Supplementary data

Charge Transfer Complex between 4-Dimethylaminopyridine and DDQ: Synthesis, Spectroscopic Characterization, DNA Binding Analysis, and Density Functional Theory (DFT)/Time-Dependent DFT/Natural Transition Orbital Studies

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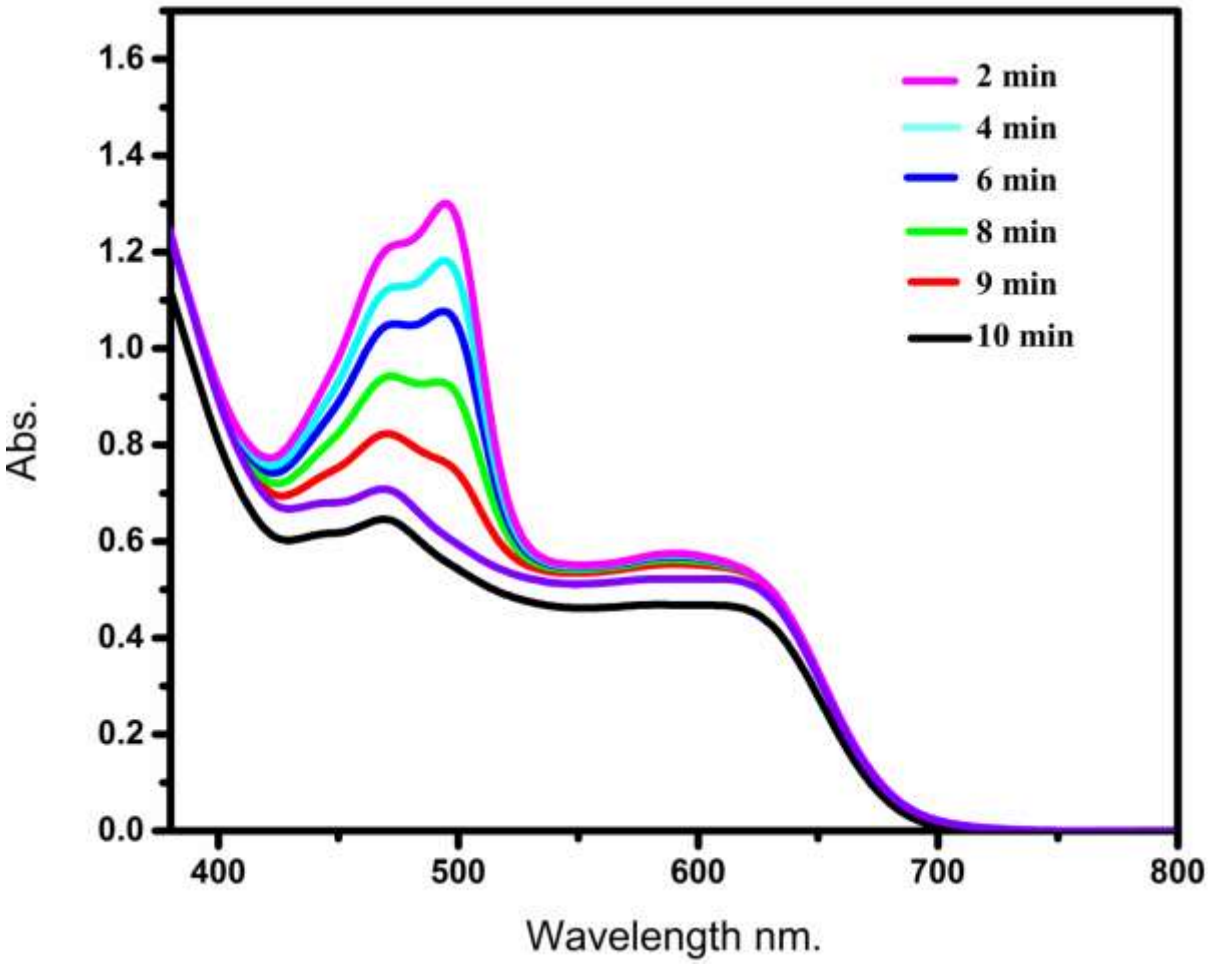

