

## Supporting Information

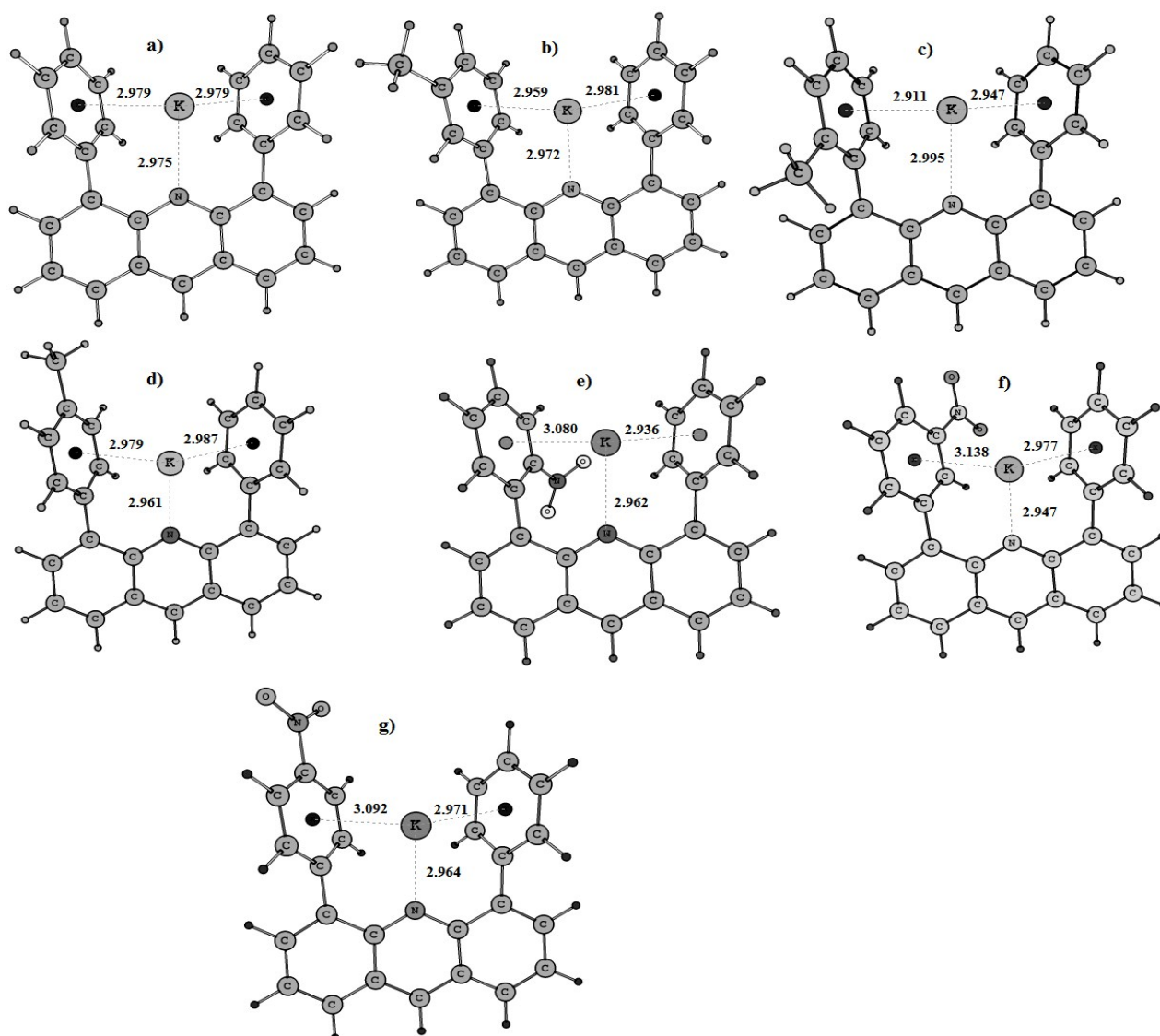
### Cation- $\pi$ Interaction in Cofacial Molecular Dyads: A DFT and TDDFT Study

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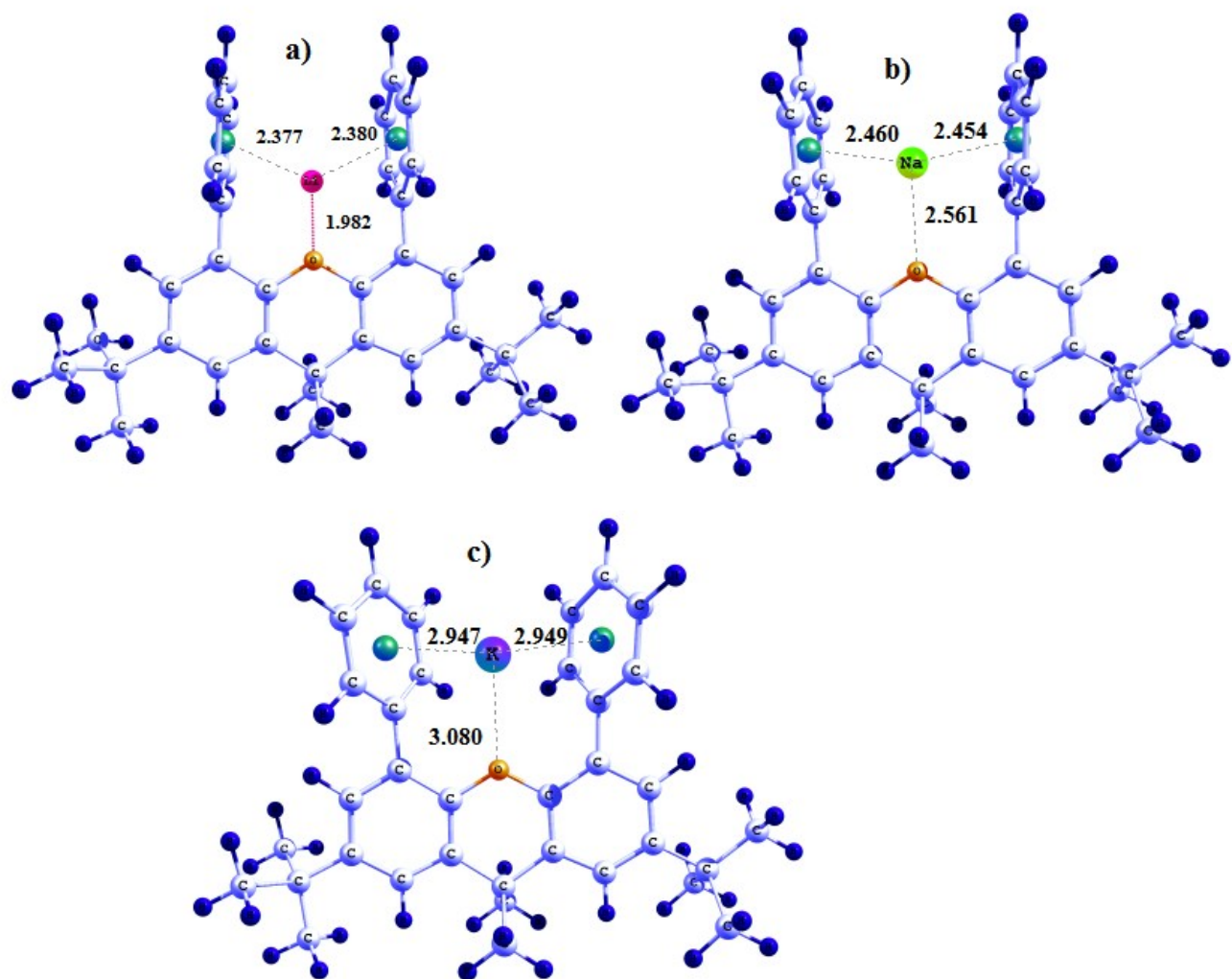
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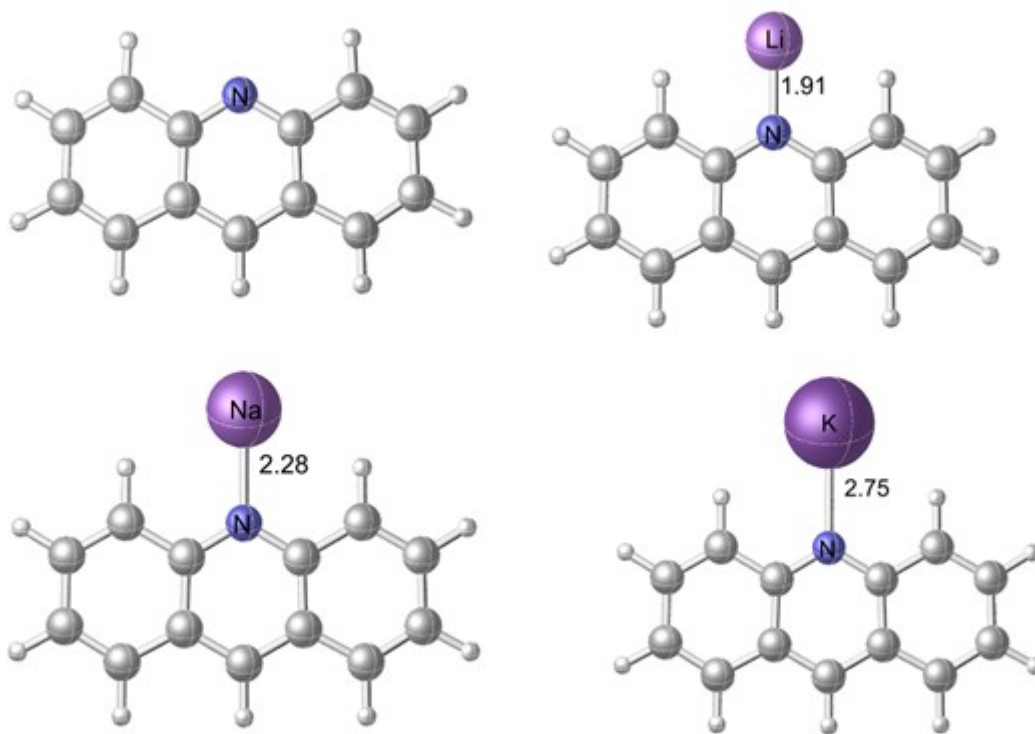
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**Figure S1.** Cation- $\pi$  complexes of  $K^+$  with  $-CH_3$  and  $-NO_2$  group substituted at different position of the phenyl ring. (b-d) are  $-CH_3$  substituted  $K^+@BPA$  complexes, (e-g) are  $-NO_2$  substituted  $K^+@BPA$  complexes.



