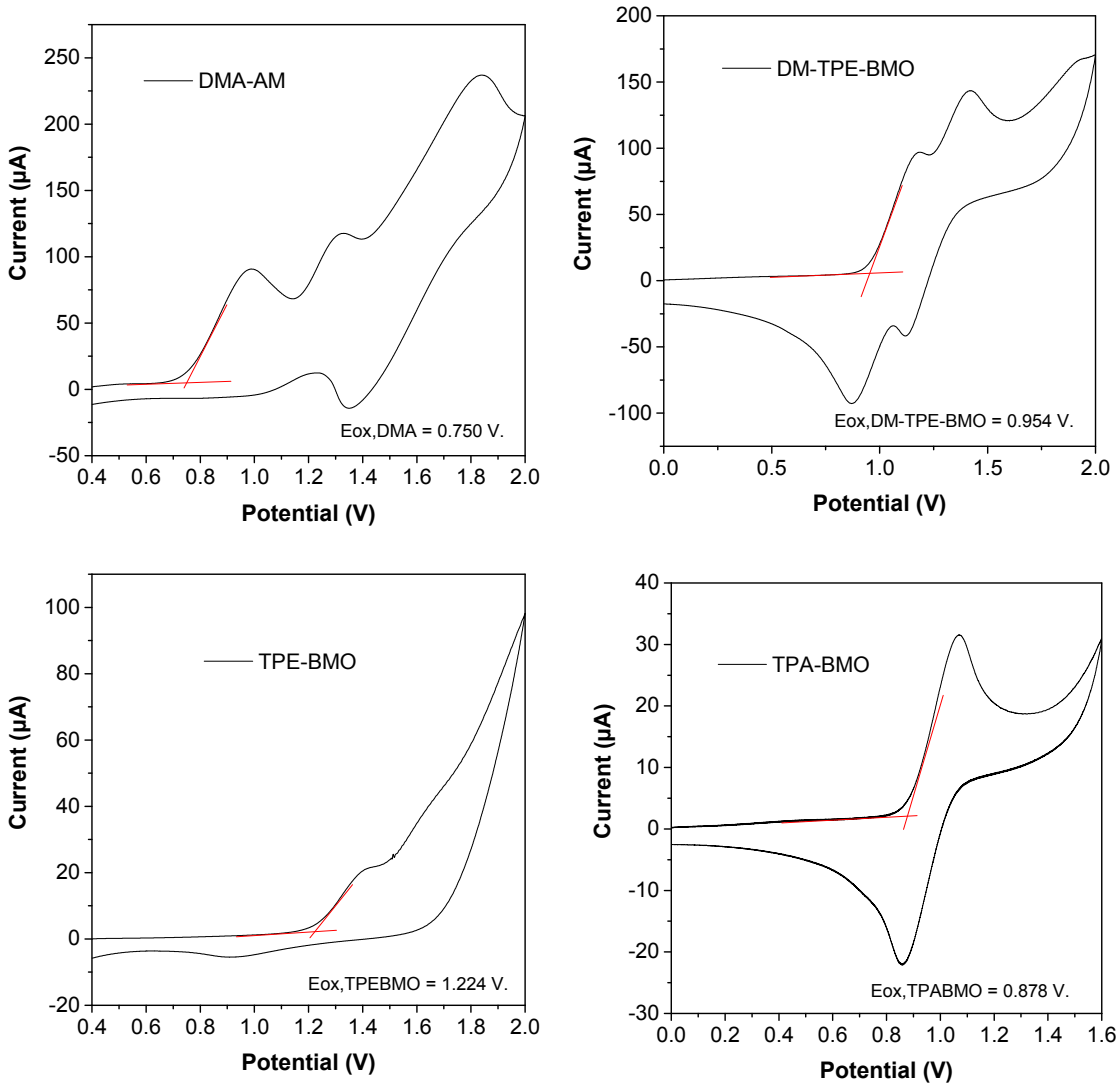

Figure S6. Cyclic voltammogram curves obtained for DMA-AM, TPA-BMO, TPE-BMO, and DM-TPE-BMO.