Figure S1. Effect of time on the stability of the formed complex

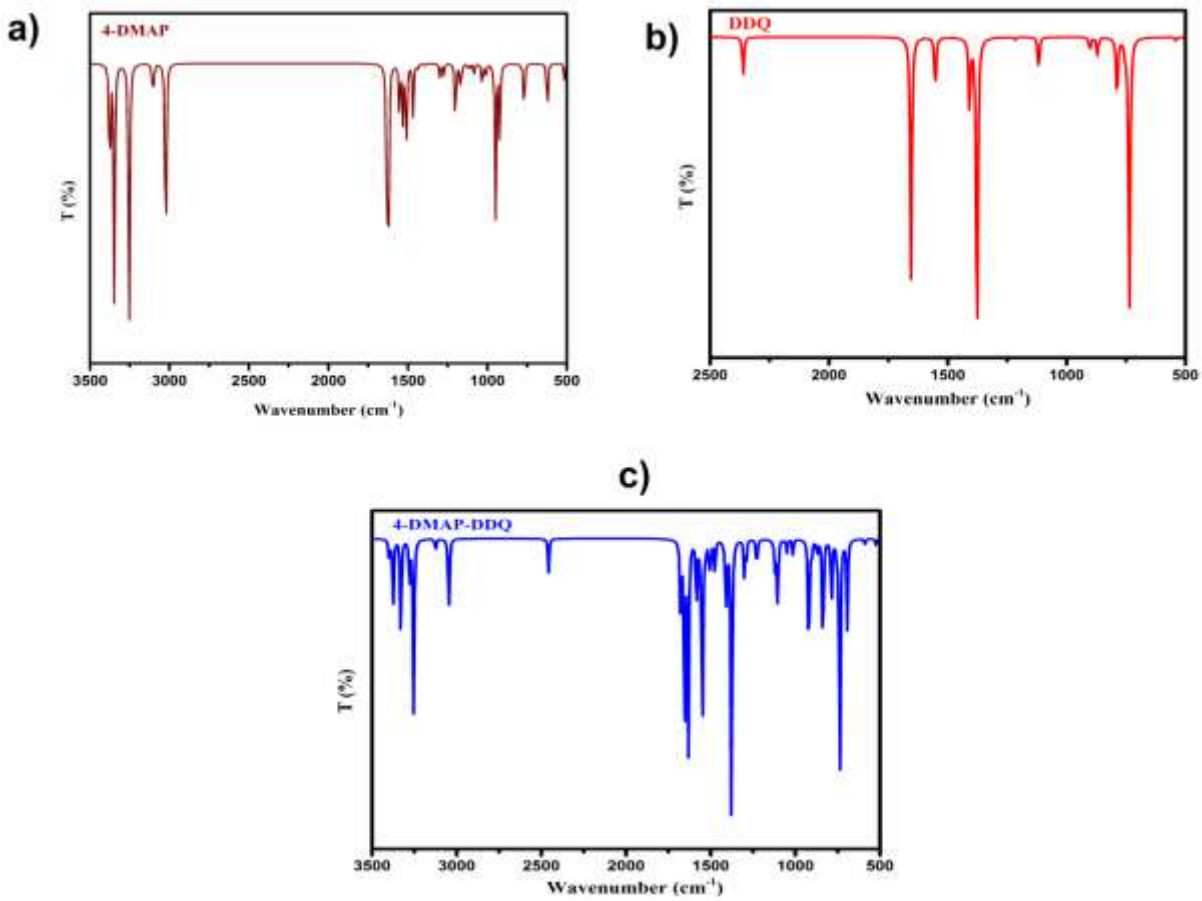

Figure S2. Calculated IR spectra of a) 4-DMAP, b) DDQ, and c) 4-DMAP-DDQ.