**Figure S2.** Cation- $\pi$  complex of a) Li<sup>+</sup> b) Na<sup>+</sup> and c) K<sup>+</sup> with the reported molecular dyad.



**Figure S3.** Optimized geometries of acridine moiety and the co-ordinated compounds of acridine with cations (Li<sup>+</sup>, Na<sup>+</sup>, K<sup>+</sup>)



**Table S1.** Interaction energy (in kcal/mol) of the cation- $\pi$  complexes in gas phase and in various solvents using B3LYP/6-31+G (d,p)

Sl.No.	Complex	Gas Phase	CCl <sub>4</sub> ( $\epsilon=2.23$ )	Chloroform ( $\epsilon=4.71$ )	DCM ( $\epsilon=8.93$ )	Acetone ( $\epsilon=20.49$ )	Ethanol ( $\epsilon=24.85$ )	Methanol ( $\epsilon=32.61$ )	DMSO ( $\epsilon=46.83$ )	Water ( $\epsilon=78.36$ )
1	Li <sup>+</sup> @BPA	-79.53	-31.19	-5.01	-0.79	1.34	2.21	3.92	4.49	4.96
2	m-CH <sub>3</sub> -Li <sup>+</sup> @BPA	-79.51	-30.97	-10.52	-2.14	2.91	1.48	4.30	4.99	5.63
3	o-CH <sub>3</sub> -Li <sup>+</sup> @BPA	-80.84	-32.22	-11.79	-3.48	1.45	1.13	2.79	3.46	4.06
4	p-CH <sub>3</sub> -Li <sup>+</sup> @BPA	-80.87	-32.45	-12.15	-3.91	1.00	1.68	2.33	3.00	3.60
5	m-NO <sub>2</sub> -Li <sup>+</sup> @BPA	-72.04	-24.74	-5.41	2.22	6.63	4.24	7.81	8.40	8.92
6	o-NO <sub>2</sub> -Li <sup>+</sup> @BPA	-88.31	-31.47	-10.73	-2.16	3.08	1.80	4.54	5.28	5.96
7	p-NO <sub>2</sub> -Li <sup>+</sup> @BPA	-70.64	-24.19	-5.44	1.84	5.96	6.56	7.05	7.58	8.05
8	Na <sup>+</sup> @BPA	-59.06	-23.00	-7.99	-1.92	1.73	2.21	2.74	3.25	3.71
9	m-CH <sub>3</sub> -Na <sup>+</sup> @BPA	-60.15	-23.90	-8.83	-2.71	1.00	1.48	2.02	2.55	3.02
10	o-CH <sub>3</sub> -Na <sup>+</sup> @BPA	-60.54	-24.29	-9.22	-3.09	0.63	1.13	1.67	2.20	2.69
11	p-CH <sub>3</sub> -Na <sup>+</sup> @BPA	-60.26	-23.94	-8.76	-2.56	1.19	1.68	2.23	2.76	3.24
12	m-NO <sub>2</sub> -Na <sup>+</sup> @BPA	-50.66	-17.27	-4.09	0.98	3.87	4.24	4.64	5.02	5.37
13	o-NO <sub>2</sub> -Na <sup>+</sup> @BPA	-65.77	-22.57	-8.03	-2.16	1.34	1.80	2.30	2.79	3.23
14	p-NO <sub>2</sub> -Na <sup>+</sup> @BPA	-49.54	-15.51	-2.01	3.19	6.18	6.56	6.98	7.38	7.74
15	K <sup>+</sup> @BPA	-39.77	-16.93	-7.56	-3.75	-1.44	-1.14	-0.80	-0.47	-0.17
16	m-CH <sub>3</sub> -K <sup>+</sup> @BPA	-40.59	-17.53	-8.05	-4.18	-1.81	-1.50	-1.15	-0.81	-0.49
17	o-CH <sub>3</sub> -K <sup>+</sup> @BPA	-39.87	-16.54	-6.95	-3.04	-0.62	-0.29	0.07	0.43	0.75
18	p-CH <sub>3</sub> -K <sup>+</sup> @BPA	-40.70	-17.53	-8.01	-4.12	-1.76	-1.44	-1.09	-0.75	-0.44
19	m-NO <sub>2</sub> -K <sup>+</sup> @BPA	-33.26	-11.85	-3.54	-0.35	1.49	1.73	1.99	2.24	2.46
20	o-NO <sub>2</sub> -K <sup>+</sup> @BPA	-43.23	-12.99	-4.08	-0.61	1.41	1.68	1.96	2.24	2.49
21	p-NO <sub>2</sub> -K <sup>+</sup> @BPA	-31.73	-10.97	-3.11	-0.18	1.46	1.67	1.89	2.10	2.29