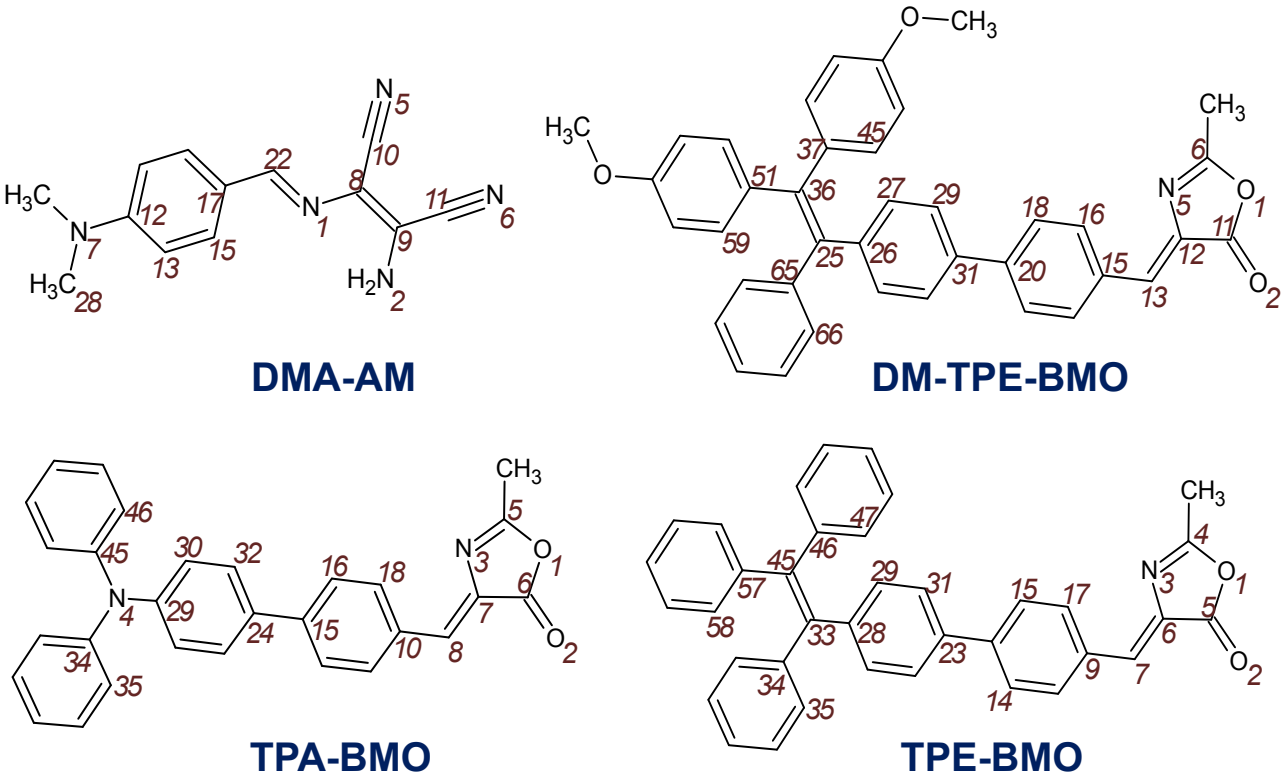

Figure S7. Molecular structures and the numbering of selected atoms for the investigated molecules.

Table S1. Selected structural parameters (bond lengths in Å, bond angles in degrees and inter-ring dihedral angles in degrees) calculated for the S_0 and S_1 states in THF solution at the PBE0/6-31G** level of theory (atom numbering is shown in **Figure 1**). $|\Delta(S_1\text{-}S_0)|$ is the numerical difference between a structural parameter calculated for the molecule in excited state with respect to the ground state. The numbering of atoms is shown in Figure S7.

Compound	BOND LENGTH				BOND ANGLE				DIHEDRAL ANGLE			
		S_0	S_1	$\|\Delta(S_1\text{-}S_0)\|$		S_0	S_1	$\|\Delta(S_1\text{-}S_0)\|$		S_0	S_1	$\|\Delta(S_1\text{-}S_0)\|$
DMA-AM	*C17-C22*	1.440	1.432	0.008	*C17-C22-N1*	123.09	120.81	2.28	*C15-C17-C22-N1*	-0.18	-0.55	0.37*
	C22-N1	1.293	1.321	0.028	*C22-N1-C8*	120.87	122.84	1.97	*C22-N1-C8-C10*	1.82	-0.06	1.88
	N1-C8	1.379	1.345	0.034	*N1-C8-C9*	117.58	117.93	0.35	*N1-C8-C9-N2*	3.82	4.01	0.19*
	C8-C10	1.427	1.422	0.005	*N1-C8-C10*	122.50	122.63	0.13	*C10-C8-C9-C11*	1.50	1.73	0.23*
	C8-C9	1.379	1.429	0.050	*C8-C9-C11*	120.12	121.73	1.61	*C13-C12-N7-C28*	-0.22	0.11	0.33
	C9-C11	1.429	1.403	0.026	*C8-C9-N2*	122.22	118.39	3.83				
	C9-N2	1.357	1.362	0.005	*C20-C12-N7*	121.33	121.07	0.26				
	C12-N7	1.362	1.362	0.000	*C12-N7-C28*	120.30	120.40	0.10				
TPA-BMO	***C24-C15***	1.472	1.459	0.013	*C24-C15-C16*	121.11	121.61	0.50	***C32-C24-C15-C16***	32.14	25.40	6.74
	C29-N4	1.404	1.403	0.001	*C30-C29-N4*	120.86	120.40	0.46	*C30-C29-N4-C45*	-34.42	-39.18	4.76*
	N4-C45	1.416	1.405	0.011	*C29-N4-C45*	120.42	119.89	0.53	*C29-N4-C45-C46*	-43.29	-37.52	5.77
	N4-C34	1.416	1.405	0.011	*C29-N4-C34*	120.39	119.86	0.53	*C29-N4-C34-C35*	-43.69	-37.62	6.07
	C10-C8	1.444	1.420	0.024	*C10-C8-C7*	129.70	129.43	0.27	*C18-C10-C8-C7*	0.50	-0.85	1.35*
	C8-C7	1.356	1.392	0.036	*C8-C7-C6*	122.26	122.85	0.59				
	C7-C6	1.472	1.443	0.029	*C7-C6-O2*	133.46	134.58	1.12				
	C7-N3	1.396	1.391	0.005	*C8-C7-N3*	129.38	128.39	0.99				
	C6-O2	1.203	1.221	0.018								
TPE-BMO	*C23-C14*	1.475	1.449	0.026	*C31-C23-C14*	121.09	121.80	0.71	*C31-C23-C14-C15*	-34.02	-18.83	15.19
	C28-C33	1.486	1.440	0.046	*C29-C28-C33*	121.46	121.87	0.41	*C29-C28-C33-C45*	-48.09	-30.08	18.01
	C33-C45	1.363	1.425	0.062	*C28-C33-C45*	122.56	121.72	0.84	*C28-C33-C45-C46*	-12.22	-29.54	17.32*
	C33-C34	1.488	1.471	0.017	*C33-C45-C46*	122.53	121.02	1.51	*C33-C45-C46-C47*	-48.96	-34.60	14.36
	C9-C7	1.445	1.421	0.024	*C33-C45-C57*	122.57	120.73	1.84	*C33-C45-C57-C58*	-48.77	-35.94	12.83
	C7-C6	1.355	1.382	0.027	*C28-C33-C34*	114.83	118.25	3.42	*C28-C33-C34-C35*	-46.64	-39.08	7.56
	C6-C5	1.472	1.450	0.022	*C17-C9-C7*	123.67	124.12	0.45	*C17-C9-C7-C6*	0.12	0.44	0.32*
	C6-N3	1.396	1.393	0.003	*C7-C6-C5*	122.25	122.61	0.36				
	C5-O2	1.203	1.215	0.012	*C7-C6-N3*	129.41	128.69	0.72				
DM-TPE-BMO	*C31-C20*	1.475	1.455	0.020	*C29-C31-C20*	121.08	121.63	0.55	***C29-C31-C20-C18***	33.59	22.38	11.21
	C26-C25	1.485	1.419	0.066	*C27-C26-C25*	121.51	121.63	0.12	*C27-C26-C25-C36*	-46.86	-32.77	14.09
	C25=C36	1.366	1.449	0.083	*C26-C25-C36*	122.60	121.62	0.98	*C26-C25-C36-C37*	-13.48	-27.62	14.14*
	C25-C65	1.488	1.469	0.019	*C25-C36-C37*	122.45	121.22	1.23	*C25-C36-C37-C45*	-46.23	-35.44	10.79
	C15-C13	1.445	1.420	0.025	*C25-C36-C51*	122.37	120.89	1.48	*C25-C36-C51-C59*	-47.03	-36.47	10.56
	C13-C12	1.355	1.387	0.032	*C26-C25-C65*	114.82	117.88	3.06	*C26-C25-C65-C66*	-46.56	-38.20	8.36
	C12-C11	1.472	1.445	0.027	*C16-C15-C13*	123.65	124.16	0.51	*C16-C15-C13-C12*	-0.06	-0.09	0.03*
	C12-N5	1.396	1.393	0.020	*C13-C12-C11*	122.26	122.75	0.49				
	C11-O2	1.203	1.219	0.066	*C13-C12-N5*	129.39	128.50	0.89				