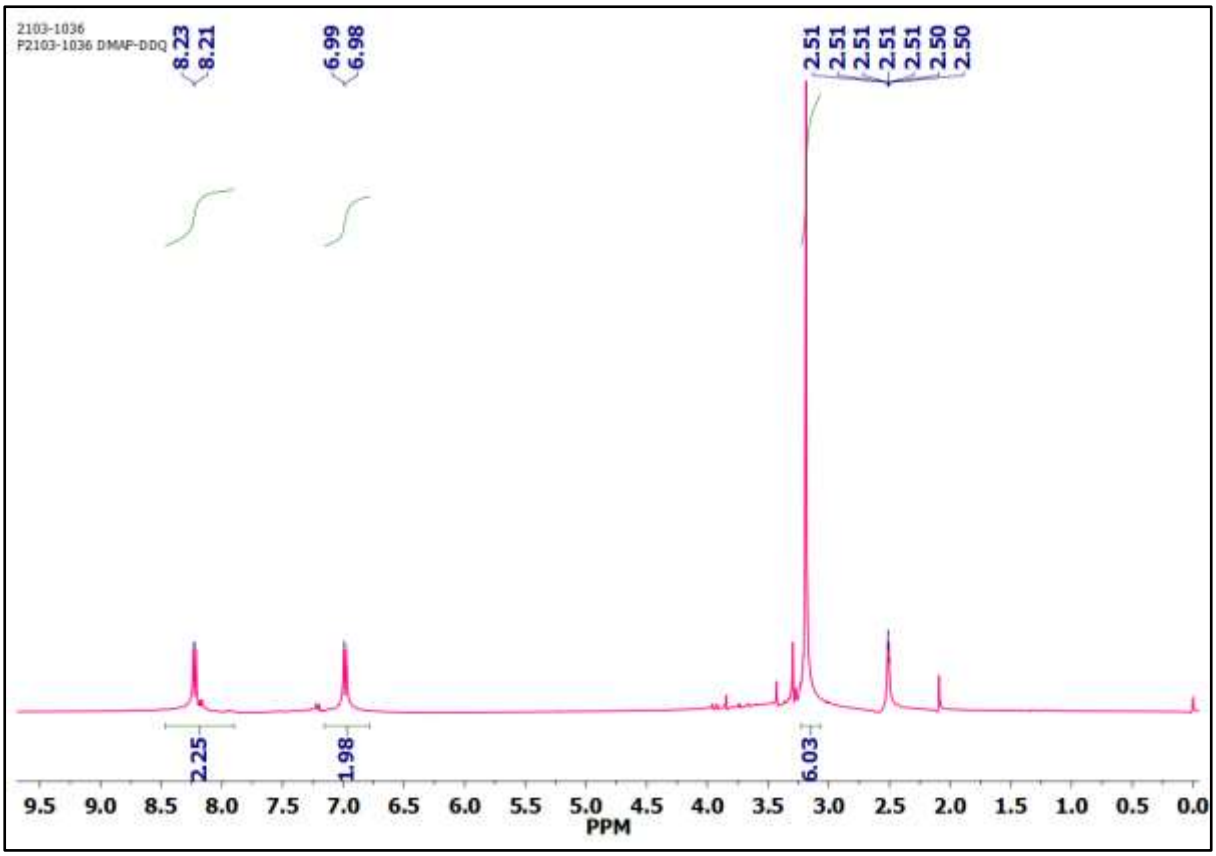

Figure S3. ^{1}H-NMR spectra of CTC in DMSO-d_6 (400 mhz).