**Table S2- TDDFT analysis in Gas Phase and in different solvent systems**

<b>In gas phase</b>				
Complex	$\lambda_{\max}$	$f$	FMO	orbital contribution
BPA	363.59	0.1867	HOMO→LUMO	0.69483
	253.47	0.3735	HOMO→LUMO+1	0.50656
	235.88	0.9821	HOMO→LUMO+2	0.54470
m-CH <sub>3</sub> -@BPA	363.19	0.1862	HOMO→LUMO	0.69480
	253.34	0.339	HOMO→LUMO+1	0.48064
	236.09	0.525	HOMO→LUMO+2	0.41793
o-CH <sub>3</sub> -@BPA	358.99	0.1681	HOMO→LUMO	0.69434
	247.95	0.5352	HOMO→LUMO+2	0.44104
			HOMO→LUMO+1	0.38789
	235.76	0.7171	HOMO→LUMO+2	0.45284
HOMO→LUMO+1			0.38789	
p-CH <sub>3</sub> -@BPA	365	0.1967	HOMO→LUMO	0.69342
	254.07	0.2861	HOMO→LUMO+1	0.40933
	236.42	0.9168	HOMO→LUMO+2	0.52578
m-NO <sub>2</sub> -@BPA	358.96	0.1828	HOMO→LUMO	0.67698
	253.22	0.2754	HOMO→LUMO+2	0.55065
o-NO <sub>2</sub> -@BPA	358.96	0.1461	HOMO→LUMO	0.58842
	308.17	0.0581	HOMO-3→LUMO+1	0.30371
	269.69	0.0322	HOMO-1→LUMO+1	0.36966
p-NO <sub>2</sub> -@BPA	363.95	0.2233	HOMO→LUMO	0.63735
	302.01	0.11	HOMO→LUMO+1	0.50748
	257.76	0.2389	HOMO-1→LUMO+1	0.48816
Li <sup>+</sup> @BPA	357.17	0.1211	HOMO→LUMO	0.69661
	247.39	0.3038	HOMO→LUMO+1	0.53330
				0.35982
	235.89	0.522	HOMO→LUMO+2	0.32347
m-CH <sub>3</sub> -Li <sup>+</sup> @BPA	357.48	0.1235	HOMO→LUMO	0.6973
	236.25	0.4225	HOMO→LUMO+1	0.4043
	235.31	0.4794	HOMO→LUMO+3	0.45792
o-CH <sub>3</sub> -Li <sup>+</sup> @BPA	354.34	0.117	HOMO→LUMO	0.69727
	306.49	0.0905	HOMO-1→LUMO+1	0.59186
	235.66	0.667	HOMO→LUMO+2	0.4445
HOMO→LUMO+1			0.33813	

p-CH <sub>3</sub> -Li <sup>+</sup> @BPA	354.73	0.1230	HOMO→LUMO	0.69696
	241	0.4664	HOMO→LUMO+1	0.44511
	231.89	0.4204	HOMO→LUMO+3	0.47462
m-NO <sub>2</sub> -Li <sup>+</sup> @BPA	356.84	0.1299	HOMO→LUMO	0.66979
	257.74	0.1796	HOMO→LUMO+2	0.61491
	238.54	0.2878	HOMO-6→LUMO+1	0.36004
o-NO <sub>2</sub> -Li <sup>+</sup> @BPA	355.24	0.1188	HOMO→LUMO+1	0.67847
	306.54	0.0998	HOMO-1→LUMO+1	0.57916
	266.27	0.0228	HOMO-5→LUMO	0.37753
p-NO <sub>2</sub> -Li <sup>+</sup> @BPA	356.01	0.1371	HOMO→LUMO	0.67417
	306.51	0.0933	HOMO-1→LUMO	0.56666
	238.47	0.7961	HOMO→LUMO+3	0.4059
Na <sup>+</sup> @BPA	349.84	0.1184	HOMO→LUMO	0.69668
	237.16	1.2756	HOMO→LUMO+2	0.57457
m-CH <sub>3</sub> -Na <sup>+</sup> @BPA	349.98	0.1202	HOMO→LUMO	0.69667
	305.87	0.0783	HOMO-1→LUMO	0.58193
	237.42	1.1901	HOMO→LUMO+1	0.49529
o-CH <sub>3</sub> -Na <sup>+</sup> @BPA	350.68	0.118	HOMO→LUMO	0.69677
			HOMO→LUMO+1	0.44215
	238.54	0.5005	HOMO→LUMO+2	0.4269
	237.25	0.6207	HOMO→LUMO+2	0.45102
p-CH <sub>3</sub> -Na <sup>+</sup> @BPA	349.9	0.1219	HOMO→LUMO	0.6967
	305.89	0.0787	HOMO-1→LUMO	0.58311
			HOMO→LUMO+1	0.47789
	237.34	1.2767	HOMO-1→LUMO	0.34783
			HOMO→LUMO+1	0.54688
m-NO <sub>2</sub> -Na <sup>+</sup> @BPA	354.86	0.1368	HOMO→LUMO	0.42937
			HOMO→LUMO+2	
	256.7	0.1184		0.58734
			HOMO→LUMO+3	0.3813
	239.21	0.4624	HOMO→LUMO+5	0.313
o-NO <sub>2</sub> -Na <sup>+</sup> @BPA	354.59	0.1272	HOMO→LUMO+1	0.68425
			HOMO-1→LUMO+1	
	305.83	0.0954		0.56409
			HOMO→LUMO+3	0.43991
	243.12	0.537	HOMO→LUMO+4	0.33026
p-NO <sub>2</sub> -Na <sup>+</sup> @BPA	350.31	0.1243	HOMO→LUMO+1	0.69632
	242.79	0.577	HOMO→LUMO+2	0.61573