* The dihedral angle increases after excitation.

Table S2. Selected structural parameters (bond lengths in Å, bond angles in degrees and inter-ring dihedral angles in degrees) calculated for the S_0 and S_1 states in solid phase at the PBE0/6-31G**//UFF level of theory (atom numbering shown in **Figure 1**). $|\Delta(S_1\text{-}S_0)|$ is the numerical difference between a structural parameter calculated for the molecule in excited state with respect to the ground state. The numbering of atoms is shown in Figure S7.

Compound	BOND LENGTH	BOND ANGLE	DIHEDRAL ANGLE

		S_0	S_1	$\lvert\Delta(S_1-S_0)\rvert$		S_0	S_1	$\lvert\Delta(S_1-S_0)\rvert$		S_0	S_1	$\lvert\Delta(S_1-S_0)\rvert$	Crystal [a]
	C17-C22	1.439	1.430	0.009	*C17-C22-N1*	123.63	121.80	1.83	*C15-C17-C22-N1*	3.34	2.31	1.03	1.65
	C22-N1	1.289	1.318	0.029	*C22-N1-C8*	119.55	120.43	0.88	*C22-N1-C8-C10*	4.09	4.05	0.04	-2.07
DMA-AM	*N1-C8*	1.381	1.351	0.030	*N1-C8-C9*	117.53	117.68	0.15	*N1-C8-C9-N2*	-4.32	-5.19	0.87*	3.11
	C8-C10	1.425	1.419	0.006	*N1-C8-C10*	121.50	121.75	0.25	*C10-C8-C9-C11*	-3.59	-5.12	1.53*	0.78
	C8-C9	1.372	1.418	0.046	*C8-C9-C11*	120.99	122.79	1.80	*C13-C12-N7-C28*	13.41	11.99	1.42	14.15
	C9-C11	1.423	1.402	0.021	*C8-C9-N2*	121.64	117.26	4.38					
	C9-N2	1.361	1.358	0.003	*C20-C12-N7*	120.89	120.28	0.61					
	C12-N7	1.369	1.373	0.004	*C12-N7-C28*	120.14	120.32	0.18					
	C24-C15	1.473	1.472	0.001	*C24-C15-C16*	121.42	121.81	0.39	*C32-C24-C15-C16*	25.54	26.87	1.33*	21.56
	C29-N4	1.403	1.418	0.015	*C30-C29-N4*	121.74	121.11	0.63	*C30-C29-N4-C45*	-33.57	-37.05	3.48*	-36.06
TPA-BMO	*N4-C45*	1.420	1.413	0.007	*C29-N4-C45*	120.01	119.70	0.31	*C29-N4-C45-C46*	-61.03	-55.89	5.14	-59.93
	N4-C34	1.411	1.387	0.024	*C29-N4-C34*	121.70	121.63	0.07	*C29-N4-C34-C35*	-32.70	-28.92	3.78	-37.34
	C10-C8	1.444	1.428	0.016	*C10-C8-C7*	130.05	129.40	0.65	*C18-C10-C8-C7*	4.23	4.12	0.11	7.18
	C8-C7	1.354	1.385	0.031	*C8-C7-C6*	121.73	121.91	0.18					
	C7-C6	1.472	1.450	0.022	*C7-C6-O2*	133.44	134.20	0.76					
	C7-N3	1.394	1.387	0.007	*C8-C7-N3*	129.73	129.22	0.51					
	C6-O2	1.198	1.212	0.014									
	C23-C14	1.474	1.459	0.015	*C31-C23-C14*	121.83	122.35	0.52	*C31-C23-C14-C15*	-33.63	-33.30	0.33	-30.43
	C28-C33	1.484	1.452	0.032	*C29-C28-C33*	122.31	123.39	1.08	*C29-C28-C33-C45*	-44.34	-37.53	6.81	-45.21
TPE-BMO	*C33=C45*	1.367	1.412	0.045	*C28-C33-C45*	122.81	122.73	0.08	*C28-C33-C45-C46*	-11.57	-16.53	4.96*	-10.50
	C33-C34	1.488	1.469	0.019	*C33-C45-C46*	122.71	121.49	1.22	*C33-C45-C46-C47*	-39.77	-34.77	5.00	-40.16
	C9-C7	1.445	1.425	0.020	*C33-C45-C57*	120.95	120.77	0.18	*C33-C45-C57-C58*	-49.23	-40.16	9.07	-50.21
	C7-C6	1.353	1.380	0.027	*C28-C33-C34*	115.22	116.10	0.88	*C28-C33-C34-C35*	-47.24	-42.53	4.71	-46.66
	C6-C5	1.476	1.454	0.022	*C17-C9-C7*	123.94	124.30	0.36	*C17-C9-C7-C6*	-4.51	-4.90	0.39*	-1.88
	C6-N3	1.395	1.390	0.005	*C7-C6-C5*	121.91	122.15	0.24					
	C5-O2	1.199	1.211	0.012	*C7-C6-N3*	129.40	128.85	0.55					
	C31-C20	1.474	1.463	0011	*C29-C31-C20*	120.67	121.24	0.57	*C29-C31-C20-C18*	20.11	16.56	3.55	18.85
	C26-C25	1.487	1.462	0025	*C27-C26-C25*	121.43	121.81	0.38	*C27-C26-C25-C36*	-45.15	-41.02	4.13	-45.24
	C25=C36	1.365	1.401	0036	*C26-C25-C36*	123.40	122.92	0.48	*C26-C25-C36-C37*	-14.77	-18.45	3.68*	-14.23
	C25-C65	1.486	1.466	0020	*C25-C36-C37*	120.10	119.90	0.20	*C25-C36-C37-C45*	-52.65	-46.67	5.98	-54.71
DM- TPE-BMO	*C15-C13*	1.442	1.422	0020	*C25-C36-C51*	121.01	120.97	0.04	*C25-C36-C51-C59*	-51.86	-42.36	9.50	-49.20
	C13-C12	1.354	1.381	0027	*C26-C25-C65*	113.83	115.67	1.84	*C26-C25-C65-C66*	-35.94	-33.88	2.06	-38.62
	C12-C11	1.473	1.450	0023	*C16-C15-C13*	122.81	123.34	0.53	*C16-C15-C13-C12*	-4.25	-2.25	2.00	-5.36
	C12-N5	1.394	1.389	0005	*C13-C12-C11*	122.48	122.58	0.10					
	C11-O2	1.198	1.211	0013	*C13-C12-N5*	128.86	128.32	0.54					