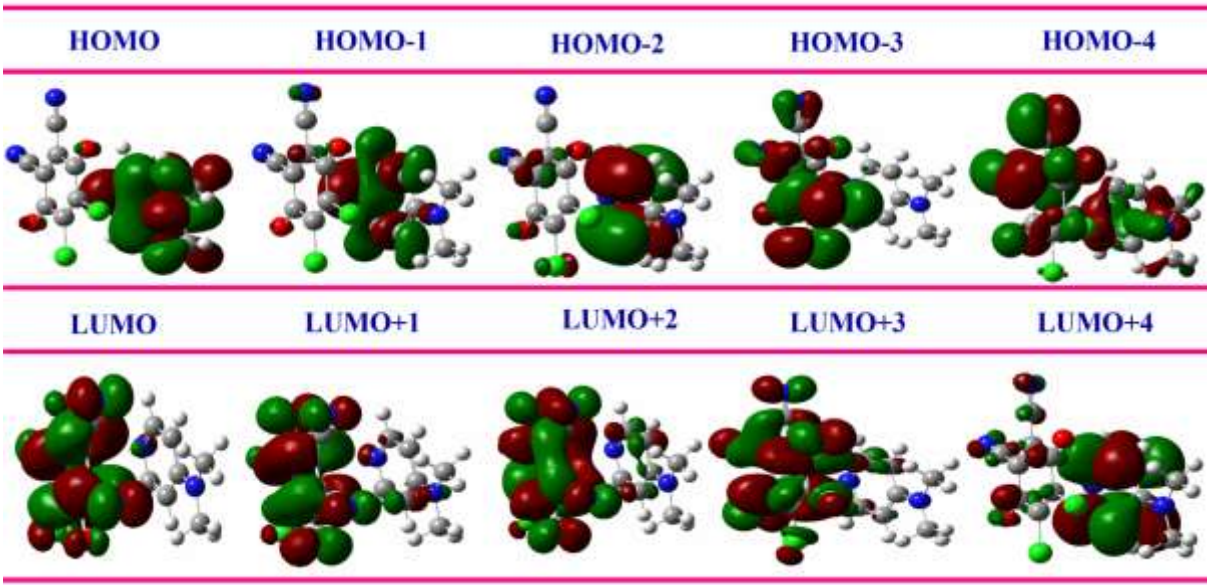

Figure S4. FMO pictures of CT-complex calculated by DFT (wB97XD).