			HOMO→LUMO+3	0.41762
	237.56	0.4446	HOMO-5→LUMO+1	0.40079
K+@BPA	358.34	0.1468	HOMO→LUMO	0.695
	252.35	0.4234	HOMO→LUMO+3	0.47908
	232.2	0.5642	HOMO→LUMO+1	0.37179
m-CH <sub>3</sub> -K+@BPA	356.33	0.1464	HOMO→LUMO	0.69492
	251.59	0.4318	HOMO→LUMO+2	0.52307
			HOMO→LUMO+4	0.32451
	232.59	0.7459	HOMO→LUMO+5	0.32038
o-CH <sub>3</sub> -K+@BPA	355.76	0.1371	HOMO→LUMO	0.69553
	251.11	0.3843	HOMO→LUMO+1	0.43527
	233.16	0.8888	HOMO→LUMO+4	0.46985
p-CH <sub>3</sub> -K+@BPA	356.97	0.1502	HOMO→LUMO	0.69472
	251.36	0.4232	HOMO→LUMO+2	0.51851
			HOMO→LUMO+5	0.36163
	232.37	0.7829	HOMO→LUMO+4	0.32424
m-NO <sub>2</sub> -K+@BPA	358.32	0.1556	HOMO→LUMO+1	0.58872
	305.99	0.0814	HOMO-1→LUMO+1	0.45259
	246.05	0.3285	HOMO→LUMO+4	0.52107
o-NO <sub>2</sub> -K+@BPA	355.66	0.132	HOMO→LUMO+1	0.69383
	307.06	0.0677	HOMO-1→LUMO+1	0.56276
	259.73	0.1649	HOMO→LUMO+2	0.54042
p-NO <sub>2</sub> -K+@BPA	358.69	0.1814	HOMO→LUMO	0.57214
	304.13	0.1135	HOMO→LUMO+1	0.52001
			HOMO→LUMO+4	0.34887
	247.45	0.4094	HOMO→LUMO+3	0.33443
<b>In CCl<sub>4</sub></b>				
Complex	$\lambda_{\max}$	$f$	FMO	orbital contribution
BPA	367.61	0.2596	HOMO→LUMO	0.6956
	256.97	0.8017	HOMO→LUMO+1	0.5645
	242.41	0.9102	HOMO→LUMO+2	0.61146
	235.62	0.3292	HOMO→LUMO+3	0.57981
m-CH <sub>3</sub> -@BPA	367.21	0.2589	HOMO→LUMO	0.69557
	256.45	0.7431	HOMO→LUMO+1	0.52415
	242.26	0.8812	HOMO→LUMO+2	0.61051
o-CH <sub>3</sub> -@BPA	362.62	0.2344	HOMO→LUMO	0.61051
	252.61	1.098	HOMO→LUMO+1	0.49752
	240.48	0.6433	HOMO→LUMO+2	0.57564



p-CH <sub>3</sub> -@BPA	369.11	0.2716	HOMO→LUMO	0.69408
	257.38	0.8152	HOMO→LUMO+1	0.54316
	257.38	0.8287	HOMO→LUMO+2	0.5993
	236.42	0.3693	HOMO→LUMO+3	0.50607
m-NO <sub>2</sub> -@BPA	365.88	0.2579	HOMO→LUMO	0.50265
	260.91	0.0984	HOMO-5→LUMO	0.31155
	256.22	0.6167	HOMO→LUMO+2	0.5368
o-NO <sub>2</sub> -@BPA	365.05	0.181	HOMO→LUMO	0.55301
	308.74	0.0985	HOMO-2→LUMO+1	0.47417
	264.51	0.0669	HOMO-6→LUMO	0.39538
	256.7	0.0697	HOMO-2→LUMO	0.55315
p-NO <sub>2</sub> -@BPA	368.89	0.3377	HOMO→LUMO	0.5541
	316.43	0.0884	HOMO-8→LUMO	0.41136
	265.82	0.2863	HOMO-1→LUMO+1	0.4739
	251.32	0.1219	HOMO-2→LUMO	0.46155
Li+@BPA	360.44	0.1707	HOMO→LUMO	0.69765
	249.05	1.0068	HOMO→LUMO+1	0.54253
	239.1	0.5353	HOMO→LUMO+3	0.44048
m-CH <sub>3</sub> -Li+@BPA	361.02	0.1713	HOMO→LUMO	0.69837
	310.87	0.155	HOMO-1→LUMO	0.59708
	245.79	1.3961	HOMO-1→LUMO+1	0.53728
o-CH <sub>3</sub> -Li+@BPA	357.42	0.1632	HOMO→LUMO	0.69834
	308.1	0.155	HOMO-1→LUMO	0.60724
	243.35	1.5995	HOMO→LUMO+1	0.52961
p-CH <sub>3</sub> -Li+@BPA	358.02	0.1707	HOMO→LUMO	0.69804
	308.1	0.1517	HOMO-1→LUMO	0.60194
	245.28	1.4401	HOMO→LUMO+1	0.53569
m-NO <sub>2</sub> -Li+@BPA	360.01	0.183	HOMO→LUMO+1	0.63136
	304.81	0.1238	HOMO→LUMO	0.45391
	258.57	0.2932	HOMO→LUMO+2	0.53349
	246.13	0.2411	HOMO-6→LUMO	0.46726
o-NO <sub>2</sub> -Li+@BPA	358.39	0.166	HOMO→LUMO+1	0.68132
	308.35	0.1693	HOMO-1→LUMO+1	0.60009
	253.16	0.0502	HOMO-7→LUMO+1	0.54885
p-NO <sub>2</sub> -Li+@BPA	359.34	0.1988	HOMO→LUMO	0.55986
	246.43	0.8936	HOMO→LUMO+3	0.37105
	240.77	0.9354	HOMO→LUMO+3 HOMO-3→LUMO	0.39069 0.31594
Na+@BPA	353.44	0.1643	HOMO→LUMO	0.69791
	244.6	1.7118	HOMO→LUMO+1	0.57075
m-CH <sub>3</sub> -Na+@BPA	353.58	0.1667	HOMO→LUMO	0.69788

	307.31	0.1342	HOMO-1→LUMO	0.59626
	244.76	1.6971	HOMO→LUMO+1	0.55888
o-CH <sub>3</sub> -Na+@BPA	354.08	0.1646	HOMO→LUMO	0.69795
	307.36	0.1355	HOMO-1→LUMO	0.60017
	244.8	1.6545	HOMO-8→LUMO	0.53746
p-CH <sub>3</sub> -Na+@BPA	353.53	0.1687	HOMO→LUMO	0.69792
	307.32	0.1351	HOMO-1→LUMO	0.59903
	244.77	1.7152	HOMO→LUMO+2	0.56712
m-NO <sub>2</sub> -Na+@BPA	358.36	0.1924	HOMO→LUMO+1	0.66148
	306.06	0.1565	HOMO-1→LUMO+1	0.50394
	255.05	0.3173	HOMO→LUMO+2	0.51384
	245.48	0.4418	HOMO-6→LUMO	0.43923
o-NO <sub>2</sub> -Na+@BPA	358.02	0.1797	HOMO→LUMO+1	0.68827
	307.64	0.157	HOMO-1→LUMO+1	0.58462
	247.22	1.2943	HOMO→LUMO+2	0.53983
p-NO <sub>2</sub> -Na+@BPA	353.71	0.1738	HOMO→LUMO+1	0.69759
	248.7	1.2099	HOMO-5→LUMO	0.36968
	241.89	0.4825	HOMO-5→LUMO	0.4562
K+@BPA	360.42	0.2025	HOMO→LUMO	0.69644
	253.07	1.0799	HOMO→LUMO+1	0.58499
	238.38	0.4779	HOMO→LUMO+4	0.58984
m-CH <sub>3</sub> -K+@BPA	360.64	0.2054	HOMO→LUMO	0.6962
	253.51	1.0565	HOMO→LUMO+2	0.55718
	237.36	0.5548	HOMO→LUMO+4	0.31416
o-CH <sub>3</sub> -K+@BPA	359.85	0.1921	HOMO→LUMO	0.69679
	252.45	1.0686	HOMO→LUMO+1	0.56573
			HOMO→LUMO+5	0.26604
	237.93	0.4635	HOMO→LUMO+3	0.26228
p-CH <sub>3</sub> -K+@BPA	361.33	0.2104	HOMO→LUMO	0.69589
	253.32	1.0992	HOMO→LUMO+2	0.42291
	237.07	0.4747	HOMO→LUMO+4	0.4152
m-NO <sub>2</sub> -K+@BPA	362.27	0.2202	HOMO→LUMO+1	0.64731
	307.75	0.1274	HOMO-1→LUMO+1	0.48668
	258.5	0.3796	HOMO→LUMO+2	0.54464
	249.84	0.322	HOMO-8→LUMO	0.34802
o-NO <sub>2</sub> -K+@BPA	359.45	0.187	HOMO→LUMO+1	0.69304
	308.23	0.1179	HOMO-1→LUMO+1	0.57191
	260.11	0.1207	HOMO-2→LUMO	0.45684
	255.77	0.4918	HOMO→LUMO+2	0.50387