[a] Experimental crystallographic parameters (references [6,7])

* The dihedral angle increases after excitation.

Table S3. Selected structural parameters (bond lengths in Å, bond angles in degrees and inter-ring dihedral angles in degrees) calculated for the neutral, anionic and cationic species in gas phase at the B3LYP/6-31G** level of theory. |Δ(A-N)| is the numerical difference between a structural parameter calculated for the molecule in anionic form with respect to the neutral state. |Δ(C-N)| is the numerical difference between a structural parameter calculated for the molecule in cationic form with respect to the neutral state. The numbering of atoms is shown in Figure S7.

Compound		BOND LENGTH						BOND ANGLE						DIHEDRAL ANGLE					
		Neutral	Anion	Cation	$\lvert\Delta(A-N)\rvert$	$\lvert\Delta(C-N)\rvert$		Neutral	Anion	Cation	$\lvert\Delta(A-N)\rvert$	$\lvert\Delta(C-N)\rvert$		Neutral	Anion	Cation	$\lvert\Delta(A-N)\rvert$	$\lvert\Delta(C-N)\rvert$
DMA-AM	*C17-C22*	1.448	1.437	1.417	0.011	0.031	*C17-C22-N1*	123.31	122.48	122.55	0.83	0.76	τ_1	0.15	0.17	-0.01	0.02	0.16
	C22-N1	1.295	1.324	1.322	0.029	0.027	*C22-N1-C8*	120.93	123.76	120.34	2.83	0.59	τ_2	2.80	0.35	0.00	2.45	2.80
	N1-C8	1.388	1.356	1.352	0.032	0.036	*N1-C8-C9*	117.34	119.01	117.47	1.67	0.13	τ_3	4.48	5.53	-0.01	1.05*	4.49
	C8-C10	1.432	1.432	1.433	0.000	0.001	*N1-C8-C10*	121.98	121.26	123.09	0.72	1.11	τ_4	2.28	3.67	0.00	1.39*	2.28