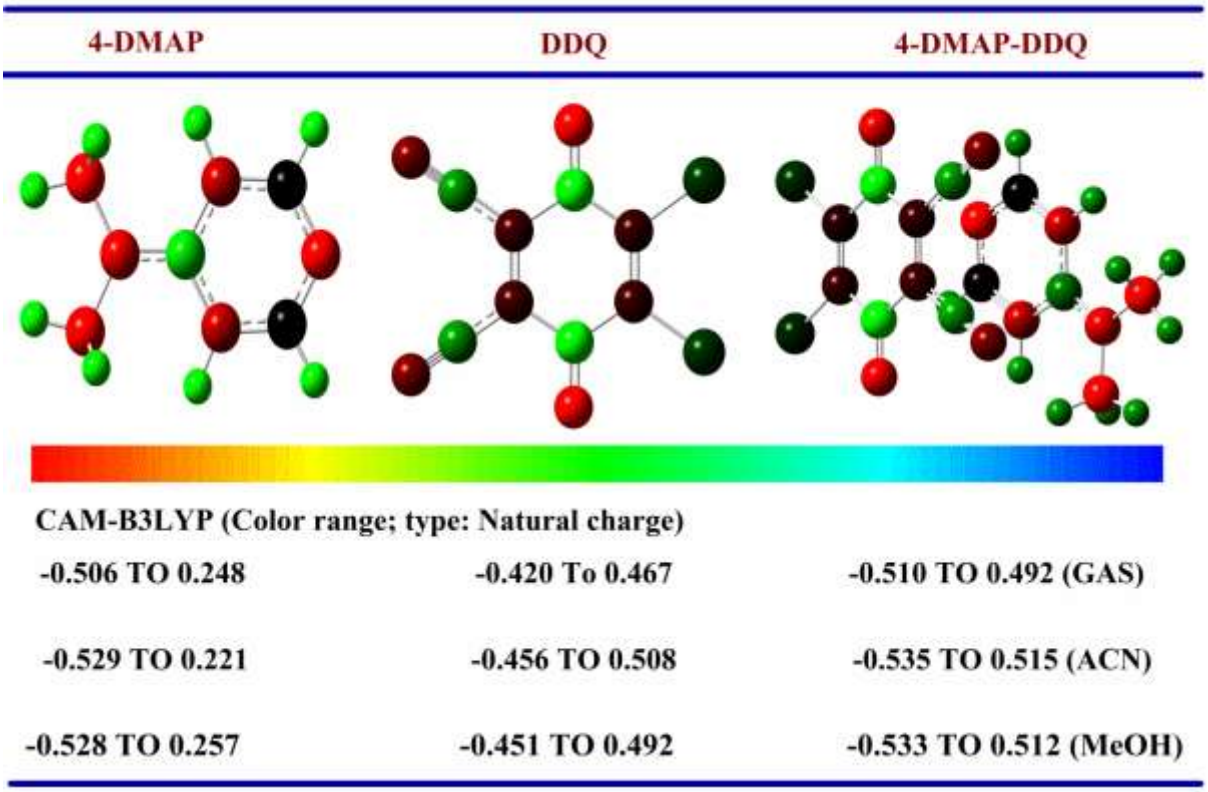

Figure S5. Natural atomic charge of CT complex

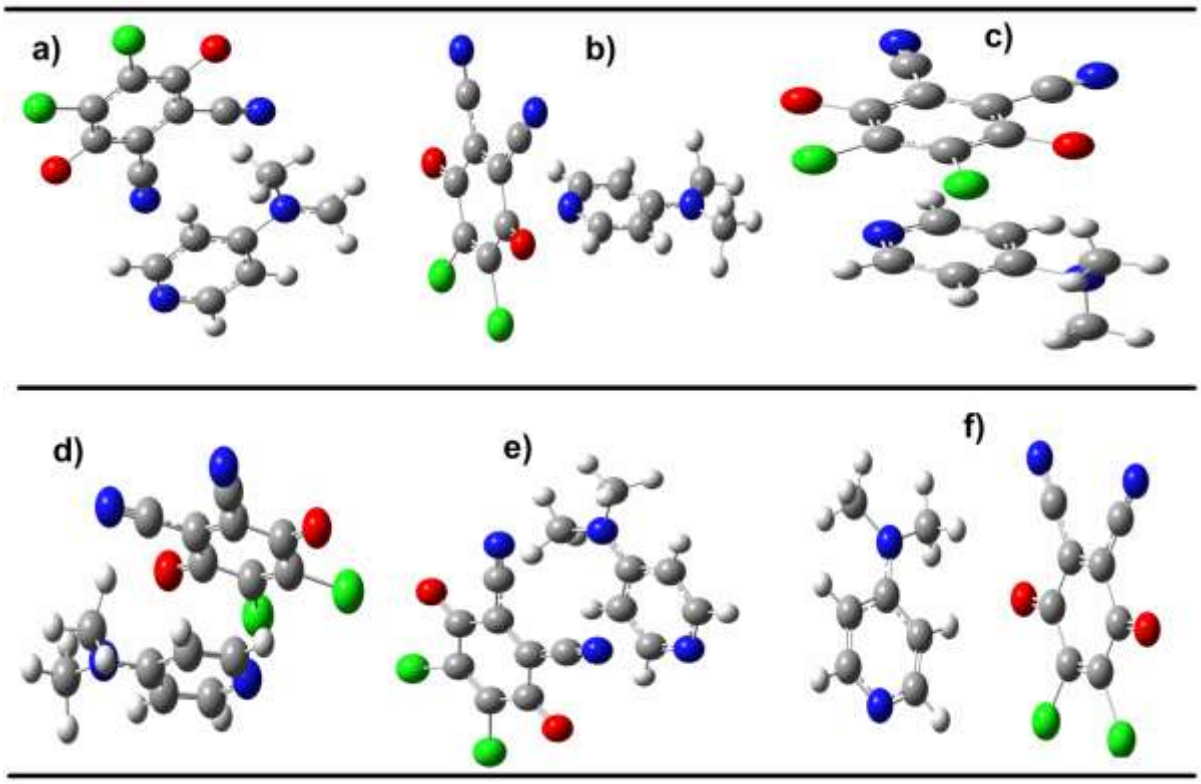

Figure S6. wB97XD optimized ground state geometric structure of the complex in gas phase. (a, c, d) Top view of 4-DMAP-DDQ CT complex. (e, f) Front view of 4-DMAP-DDQ CT complex. (b) Side view of 4-DMAP-DDQ CT complex.