p-NO <sub>2</sub> -K+@BPA	363.54	0.2696	HOMO→LUMO+1	0.50918
			HOMO-1→LUMO+1	0.27034
	252.69	0.5455	HOMO→LUMO+3	0.26075
			HOMO→LUMO+3	0.36963
	248.72	0.9316	HOMO-1→LUMO	0.34072
<b>In Ethanol</b>				
Complex	$\lambda_{\max}$	$f$	FMO	orbital contribution
BPA	365.11	0.2429	HOMO→LUMO	0.69564
	256.86	0.6481	HOMO→LUMO+1	0.57645
	241.04	1.0364	HOMO→LUMO+2	0.60204
	236.08	0.2607	HOMO→LUMO+3	0.58861
m-CH <sub>3</sub> -@BPA	364.81	0.2424	HOMO→LUMO	0.69563
	256.62	0.6081	HOMO→LUMO+1	0.56634
	240.94	0.9892	HOMO→LUMO+2	0.60346
	235.5	0.2457	HOMO→LUMO+4	0.55868
o-CH <sub>3</sub> -@BPA	360.26	0.2202	HOMO→LUMO	0.69568
	252.02	0.8961	HOMO→LUMO+1	0.4929
	240.13	0.7842	HOMO-4→LUMO	0.46335
p-CH <sub>3</sub> -@BPA	366.57	0.2543	HOMO→LUMO	0.69432
	257.07	0.6877	HOMO→LUMO+1	0.5646
	241.31	0.9509	HOMO→LUMO+2	0.60301
	236.52	0.3405	HOMO→LUMO+3	0.53788
m-NO <sub>2</sub> -@BPA	363.1	0.2466	HOMO→LUMO+1	0.65313
	307.87	0.0699	HOMO-2→LUMO+1	0.54927
	267.96	0.1181	HOMO-6→LUMO	0.42731
o-NO <sub>2</sub> -@BPA	373.72	0.0798	HOMO→LUMO	0.62021
	354.59	0.1462	HOMO→LUMO+1	0.66861
	307.72	0.0848	HOMO-2→LUMO+1	0.53339
			HOMO-5→LUMO	0.34642
	270.92	0.0715	HOMO-6→LUMO	0.34309
p-NO <sub>2</sub> -@BPA	368.41	0.3609	HOMO→LUMO HOMO→LUMO+1	0.49453 0.48097
	269.72	0.2161	HOMO-1→LUMO+1	0.50263
	250.83	0.9077	HOMO→LUMO+1	0.48453
Li+@BPA	358.49	0.1656	HOMO→LUMO	0.6974
	307.48	0.1239	HOMO-1→LUMO	0.57243
	246.5	1.2308	HOMO→LUMO+1	0.54721
m-CH <sub>3</sub> -Li+@BPA	359.14	0.1647	HOMO→LUMO	0.69817

	244.44	1.3918	HOMO→LUMO+1	0.54768
o-CH <sub>3</sub> -Li <sup>+</sup> @BPA	355.21	0.1569	HOMO→LUMO	0.69816
	242.14	1.5511	HOMO→LUMO+1	0.56317
p-CH <sub>3</sub> -Li <sup>+</sup> @BPA	356.03	0.1647	HOMO→LUMO	0.69782
	243.71	1.4678	HOMO→LUMO+1	0.56106
m-NO <sub>2</sub> -Li <sup>+</sup> @BPA	357.95	0.1782	HOMO→LUMO+1	0.68179
	306.44	0.1479	HOMO-1→LUMO+1	0.5465
	254.73	0.1978	HOMO-5→LUMO	0.55726
	253.34	0.4031	HOMO→LUMO+2	0.58453
o-NO <sub>2</sub> -Li <sup>+</sup> @BPA	356.67	0.1601	HOMO→LUMO+1	0.68115
	325.71	0.026	HOMO-6→LUMO	0.5118
	307.74	0.1477	HOMO-1→LUMO+1	0.59233
p-NO <sub>2</sub> -Li <sup>+</sup> @BPA	357.38	0.2042	HOMO→LUMO+1	0.59244
	254.14	0.3451	HOMO-6→LUMO	0.46688
			HOMO→LUMO+3	0.38695
	241.7	1.4141	HOMO→LUMO+4	0.38249
Na <sup>+</sup> @BPA	351.96	0.1566	HOMO→LUMO	0.69786
	242.99	1.7505	HOMO→LUMO+1	0.57598
m-CH <sub>3</sub> -Na <sup>+</sup> @BPA	325.1	0.1591	HOMO→LUMO	0.69779
	243.3	1.6823	HOMO→LUMO+1	0.5678
o-CH <sub>3</sub> -Na <sup>+</sup> @BPA	352.49	0.1573	HOMO→LUMO	0.69786
	243.3	1.594	HOMO→LUMO+1	0.55176
p-CH <sub>3</sub> -Na <sup>+</sup> @BPA	352.04	0.1617	HOMO→LUMO	0.69785
	243.17	1.7505	HOMO→LUMO+1	0.57507
m-NO <sub>2</sub> -Na <sup>+</sup> @BPA	356.66	0.1861	HOMO→LUMO+1	0.68149
	306.38	0.1254	HOMO-1→LUMO+1	0.54041
	254.57	0.2185	HOMO-5→LUMO	0.51059
	250.95	0.5368	HOMO-1→LUMO+2	0.56531
o-NO <sub>2</sub> -Na <sup>+</sup> @BPA	356.69	0.1728	HOMO→LUMO+1	0.68742
	307.22	0.1344	HOMO-2→LUMO+1	0.56547
	246.41	0.4214	HOMO-3→LUMO	0.38269
p-NO <sub>2</sub> -Na <sup>+</sup> @BPA	351.87	0.1695	HOMO→LUMO+1	0.69747
	255.71	0.5299	HOMO-5→LUMO	0.56733
	242.18	1.4399	HOMO→LUMO+1	0.5102
K <sup>+</sup> @BPA	359.65	0.1944	HOMO→LUMO	0.69628
	250.61	1.1906	HOMO→LUMO+1	0.55536
	236.02	0.4145	HOMO→LUMO+3	0.42162
m-CH <sub>3</sub> -K <sup>+</sup> @BPA	359.92	0.1969	HOMO→LUMO	0.69594
	251.07	1.1595	HOMO→LUMO+1	0.55494
	236.09	0.5207	HOMO→LUMO+3	0.4635