	C8-C9	1.380	1.420	1.415	0.040	0.035	*C8-C9-C11*	121.42	123.79	120.74	2.37	0.68	τ_5	-1.00	-22.31	0.12	21.31*	1.12
	C9-C11	1.431	1.402	1.430	0.029	0.001	*C8-C9-N2*	121.75	118.31	121.30	3.44	0.45						
	C9-N2	1.373	1.424	1.336	0.051	0.037	*C20-C12-N7*	121.35	121.76	121.06	0.41	0.29						
	C12-N7	1.376	1.421	1.349	0.045	0.027	*C12-N7-C28*	120.29	120.96	121.01	0.67	0.72						
TPA-BMO	*C24-C15*	1.478	1.460	1.460	0.018	0.018	*C24-C15-C16*	121.22	122.14	121.25	-0.92	-0.03	τ_1	33.24	21.74	24.62	11.50	8.62
	C29-N4	1.414	1.436	1.390	0.022	0.024	*C30-C29-N4*	120.90	120.87	120.77	0.03	0.13	τ_2	-36.59	-58.11	-28.81	21.52*	7.78
	N4-C45	1.424	1.413	1.427	0.011	0.003	*C29-N4-C45*	120.32	119.04	120.83	1.28	-0.51	τ_3	-43.96	-33.17	-45.57	10.79	1.61*
	N4-C34	1.424	1.413	1.427	0.011	0.003	*C29-N4-C34*	120.30	119.04	120.82	1.26	-0.52	τ_4	-44.01	-33.18	-45.53	10.83	1.52*
	C10-C8	1.448	1.416	1.443	0.032	0.005	*C10-C8-C7*	129.91	124.60	128.92	5.31	0.99	τ_5	0.29	-0.12	0.30	0.41	0.01*
	C8-C7	1.358	1.398	1.362	0.040	0.004	*C8-C7-C6*	122.32	130.33	121.89	-8.01	0.43						
	C7-C6	1.479	1.444	1.490	0.035	0.011	*C7-C6-O2*	133.60	135.34	133.02	-1.74	0.58						
	C7-N3	1.403	1.401	1.390	0.002	0.013	*C8-C7-N3*	129.15	127.84	129.58	1.31	-0.43						
	C6-O2	1.202	1.222	1.197	0.020	0.005												
TPE-BMO	*C23-C14*	1.480	1.458	1.466	0.022	0.014	*C31-C23-C14*	121.23	122.25	121.35	-1.02	-0.12	τ_1	-34.56	-20.31	-27.22	14.25	7.34
	C28-C33	1.493	1.471	1.461	0.022	0.032	*C29-C28-C33*	121.65	122.37	121.85	-0.72	-0.20	τ_2	-48.59	-36.75	-36.88	11.84	11.71
	C33-C45	1.367	1.391	1.414	0.024	0.047	*C28-C33-C45*	122.73	123.50	121.85	-0.77	0.88	τ_3	-12.25	-20.13	-24.02	7.88*	11.77*
	C33-C34	1.496	1.494	1.477	0.002	0.019	*C33-C45-C46*	122.67	122.37	121.39	0.30	1.28	τ_4	-49.81	-43.24	-40.32	6.57	9.49
	C9-C7	1.449	1.421	1.456	0.028	0.007	*C33-C45-C57*	122.64	122.16	121.65	0.48	0.99	τ_5	-49.62	-43.35	-40.10	6.27	9.52
	C7-C6	1.358	1.389	1.360	0.031	0.002	*C28-C33-C34*	114.6	115.73	117.00	-1.13	-2.40	τ_6	-45.47	-45.16	-41.27	0.31	4.20
	C6-C5	1.479	1.450	1.489	0.029	0.010	*C17-C9-C7*	123.78	124.52	123.68	-0.74	0.10	τ_7	-0.27	-0.04	-0.33	0.23	0.06*
	C6-N3	1.403	1.402	1.393	0.001	0.010	*C7-C6-C5*	122.30	122.85	121.95	-0.55	0.35						
	C5-O2	1.202	1.218	1.197	0.016	0.005	*C7-C6-N3*	129.17	128.08	129.55	1.09	-0.38						
DM-TPE-BMO	*C31-C20*	1.478	1.458	1.470	0.020	0.008	*C29-C31-C20*	121.21	122.20	121.36	-0.99	-0.15	τ_1	34.61	20.56	28.72	14.05	5.89
	C26-C25	1.492	1.472	1.461	0.020	0.031	*C27-C26-C25*	121.70	122.28	121.86	-0.58	-0.16	τ_2	-47.58	-36.98	-35.94	10.60	11.64
	C25-C36	1.396	1.389	1.419	0.007	0.023	*C26-C25-C36*	122.75	123.51	121.80	-0.76	0.95	τ_3	-13.35	-19.96	-26.03	6.61*	12.68*
	C25-C65	1.496	1.495	1.476	0.001	0.020	*C25-C36-C37*	122.60	122.52	121.23	0.08	1.37	τ_4	-47.47	-42.97	-37.58	4.50	9.89
	C15-C13	1.449	1.420	1.449	0.029	0.000	*C25-C36-C51*	122.47	122.07	121.33	0.40	1.14	τ_5	-48.03	-43.93	-38.12	4.10	9.91
	C13-C12	1.358	1.391	1.358	0.033	0.000	*C26-C25-C65*	114.63	115.68	117.23	-1.05	-2.60	τ_6	-47.61	-45.24	-40.48	2.37	7.13
	C12-C11	1.479	1.449	1.487	0.030	0.008	*C16-C15-C13*	123.79	124.54	123.67	-0.75	0.12	τ_7	0.26	-0.01	0.28	0.27	0.02*
	C12-N5	1.403	1.402	1.397	0.001	0.006	*C13-C12-C11*	122.31	122.87	122.02	-0.56	0.29						
	C11-O2	1.202	1.219	1.198	0.017	0.004	*C13-C12-N5*	129.16	128.04	129.50	1.12	-0.34						

*The dihedral angle departs from zero from neutral to charged state.

Table S4. Vertical transition energies (E_{ab}^{C}), oscillator strength (f) and main components of the transitions (% Contribution) computed for a single molecule, three molecular dimers and a tetramer extracted from the crystal of DMA-AM (without further optimization) and shown in Figure 3(a).