Table S1. Elemental analysis by EDX spectroscopy

Element	Experimental (%)	Theoretical (%)
C	51.51	51.60
Cl	20.19	20.31
N	16.01	16.01
O	9.15	9.15

Table S2. Optimized bond length values of 4-DMAP, DDQ and CT-complex

Bond length (A^0)	4-DMAP	DDQ	CTC		
			Gas	ACN	MeOH
C1-C2	1.362		1.386	1.387	1.386
C2-C3	1.454		1.419	1.414	1.414
C3-C4	1.454		1.415	1.417	1.417
C4-C5	1.374		1.386	1.383	1.383
C5-N6	1.375		1.355	1.353	1.355
C1-N6	1.375		1.349	1.352	1.352
C3-N11	1.415		1.369	1.371	1.373
C16-N11	1.455		1.463	1.459	1.460
C12-N11	1.464		1.462	1.460	1.461
C1-C2		1.495	1.489	1.488	1.489
C2-C3		1.484	1.479	1.478	1.477
C3-C4		1.347	1.338	1.337	1.338
C4-C5		1.485	1.480	1.482	1.479
C5-C6		1.498	1.494	1.491	1.493
C1-C6		1.363	1.356	1.357	1.352
C5-O7		1.26	1.252	1.253	1.255
C2-O8		1.26	1.252	1.254	1.252
C3-Cl10		1.781	1.773	1.769	1.768
C4-Cl9		1.781	1.766	1.768	1.767
C1-C12		1.425	1.433	1.432	1.434
C12-N14		1.174	1.166	1.167	1.164
C6-C11		1.421	1.421	1.421	1.420
C11-N13		1.176	1.167	1.163	1.164

Table S3. Optimized bond angle values of 4-DMAP, DDQ and CT-complex

Bond angles (A^0)	4-DMAP	DDQ	CTC		
			Gas	ACN	MeOH
C1-C2-C3	117.8		119.3	119.3	119.4
C2-C3-C4	115.5		116.3	116.4	116.1
C3-C4-C5	118.5		119.7	119.6	119.1
C4-C5-N6	125.3		124	124.6	124.4
C5-N6-C1	115		116.6	116.3	116.3
C2-C1-N6	125.7		124.3	124.4	124.5
C3-N11-C12	120.5		120.4	120.6	120.6
C3-N11-C16	119.7		120.2	120.1	120.2
C12-N11-C16	120.6		119.6	119.5	119.7
C1-C2-C3		117.6	116.3	116.6	116.3
C2-C3-C4		121.8	121.3	121.7	121.7
C3-C4-C5		121.5	121.8	121.3	121.4
C4-C5-C6		117.1	117.8	117.9	117.7
C5-C6-C1		121.4	120.3	120.2	120.4
C1-C2-O8		120.5	121	121.4	121.5
C3-C2-O8		122.1	122.4	122.5	122.3
C4-C5-O7		122.6	120.4	122.6	122.7
C6-C5-O7		120.5	121.7	121.6	121.7
C2-C3-Cl10		115.1	115.4	115.3	115.1
C4-C3-Cl10		122.9	122.9	123.4	123.8
C3-C4-Cl9		122.9	123.1	123.4	123.6
C5-C4-Cl9		115.1	115.3	115.6	115.2
C2-C1-C12		116.7	115.7	115.2	115.5
C6-C1-C12		122.7	121.1	121.4	121.3
C5-C6-C11		116.7	115.7	115.4	115.1
C1-C6-C11		122.7	121.3	121.6	121.7

Table S4. Natural atomic charge of 4-DMAP, DDQ, and CT-complex calculated using the wB97XD function.