o-CH <sub>3</sub> -K+@BPA	358.94	0.1838	HOMO→LUMO	0.69663
	249.76	1.2332	HOMO→LUMO+1	0.55605
	236.06	0.3804	HOMO→LUMO+3	0.39968
p-CH <sub>3</sub> -K+@BPA	360.67	0.2025	HOMO→LUMO	0.69549
	250.99	1.2022	HOMO→LUMO+1	0.54692
	236.17	0.4781	HOMO→LUMO+3	0.4628
m-NO <sub>2</sub> -K+@BPA	360.79	0.2123	HOMO→LUMO+1	0.6679
			HOMO-2→LUMO+1	0.40263
	307.5	0.1005	HOMO-1→LUMO+1	0.40139
	257.9	0.1641	HOMO-6→LUMO	0.42633
			HOMO→LUMO+2	0.5542
	255.21	0.4724		
o-NO <sub>2</sub> -K+@BPA	359.04	0.1378	HOMO→LUMO+1	0.62283
	307.63	0.0988	HOMO-1→LUMO+1	0.51726
	252.27	0.3232	HOMO→LUMO+2	0.41065
p-NO <sub>2</sub> -K+@BPA	362.92	0.2788	HOMO→LUMO+1	0.55117
	259.64	0.2944	HOMO-8→LUMO	0.32762
	247.9	1.1584	HOMO→LUMO+2	0.41611
<b>In Methanol</b>				
Complex	$\lambda_{\max}$	$f$	FMO	orbital contribution
BPA	364.74	0.2382	HOMO→LUMO	0.69561
	256.69	0.6164	HOMO→LUMO+1	0.57726
	240.63	1.0478	HOMO→LUMO+2	0.60012
	236.04	0.2546	HOMO→LUMO+3	0.5896
m-CH <sub>3</sub> -@BPA	364.45	0.2377	HOMO→LUMO	0.6956
	256.44	0.5776	HOMO→LUMO+1	0.56669
	240.55	1.001	HOMO→LUMO+3	0.60152
	235.47	0.2397	HOMO→LUMO+4	0.55918
o-CH <sub>3</sub> -@BPA	359.61	0.216	HOMO→LUMO	0.69565
	251.78	0.8513	HOMO→LUMO+1	0.48901
	239.83	0.8056	HOMO→LUMO+2	0.55793
p-CH <sub>3</sub> -@BPA	366.2	0.2495	HOMO→LUMO	0.6943
	256.88	0.6554	HOMO→LUMO+1	0.56467
	240.92	0.9662	HOMO→LUMO+3	0.60127
	236.42	0.3336	HOMO→LUMO+4	0.53882
m-NO <sub>2</sub> -@BPA	362.74	0.242	HOMO→LUMO+1	0.65337
	307.75	0.0674	HOMO-2→LUMO+1	0.55061
	268.06	0.116	HOMO-6→LUMO	0.42655

o-NO <sub>2</sub> -@BPA	374.11	0.0752	HOMO→LUMO	0.62224
	354.43	0.1465	HOMO→LUMO+1	0.67095
	307.62	0.0819	HOMO-2→LUMO+1	0.53323
	271.04	0.0682	HOMO-5→LUMO	0.3452
p-NO <sub>2</sub> -@BPA	368.1	0.3557	HOMO→LUMO	0.49433
	269.65	0.2107	HOMO-1→LUMO+1	0.50414
	250.6	0.8322	HOMO→LUMO+2	0.47105
Li+@BPA	358.19	0.1627	HOMO-2→LUMO+5	0.25195
	307.37	0.1184	HOMO-1→LUMO	0.56953
m-CH <sub>3</sub> -Li+@BPA	358.84	0.1618	HOMO→LUMO	0.69811
	244.05	1.3125	HOMO-1→LUMO	0.56138
o-CH <sub>3</sub> -Li+@BPA	354.91	0.1541	HOMO→LUMO	0.6981
	307.28	0.1271	HOMO-1→LUMO	0.58911
	241.71	1.5302	HOMO→LUMO+1	0.56265
p-CH <sub>3</sub> -Li+@BPA	355.74	0.1619	HOMO→LUMO	0.69776
	307.23	0.1228	HOMO-1→LUMO	0.5688
	243.26	1.4949	HOMO-2→LUMO	0.4239
m-NO <sub>2</sub> -Li+@BPA	357.66	0.1751	HOMO→LUMO+1	0.68194
	306.33	0.1425	HOMO-1→LUMO	0.54586
	254.93	0.1874	HOMO-5→LUMO	0.55932
	253.05	0.3756	HOMO→LUMO+2	0.57232
o-NO <sub>2</sub> -Li+@BPA	356.39	0.1572	HOMO→LUMO+1	0.68111
	325.64	0.0257	HOMO-6→LUMO	0.51009
			HOMO-1→LUMO+2	
	307.62	0.1427		0.59081
p-NO <sub>2</sub> -Li+@BPA	357.07	0.2011	HOMO→LUMO+1	0.59389
	254.32	0.3349	HOMO-6→LUMO	0.46872
			HOMO→LUMO+2	0.39886
	241.29	1.3829	HOMO→LUMO+3	0.36567
Na+@BPA	351.68	0.1538	HOMO→LUMO	0.6978
	242.48	1.7356	HOMO→LUMO+1	0.57524
m-CH <sub>3</sub> -Na+@BPA	351.83	0.1563	HOMO→LUMO	0.69773
	242.82	1.6482	HOMO→LUMO+1	0.56438
o-CH <sub>3</sub> -Na+@BPA	352.22	0.1545	HOMO→LUMO	0.6978
	242.89	1.417	HOMO→LUMO+1	0.52146
p-CH <sub>3</sub> -Na+@BPA	351.76	0.1588	HOMO→LUMO	0.69779
	242.67	1.7356	HOMO→LUMO+1	0.57428
m-NO <sub>2</sub> -Na+@BPA	356.37	0.1828	HOMO→LUMO+1	0.68171
	306.28	0.1203	HOMO-1→LUMO+1	0.53802

	254.78	0.2087	HOMO-6→LUMO	0.50921
	250.63	0.5261	HOMO→LUMO+2	0.56921
o-NO <sub>2</sub> -Na+@BPA	356.43	0.1696	HOMO→LUMO+1	0.68732
	307.11	0.1297	HOMO-1→LUMO+1	0.56294
	246.35	0.252	HOMO-2→LUMO	0.39797
p-NO <sub>2</sub> -Na+@BPA	351.58	0.1666	HOMO→LUMO+1	0.69741
	255.82	0.5086	HOMO-5→LUMO	0.5676
	241.72	1.4391	HOMO→LUMO+2	0.51515
K+@BPA	359.38	0.1908	HOMO→LUMO	0.69622
	250.22	1.1579	HOMO→LUMO+1	0.55107
	235.85	0.5071	HOMO→LUMO+3	0.48373
m-CH <sub>3</sub> -K+@BPA	359.66	0.1934	HOMO→LUMO	0.69588
	250.69	1.1262	HOMO→LUMO+1	0.55071
	235.84	0.5287	HOMO→LUMO+3	0.46215
o-CH <sub>3</sub> -K+@BPA	358.68	0.1804	HOMO→LUMO	0.69657
	249.37	1.2	HOMO→LUMO+1	0.55157
	235.89	0.3465	HOMO→LUMO+3	0.37469
p-CH <sub>3</sub> -K+@BPA	360.41	0.1988	HOMO→LUMO	0.69543
	250.62	1.1697	HOMO→LUMO+1	0.5425
	235.98	0.4625	HOMO→LUMO+3	0.45826
m-NO <sub>2</sub> -K+@BPA	360.5	0.2085	HOMO→LUMO+1	0.66813
	307.41	0.0964	HOMO-2→LUMO+1	0.40649
	258.09	0.1554	HOMO-6→LUMO+1	0.42566
	254.97	0.4614	HOMO→LUMO+2	0.5576
o-NO <sub>2</sub> -K+@BPA	358.9	0.1271	HOMO→LUMO+1	0.6066
	354.93	0.0615	HOMO→LUMO	0.56894
	307.54	0.0951	HOMO-1→LUMO+1	0.51168
	252.25	0.236	HOMO→LUMO+2	0.37793
p-NO <sub>2</sub> -K+@BPA	362.63	0.2745	HOMO→LUMO+1	0.55165
	259.73	0.288	HOMO-7→LUMO	0.32771
	247.55	1.1172	HOMO→LUMO+2	0.41922
<b>In DMSO</b>				
Complex	$\lambda_{\max}$	$f$	FMO	orbital contribution
BPA	365.51	0.2502	HOMO→LUMO	0.6957
	257.25	0.6945	HOMO→LUMO+1	0.5752
	241.64	1.0243	HOMO→LUMO+2	0.6024
	236.25	0.2591	HOMO→LUMO+3	0.58528
				0.69569
m-CH <sub>3</sub> -@BPA	365.21	0.2496	HOMO→LUMO	
	256.97	0.669	HOMO→LUMO+1	0.57089
	241.53	0.975	HOMO→LUMO+2	0.60466
	235.68	0.2519	HOMO→LUMO+3	0.55879