Species	E_{ab}^{C} /eV(nm)	f [a]	% Contribution
Molecule 1	3.33 (373)	1.025	H→L (99.7)
	4.17 (298)	0.105	H-1→L (59.2), H→L+1 (37.3)
	4.43 (280)	0.048	H→L+2 (54.5), H-2→L (23.3)
	4.51 (275)	0.013	H→L+1 (92.0)
	4.77 (260)	0.146	H→L+1 (49.2), H-1→L (28.3) , H-2→L (11.0)
	4.93 (252)	0.014	H→L+3 (76.1), H-1→L+3 (10.8)
	4.96 (250)	0.036	H-2→L (54.1), H→L+2 (29.9)
	5.49 (226)	0.052	H-1→L+1 (88.4)
	5.90 (210)	0.081	H-4→L (73.7)
	6.32 (196)	0.050	H-1→L+1 (84.9)
	6.75 (184)	0.165	H-6→L (78.5)
	6.81 (182)	0.121	H-7→L (70.4), H-2→L+2 (18.9)
Dimer A	2.74 (453)	0.023	H→L+1 (52.6), H-1→L (46.9)
	3.34 (371)	1.513	H→L+1 (45.8), H-1→L (51.2)
	3.83 (324)	0.017	H-2→L (58.7), H-1→L+1 (20.7), H→L+2 (17.2)
	3.95 (314)	0.299	H→L+2 (68.5), H-2→L (26.5)
	4.27 (291)	0.066	H-2→L+1 (59.1), H-1→L+3 (12.2)
	4.34 (286)	0.062	H→L+4 (46.8), H-5→L (24.8)
	4.50 (275)	0.010	H-6→L (55.4), H-7→L+1 (32.2)
	4.56 (272)	0.086	H-1→L+3 (39.2), H→L+4 (29.3)
	4.65 (267)	0.086	H-4→L+1 (39.9), H-5→L (33.4), H-1→L+5 (15.3)
	4.76 (261)	0.084	H→L+6 (33.4), H-1→L+3 (32.1)
Dimer B	2.51 (494)	0.037	H→L (97.6)
	3.17 (391)	0.158	H→L+1 (62.4), H-1→L (36.6)
	3.31 (375)	1.167	H→L+1 (30.7), H-1→L (53.5)
	3.41 (363)	0.415	H-1→L+1 (85.1)
	4.13 (300)	0.185	H-2→L+1 (51.5), H→L+3 (36.6)
	4.17 (286)	0.068	H-3→L (54.7), H-1→L+2 (38.0)
	4.34 (286)	0.021	H-4→L (33.3), H→L+4 (15.4), H→L+3 (12.7)
	4.36 (284)	0.055	H-4→L (25.6), H→L+3 (20.7), H→L+4 (18.7)
	4.44 (279)	0.015	H-1→L+3 (14.9), H→L+4 (14.3) , H-4→L (13.0)
	4.48 (277)	0.019	H-4→L (22.5), H→L+4 (15.8), H→L+5 (12.8)
	4.51 (275)	0.011	H-6→L+1 (84.5)
	4.74 (262)	0.237	H-1→L+2 (22.5), H-3→L+1 (14.9), H-3→L (11.8)
	4.85 (256)	0.019	H→L+7 (61.3), H-4→L+1 (12.6)
Dimer C	2.51 (494)	0.037	H→L (97.6)
	3.17 (391)	0.158	H→L+1 (62.4), H-1→L (36.6)
	3.31 (375)	1.168	H-1→L (53.5), H→L+1 (30.7), H-1→L+1 (14.6)
	3.41 (364)	0.419	H-1→L+1 (84.9)
	4.13 (300)	0.185	H-2→L+1 (51.6), H→L+3 (36.6)
	4.17 (297)	0.069	H-3→L (54.7), H-1→L+2 (38.0)
	4.34 (286)	0.021	H-4→L (33.1), H→L+4 (15.4), H→L+3 (12.8)
	4.36 (284)	0.055	H-4→L (25.8), H→L+3 (20.5), H→L+4 (18.5)
	4.44 (279)	0.015	H-1→L+3 (14.8), H→L+4 (14.6), H-4→L (12.8)
	4.48 (277)	0.019	H-4→L (22.7), H→L+4 (15.8) , H→L+5 (12.6)
	4.51 (275)	0.011	H-6→L+1 (84.4)
	4.74 (262)	0.237	H-1→L+2 (22.7), H-3→L+1 (14.9) , H-3→L (11.9)
	4.85 (256)	0.019	H→L+7 (60.9), H-4→L+1 (12.5)

Tetramer	2.37 (522)	0.018	H→L+1 (77.4), H-1→L (9.3)
	2.39 (518)	0.040	H-1→L (69.7),H-2→L (15.2)
	2.70 (459)	0.014	H→L+2 (37.9),H-1→L+2 (23.8),H-2→L+1 (19.7)
	3.06 (405)	0.039	H-2→L+2 (66.9),H-2→L+1 16.3)
	3.19 (389)	0.040	H-3→L (76.6), H→L+3 (18.1)
	3.24 (382)	0.213	H→L+3 (29.2),H-1→L+2 (25.2), H-2→L+2 (22.3)
	3.29 (377)	0.064	H-3→L+1 (37.9),H→L+3 (23.8)
	3.39 (366)	1.401	H-1→L+3 (30.8),H→L+3 (24.6)
	3.43 (362)	0.952	H-1→L+3 (58.4)

Table S5. Selected normal modes ν_i of the ground state along with the vibrational reorganization energy and Huang-

Rhys (HR) factor calculated for the studied compounds in THF solution at the PBE0/6-31G** level of theory.