Atom	4-DMAP	DDQ	CTC		
			Gas	ACN	MeOH
C1	0.00617		-0.0182	-0.0056	-0.0056
C2	-0.3479		-0.3415	-0.3519	-0.3527
C3	0.2041		0.2119	0.2109	0.2115
C4	-0.3478		-0.3461	-0.3512	-0.3521
C5	0.0069		-0.0041	-0.0054	-0.0059
N6	-0.4843		-0.5262	-0.5359	-0.5357
H7	0.2375		0.2467	0.2418	0.2411
H8	0.2489		0.2611	0.2607	0.2599
H9	0.2488		0.2626	0.2656	0.2652
H10	0.2367		0.2539	0.2389	0.2406
N11	-0.4331		-0.4264	-0.4242	-0.4247
C12	-0.5066		-0.5085	-0.5117	-0.5114
H13	0.2455		0.2384	0.2378	0.2368
H14	0.2352		0.2514	0.2549	0.2533
H15	0.2352		0.2467	0.2438	0.2479
C16	-0.5072		-0.5099	-0.5108	-0.5108
H17	0.2459		0.2446	0.2409	0.2405
H18	0.2341		0.2524	0.2543	0.2573
H19	0.2342		0.2391	0.2381	0.2386
C1		-0.1078	-0.1129	-0.0943	-0.0946
C2		0.4673	0.4861	0.5171	0.5159
C3		-0.0932	-0.1029	-0.0808	-0.0809
C4		-0.0937	-0.0739	-0.0769	-0.0788
C5		0.4679	0.4932	0.5072	0.5071
C6		-0.1074	-0.1023	-0.0893	-0.0893
O8		-0.4214	-0.4470	-0.4665	-0.4671
O7		-0.4214	-0.4372	-0.4550	-0.4546
Cl10		0.0947	0.0728	0.0779	0.0772
Cl9		0.0947	0.0865	0.0827	0.0845
C12		0.2474	0.2629	0.2830	0.2944
C11		0.2474	0.2608	0.2850	0.2892
N14		-0.1864	-0.2301	-0.2443	-0.2529
N13		-0.1864	-0.2466	-0.2459	-0.2472

Table S5. The reactivity parameters of 4-DMAP, DDQ, and CTC in gas phase, acetonitrile and methanol.

Parameter	4-DMAP	DDQ	CTC		
			Gas	ACN	MeOH
E_{HOMO} (eV)	-6.96	-10.32	-6.386	-6.128	-6.141
E_{LUMO} (eV)	1.425	-5.041	-3.807	-3.881	-3.877
I	6.96	10.32	6.38	6.12	6.14
A	-1.425	5.041	3.807	3.881	3.877
η	2.7675	2.64	1.286	1.119	1.131
μ	-4.192	-7.681	-5.093	-5.00	-5.00
ω	3.174	11.172	10.081	11.17	11.052
σ	0.3613	0.3787	0.7776	0.8936	0.8841

1eV= 96.485 kJ mol^{-1}

Table S6. Cartesian coordinates of CT complex.

Symbol	X	Y	Z
C	0.000461070	-0.002287811	0.000601419
C	-0.001762861	-0.001339735	0.000860785
C	0.000017942	-0.006864873	0.000294368
C	-0.003221543	0.000528848	0.000363441
C	-0.000215909	0.003326746	0.000694308
N	0.001114505	0.000637104	0.000596033
H	0.001496960	0.001788145	0.000540586
H	-0.000020693	0.001983101	0.000553686
H	-0.001911383	-0.001254853	0.000322453
H	0.001352289	-0.001642692	0.000279655
N	-0.010523909	0.011547038	0.001314359
C	0.004276591	-0.007226475	0.000797893
H	0.000943939	0.005689257	0.002203863
H	0.002966519	0.000111158	0.000556808
H	-0.000845371	0.000690866	0.008561909
C	0.001767956	-0.006356331	0.000875792
H	0.000768637	-0.002082728	0.003011242
H	0.002682414	-0.000208277	0.000780591
H	0.000824571	0.003804763	0.004546963
C	0.020493245	-0.016171219	0.005041153
C	-0.020569134	-0.018374318	0.004815963
C	-0.035972544	0.005542201	0.003219001
C	-0.019270602	0.011224049	0.003508754
C	0.020601255	0.010141883	0.002846834
C	0.048183408	0.000776103	0.000473892
O	0.062338198	-0.004090934	0.001966680
O	-0.075881686	0.001935135	0.001986089
Cl	0.004520219	0.001465124	0.000397691
Cl	-0.004409689	0.001727721	0.000688904
C	-0.001185501	0.003401485	0.001272643
N	0.000513174	-0.000854524	0.000223653

C	0.001036602	0.003297447	0.001045568
N	-0.000568670	-0.000863401	0.000280860