o-CH <sub>3</sub> -@BPA	360.6	0.2268	HOMO→LUMO	0.69577
	252.5	0.9457	HOMO→LUMO+1	0.50036
	240.62	0.7613	HOMO→LUMO+2	0.57211
p-CH <sub>3</sub> -@BPA	366.96	0.2617	HOMO→LUMO	0.69438
	257.46	0.7321	HOMO→LUMO+1	0.56704
	241.89	0.9301	HOMO→LUMO+2	0.60536
	236.7	0.3458	HOMO→LUMO+3	0.53626
m-NO <sub>2</sub> -@BPA	363.48	0.2542	HOMO→LUMO+1	0.65435
	307.89	0.0741	HOMO-2→LUMO+1	0.55512
	268.72	0.1257	HOMO-6→LUMO	0.43246
o-NO <sub>2</sub> -@BPA	374.86	0.0798	HOMO→LUMO	0.62222
	355.03	0.1533	HOMO→LUMO+1	0.67056
	307.78	0.0892	HOMO-2→LUMO+1	0.53648
	271.5	0.0779	HOMO-5→LUMO	0.34596
				0.49391
p-NO <sub>2</sub> -@BPA	369.03	0.3744	HOMO→LUMO HOMO→LUMO+1	0.48099
	270.04	0.2167	HOMO-1→LUMO+1	0.50359
	251.4	0.982	HOMO→LUMO+2	0.49829
Li+@BPA	358.84	0.1709	HOMO→LUMO	0.69748
	247.01	1.3155	HOMO→LUMO+1	0.55145
m-CH <sub>3</sub> -Li+@BPA	359.49	0.1697	HOMO→LUMO	0.69826
	245.18	1.4395	HOMO→LUMO+1	0.55268
o-CH <sub>3</sub> -Li+@BPA	355.51	0.1619	HOMO→LUMO	0.69826
	307.51	0.1385	HOMO-1→LUMO	0.59021
	242.93	1.5832	HOMO→LUMO+1	0.56631
p-CH <sub>3</sub> -Li+@BPA	356.36	0.1698	HOMO→LUMO	0.69791
	307.5	0.1339	HOMO-1→LUMO	0.56702
	244.46	0.887	HOMO→LUMO+1	0.43360
m-NO <sub>2</sub> -Li+@BPA	358.3	0.1839	HOMO→LUMO+1	0.68226
	306.62	0.1549	HOMO-1→LUMO+1	0.54718
	255.69	0.1983	HOMO-5→LUMO	0.56399
	253.21	0.4269	HOMO→LUMO+2	0.56399
o-NO <sub>2</sub> -Li+@BPA	357	0.1651	HOMO→LUMO+1	0.68186
	325.79	0.0273	HOMO-6→LUMO	0.50903
	307.91	0.1553	HOMO-1→LUMO+1	0.59357
p-NO <sub>2</sub> -Li+@BPA	357.73	0.2115	HOMO→LUMO+1	0.59496
	255.02	0.3468	HOMO-6→LUMO	0.46921
	242.48	1.48	HOMO→LUMO+2	0.42130
Na+@BPA	352.3	0.1615	HOMO→LUMO	0.69798
	243.82	1.7831	HOMO→LUMO+1	0.57755
m-CH <sub>3</sub> -Na+@BPA	352.46	0.1641	HOMO→LUMO	0.69789



	244.11	1.7181	HOMO→LUMO+1	0.57028
o-CH <sub>3</sub> -Na+@BPA	352.83	0.1626	HOMO→LUMO	0.69796
	244.09	1.6455	HOMO→LUMO+1	0.5572
p-CH <sub>3</sub> -Na+@BPA	352.39	0.166	HOMO→LUMO	0.69798
	244	1.7827	HOMO→LUMO+1	0.57676
m-NO <sub>2</sub> -Na+@BPA	357.04	0.192	HOMO→LUMO+1	0.68213
	306.52	0.1294	HOMO-1→LUMO+1	0.53532
	255.62	0.2197	HOMO-6→LUMO	0.50596
	250.93	0.6289	HOMO→LUMO+2	0.50596
o-NO <sub>2</sub> -Na+@BPA	357.08	0.1782	HOMO→LUMO+1	0.68733
	307.38	0.1412	HOMO-1→LUMO+1	0.56452
			HOMO→LUMO+2	0.37547
	246.74	1.4959	HOMO-2→LUMO	0.33186
p-NO <sub>2</sub> -Na+@BPA	352.2	0.175	HOMO→LUMO+1	0.69757
	256.61	0.524	HOMO-5→LUMO	0.55873
	242.9	1.4959	HOMO→LUMO+2	0.50989
K+@BPA	360.09	0.2005	HOMO→LUMO	0.69637
	251.09	1.2691	HOMO→LUMO+1	0.55817
	236.3	0.2843	HOMO→LUMO+3	0.32873
m-CH <sub>3</sub> -K+@BPA	360.37	0.2031	HOMO→LUMO	0.69602
	251.53	1.238	HOMO→LUMO+1	0.55797
	236.39	0.4736	HOMO→LUMO+2	0.55797
o-CH <sub>3</sub> -K+@BPA	359.37	0.1896	HOMO→LUMO	0.69672
	250.25	1.3163	HOMO→LUMO+1	0.55681
	236.64	0.3563	HOMO→LUMO+2	0.39469
p-CH <sub>3</sub> -K+@BPA	361.33	0.2087	HOMO→LUMO	0.69555
	251.48	1.2792	HOMO→LUMO+1	0.54907
	236.5	0.4517	HOMO→LUMO+2	0.45264
m-NO <sub>2</sub> -K+@BPA	361.2	0.219	HOMO→LUMO+1	0.66878
	307.62	0.1048	HOMO-2→LUMO+1	0.41108
	258.83	0.1664	HOMO-6→LUMO	0.42608
	255.27	0.5362	HOMO→LUMO+2	0.54641
o-NO <sub>2</sub> -K+@BPA	359.48	0.1416	HOMO→LUMO+1	0.62073
	307.74	0.1041	HOMO-1→LUMO+1	0.50955
	252.62	0.305	HOMO→LUMO+2	0.38829
p-NO <sub>2</sub> -K+@BPA	363.4	0.2886	HOMO→LUMO+1	0.5518
	260.25	0.2977	HOMO-7→LUMO	0.32978
	248.44	1.2384	HOMO→LUMO+2	0.4321
<b>In Water</b>				
Complex	$\lambda_{\max}$	$f$	FMO	orbital contribution
BPA	364.48	0.2389	HOMO→LUMO	0.69561