DMA-AM			TPA-BMO			TPE-BMO			DM-TPE-BMO		
ν_i (cm^{-1})	λ (eV)	HR	ν_i (cm^{-1})	λ (eV)	HR	ν_i (cm^{-1})	λ (eV)	HR	ν_i (cm^{-1})	λ (eV)	HR
29	1	0.28	15	4	2.15	12	9	6.04	9	5	4.48
48	10	1.68	20	1	0.40	18	54	24.18	14	11	6.33
272	1	0.03	41	3	0.59	20	18	7.25	17	19	9.01
388	1	0.02	98	5	0.41	34	37	8.77	27	16	4.78
425	1	0.02	276	8	0.23	38	1	0.21	33	11	2.69
479	3	0.05	318	5	0.13	47	1	0.17	38	2	0.42
535	3	0.05	344	2	0.05	48	9	1.51	39	1	0.21
540	4	0.06	414	1	0.02	58	3	0.42	49	1	0.16
567	2	0.03	423	1	0.02	59	2	0.27	56	1	0.14
669	4	0.05	430	1	0.02	65	1	0.12	65	4	0.50
788	1	0.01	626	1	0.01	66	7	0.85	85	13	1.23
896	1	0.01	630	3	0.04	70	16	1.84	87	10	0.93
986	4	0.03	714	1	0.01	94	1	0.09	99	4	0.33
1157	1	0.01	716	3	0.03	103	1	0.08	115	4	0.28
1192	4	0.03	764	2	0.02	257	4	0.13	129	1	0.06
1203	1	0.01	781	1	0.01	264	3	0.09	222	2	0.07
1265	1	0.01	843	1	0.01	300	1	0.03	245	4	0.13
1405	3	0.02	855	2	0.02	325	5	0.12	252	3	0.10
1410	10	0.06	956	6	0.05	333	1	0.02	289	1	0.03
1431	4	0.02	985	1	0.01	419	1	0.02	328	4	0.10
1489	1	0.01	1017	1	0.01	423	2	0.04	349	1	0.02
1592	2	0.01	1198	2	0.01	425	5	0.09	418	2	0.04
1601	22	0.11	1201	5	0.03	516	2	0.03	431	1	0.02
1658	37	0.18	1219	1	0.01	549	5	0.07	552	5	0.07
1702	3	0.01	1289	1	0.01	573	2	0.03	572	1	0.01
2372	12	0.04	1330	1	0.01	591	1	0.01	608	1	0.01
			1337	2	0.01	628	1	0.01	630	2	0.03
			1351	1	0.01	634	1	0.01	670	1	0.01
			1423	1	0.01	641	1	0.01	713	2	0.02
			1546	1	0.01	714	4	0.05	744	1	0.01
			1609	2	0.01	716	1	0.01	749	1	0.01
			1636	1	0.00	745	2	0.02	831	1	0.01
			1659	23	0.11	777	1	0.01	833	1	0.01
			1663	3	0.01	785	1	0.01	857	1	0.01
			1677	8	0.04	860	1	0.01	957	5	0.04
			1696	2	0.01	867	2	0.02	1169	5	0.03
			1738	10	0.05	956	3	0.03	1201	7	0.05
			1886	10	0.04	1018	1	0.01	1202	1	0.01

Table S6. HOMO and LUMO energy (E_{HOMO} and E_{LUMO}) and energy gap (E_{H-L}) calculated at the B3LYP/6-31G** level of theory in gas phase

Compound	E_{HOMO} (eV)	E_{LUMO} (eV)	E_{H-L} (eV)
DMA-AM	-5.32	-2.12	3.20
TPA-BMO	-5.06	-2.28	2.78
TPE-BMO	-5.37	-2.35	3.02
DM-TPE-BMO	-5.05	-2.29	2.75

Table S7. Summary of Electrochemical Parameters.

Compound	$\lambda_{onset.abs}$ (nm)	E_g (eV)	E_{ox} (eV)	E_{HOMO} (eV)	E_{LUMO} (eV)
DMA-AM	464	2.67	0.75	-5.20	-2.53
TPA-BMO	491	2.53	0.88	-5.33	-2.80
TPE-BMO	435	2.85	1.22	-5.67	-2.82
DM-TPE-BMO	455	2.73	0.95	-5.40	-2.67

E_g is estimated from the UV-vis absorption spectra. $E_g = hc/\lambda_{onest.abs} = 1240/\lambda_{onset.abs}$
E_{HOMO} is calculated from the oxidation potentials: $E_{HOMO} = -(E^{ox} - E(Fc/Fc^+)+4.8)$ eV
E_{LUMO} is deduced from the HOMO and E_g: $E_{LUMO} = E_{HOMO} - E_g$

Table S8. Harmonic vibrational wavenumbers (cm^{-1}) calculated for S_0 and S_1 states in THF solution (PBE0/6-31G**) in solution and in solid state (ONIOM: PBE0/6-31G**:UFF).

DMA-AM				**TPA-BMO**				**TPE-BMO**				**DM- TPE-BMO**			
Isolated molecule		Cluster		Isolated molecule		Cluster		Isolated		Cluster		Isolated		Cluster	
S_0	S_1	S_0	S_1	S_0	S_1	S_0	S_1	S_0	S_1	S_0	S_1	S_0	S_1	S_0	S_1
32	31	54	102	14	15	80	78	12	12	66	68	10	9	65	66
36	36	60	103	19	20	85	84	18	17	70	78	14	16	69	70
50	51	67	111	24	26	87	86	20	21	77	80	18	18	71	71
70	59	82	121	36	46	95	96	34	33	80	81	27	26	72	75
82	81	91	139	38	49	99	101	38	38	86	87	33	36	79	81
88	111	92	144	47	53	117	119	47	50	94	94	37	40	82	84
113	113	104	150	60	65	121	124	48	59	96	96	40	44	84	87
132	134	107	164	65	70	126	131	58	60	103	102	46	51	97	97
135	134	114	199	72	81	131	133	59	66	110	111	49	57	104	100
181	187	127	207	90	93	139	141	65	71	114	116	55	59	114	114
189	190	144	245	97	106	142	143	66	73	122	124	59	71	119	118
209	202	149	257	112	112	154	161	69	90	133	133	64	78	128	126
261	259	158	270	133	132	165	168	91	95	135	133	85	87	133	134
265	267	169	271	153	155	173	172	94	106	143	143	87	99	138	140
272	279	200	305	160	160	181	191	103	110	149	147	94	101	147	147
278	308	208	316	180	186	213	216	120	124	154	158	99	112	150	156
339	331	238	354	201	212	220	225	135	136	174	177	106	114	153	159
380	363	265	368	220	228	238	241	159	157	189	192	115	123	162	164
388	374	273	380	242	244	251	249	175	178	193	197	130	135	172	172
426	386	279	420	249	251	269	268	176	186	204	204	150	151	173	175
433	414	296	429	276	276	285	285	180	194	220	223	156	163	182	184
443	427	309	438	289	284	310	299	208	217	239	238	165	172	186	187
479	462	381	478	318	317	326	326	231	235	251	252	174	178	195	190
509	480	399	497	328	327	335	333	242	240	262	260	180	188	203	204
527	509	428	518	344	345	358	354	258	259	270	266	187	195	210	216
536	521	438	530	379	365	391	377	260	267	273	274	207	212	212	221
539	532	445	539	414	414	419	418	264	274	279	281	215	222	228	228
568	535	476	574	419	415	432	425	284	284	298	292	221	225	239	240
581	568	487	594	420	417	435	434	300	305	311	311	245	240	244	243
648	627	507	638	422	422	441	437	325	325	338	333	251	246	255	246

669	636	533	642	430	427	451	443	333	331	343	337	254	252	258	258
681	675	545	669	442	435	454	450	386	362	385	372	259	265	270	269
726	724	575	728	448	449	459	459	395	404	407	406	279	277	279	272
742	730	578	732	499	470	507	480	415	410	418	416	289	287	302	295
789	787	638	794	521	505	529	515	416	413	425	422	297	300	322	318
818	798	654	797	523	512	533	531	418	419	430	424	327	326	330	322
838	828	675	822	540	548	552	560	419	423	435	434	337	333	352	351
896	866	697	864	574	570	579	573	423	424	439	440	349	343	368	355
963	880	737	888	574	572	586	579	425	430	449	444	363	354	376	362
982	965	750	953	626	620	631	621	463	442	468	451	381	368	387	381
982	968	798	958	628	622	633	628	487	465	497	475	404	403	412	411
986	973	820	987	630	626	636	630	497	483	505	490	416	415	424	424
1012	991	845	1012	634	631	641	639	516	496	521	506	417	422	436	426
1021	1005	906	1029	642	638	647	645	549	513	558	535	425	423	443	435
1091	1092	956	1099	649	650	654	656	564	545	566	561	427	431	447	445
1140	1120	981	1141	655	652	662	657	573	560	583	564	431	434	450	447
1142	1139	997	1154	675	661	681	663	591	572	596	581	438	436	457	457
1157	1153	1018	1163	699	693	703	695	598	597	600	597	470	457	473	461
1193	1177	1020	1174	713	700	721	708	627	622	632	627	478	470	476	473
1205	1182	1035	1205	714	703	723	717	628	623	633	628	482	476	481	480
1215	1204	1100	1210	716	711	732	722	631	625	636	630	501	485	506	488
1265	1244	1161	1252	737	722	742	730	634	627	640	632	527	512	531	522
1300	1284	1167	1296	761	743	768	753	641	637	645	640	530	518	544	526
1309	1311	1170	1323	763	749	768	756	645	643	651	649	552	541	559	546
1352	1329	1211	1344	774	761	783	766	653	651	657	654	556	545	568	555
1406	1376	1221	1378	781	781	787	792	658	655	661	658	572	557	575	571
1410	1390	1234	1396	782	783	804	805	675	666	679	666	580	567	589	580
1431	1425	1277	1419	843	811	853	824	691	687	695	693	588	587	594	587
1442	1435	1309	1441	843	831	860	855	705	693	707	697	608	605	608	607
1449	1447	1321	1457	852	843	864	858	714	703	718	710	629	625	634	629
1485	1463	1360	1473	854	847	868	861	716	708	718	712	630	626	637	632
1491	1478	1415	1486	859	849	876	870	718	712	724	716	639	634	644	641
1492	1481	1425	1494	865	853	878	875	720	713	732	724	644	639	652	650
1498	1487	1442	1502	878	858	890	875	745	729	749	738	647	645	654	653
1522	1497	1452	1516	907	868	908	887	750	745	755	747	649	648	656	654
1534	1508	1460	1524	918	888	925	890	768	755	776	762	655	650	663	660
1592	1527	1495	1547	921	928	935	934	777	758	780	764	670	666	673	666

1601	1530	1504	1556	949	935	954	939	783	775	792	782	675	670	680	670
1613	1561	1508	1560	953	949	960	952	785	785	797	799	702	694	709	701
1658	1566	1512	1577	954	953	965	962	799	801	816	815	713	710	718	717
1665	1609	1553	1617	956	965	970	965	840	821	850	830	717	712	725	720
1702	1665	1564	1665	976	972	984	967	857	829	862	848	729	727	734	731
2341	2279	1599	2311	982	980	994	1000	859	842	864	857	744	732	749	735
2372	2309	1612	2334	984	986	996	1002	864	855	867	858	748	744	755	750
3037	3044	1629	3034	984	994	1001	1006	866	857	869	861	757	750	759	752
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3077	3109	1696	3101	1004	995	1011	1010	867	860	878	872	783	765	786	769
3101	3111	1716	3115	1004	1002	1015	1012	869	865	896	885	785	788	799	804
3102	3118	2363	3124	1009	1008	1021	1012	887	867	899	886	806	809	810	814
3185	3200	2393	3199	1012	1013	1024	1018	891	896	903	889	811	816	815	816
3194	3207	3035	3217	1017	1014	1025	1025	907	897	903	894	830	821	836	819
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				1150	1147	1153	1148	992	996	1005	1002	898	883	903	889
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