	256.77	0.6164	HOMO→LUMO+1	0.57741
	240.66	1.0512	HOMO→LUMO+2	0.59905
	236.12	0.2489	HOMO→LUMO+3	0.58844
m-CH <sub>3</sub> -@BPA	364.39	0.2391	HOMO→LUMO	0.69561
	256.5	0.5868	HOMO→LUMO+1	0.57020
	240.58	1.004	HOMO→LUMO+2	0.60095
	235.55	0.2387	HOMO→LUMO+3	0.55985
o-CH <sub>3</sub> -@BPA	359.83	0.1554	HOMO→LUMO	0.69569
	251.86	0.8432	HOMO→LUMO+1	0.49086
	239.99	0.8122	HOMO→LUMO+2	0.55988
p-CH <sub>3</sub> -@BPA	366.12	0.2498	HOMO→LUMO	0.69432
	256.95	0.6566	HOMO→LUMO+1	0.56637
	240.94	0.9697	HOMO→LUMO+2	0.60168
	236.54	0.3312	HOMO→LUMO+3	0.53856
m-NO <sub>2</sub> -@BPA	362.68	0.2426	HOMO→LUMO+1	0.65396
	307.71	0.0676	HOMO-2→LUMO+1	0.55430
	268.56	0.1185	HOMO-6→LUMO	0.42884
o-NO <sub>2</sub> -@BPA	375.1	0.0717	HOMO→LUMO	0.62484
	354.54	0.1504	HOMO→LUMO+1	0.67363
	307.58	0.082	HOMO-2→LUMO+1	0.53475
	271.46	0.0688	HOMO-5→LUMO	0.34320
p-NO <sub>2</sub> -@BPA	368.22	0.3592	HOMO→LUMO HOMO→LUMO+1	0.49404 0.48101
	269.77	0.2069	HOMO-1→LUMO+1	0.50581
	250.74	0.8264	HOMO→LUMO+2	0.47168
Li <sup>+</sup> @BPA	358.16	0.1634	HOMO→LUMO	0.69733
	246.04	1.2319	HOMO→LUMO+1	0.54192
	232.36	0.2012	HOMO→LUMO+2	0.37856
m-CH <sub>3</sub> -Li <sup>+</sup> @BPA	358.8	0.1623	HOMO-1→LUMO	0.55556
	244.2	1.2467	HOMO→LUMO+1	0.52297
o-CH <sub>3</sub> -Li <sup>+</sup> @BPA	354.84	0.1547	HOMO→LUMO	0.69811
	241.82	1.5267	HOMO-1→LUMO	0.56296
p-CH <sub>3</sub> -Li <sup>+</sup> @BPA	355.69	0.1625	HOMO→LUMO	0.69776
	243.32	1.5046	HOMO→LUMO+1	0.56796
m-NO <sub>2</sub> -Li <sup>+</sup> @BPA	357.62	0.1759	HOMO→LUMO+1	0.68226
	306.34	0.142	HOMO-1→LUMO+1	0.54535
	255.64	0.185	HOMO-2→LUMO	0.41603
	252.83	0.272	HOMO→LUMO+2	0.48692
o-NO <sub>2</sub> -Li <sup>+</sup> @BPA	356.37	0.1579	HOMO→LUMO+1	0.68152
	325.63	0.0262	HOMO→LUMO	0.65986
	307.61	0.1428	HOMO-1→LUMO+1	0.59023
p-NO <sub>2</sub> -Li <sup>+</sup> @BPA	357.03	0.2026	HOMO→LUMO+1	0.59613
	254.97	0.3284	HOMO-7→LUMO+1	0.47085
	241.39	1.4025	HOMO→LUMO+2	0.43379
Na <sup>+</sup> @BPA	351.65	0.1543	HOMO→LUMO	0.69783

	242.55	1.7434	HOMO→LUMO+1	0.57548
m-CH <sub>3</sub> -Na <sup>+</sup> @BPA	351.81	0.1569	HOMO→LUMO	0.69774
	242.92	1.6363	HOMO→LUMO+1	0.56223
o-CH <sub>3</sub> -Na <sup>+</sup> @BPA	352.19	0.1554	HOMO→LUMO	0.69781
	243.07	1.1396	HOMO→LUMO+1	0.46627
	242.07	0.5551	HOMO-2→LUMO	0.47398
p-CH <sub>3</sub> -Na <sup>+</sup> @BPA	351.73	0.1587	HOMO→LUMO	0.69783
	242.73	1.7422	HOMO→LUMO+1	0.57452
m-NO <sub>2</sub> -Na <sup>+</sup> @BPA	356.36	0.1835	HOMO→LUMO+1	0.68223
	306.28	0.1183	HOMO-1→LUMO+1	0.53254
	255.55	0.2045	HOMO-6→LUMO	0.50413
	250.35	0.5639	HOMO→LUMO+2	0.56601
o-NO <sub>2</sub> -Na <sup>+</sup> @BPA	356.45	0.1702	HOMO→LUMO	0.68716
	307.12	0.1297	HOMO-1→LUMO+1	0.56000
	246.44	0.2337	HOMO-2→LUMO	0.38815
p-NO <sub>2</sub> -Na <sup>+</sup> @BPA	351.53	0.1674	HOMO→LUMO+1	0.69742
	256.41	0.4881	HOMO-5→LUMO	0.56138
	241.76	1.4704	HOMO→LUMO+3	0.51843
K <sup>+</sup> @BPA	359.43	0.1915	HOMO→LUMO	0.69622
	250.18	1.1772	HOMO→LUMO+1	0.54935
	235.89	0.5164	HOMO→LUMO+3	0.49235
m-CH <sub>3</sub> -K <sup>+</sup> @BPA	359.71	0.194	HOMO→LUMO	0.69587
	250.65	1.1448	HOMO→LUMO+1	0.54915
	235.83	0.509	HOMO→LUMO+3	0.44395
o-CH <sub>3</sub> -K <sup>+</sup> @BPA	358.71	0.1811	HOMO→LUMO	0.69658
	249.32	1.2221	HOMO→LUMO+1	0.54825
	235.86	0.2977	HOMO→LUMO+3	0.34149
p-CH <sub>3</sub> -K <sup>+</sup> @BPA	360.46	0.1995	HOMO→LUMO	0.69541
	250.58	1.188	HOMO→LUMO+1	0.54008
	236.02	0.4668	HOMO→LUMO+3	0.44420
m-NO <sub>2</sub> -K <sup>+</sup> @BPA	360.5	0.2093	HOMO→LUMO	0.66880
	307.41	0.0956	HOMO-2→LUMO+1	0.41409
	258.76	0.1529	HOMO-6→LUMO	0.42413
	254.8	0.4529	HOMO→LUMO+2	0.55582
o-NO <sub>2</sub> -K <sup>+</sup> @BPA	359.05	0.1196	HOMO→LUMO+1	0.58955
	355.23	0.0695	HOMO→LUMO	0.55307
	307.53	0.0949	HOMO-1→LUMO+1	0.50166
	252.49	0.1677	HOMO→LUMO+2	0.33470
p-NO <sub>2</sub> -K <sup>+</sup> @BPA	362.68	0.2766	HOMO→LUMO+1	0.55229
	260.14	0.2851	HOMO-7→LUMO	0.32895
	247.56	1.1311	HOMO→LUMO+2	0.43041

