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Supplementary Information for

Ruthenium(II) Multi Carboxylic Acid Complexes : Chemistry and Application in Dye Sensitizers Solar Cells

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Figure S1. General procedure of synthesized RMCCs(1-4) in different conditions and molecular structure of the investigated ruthenium complexes.

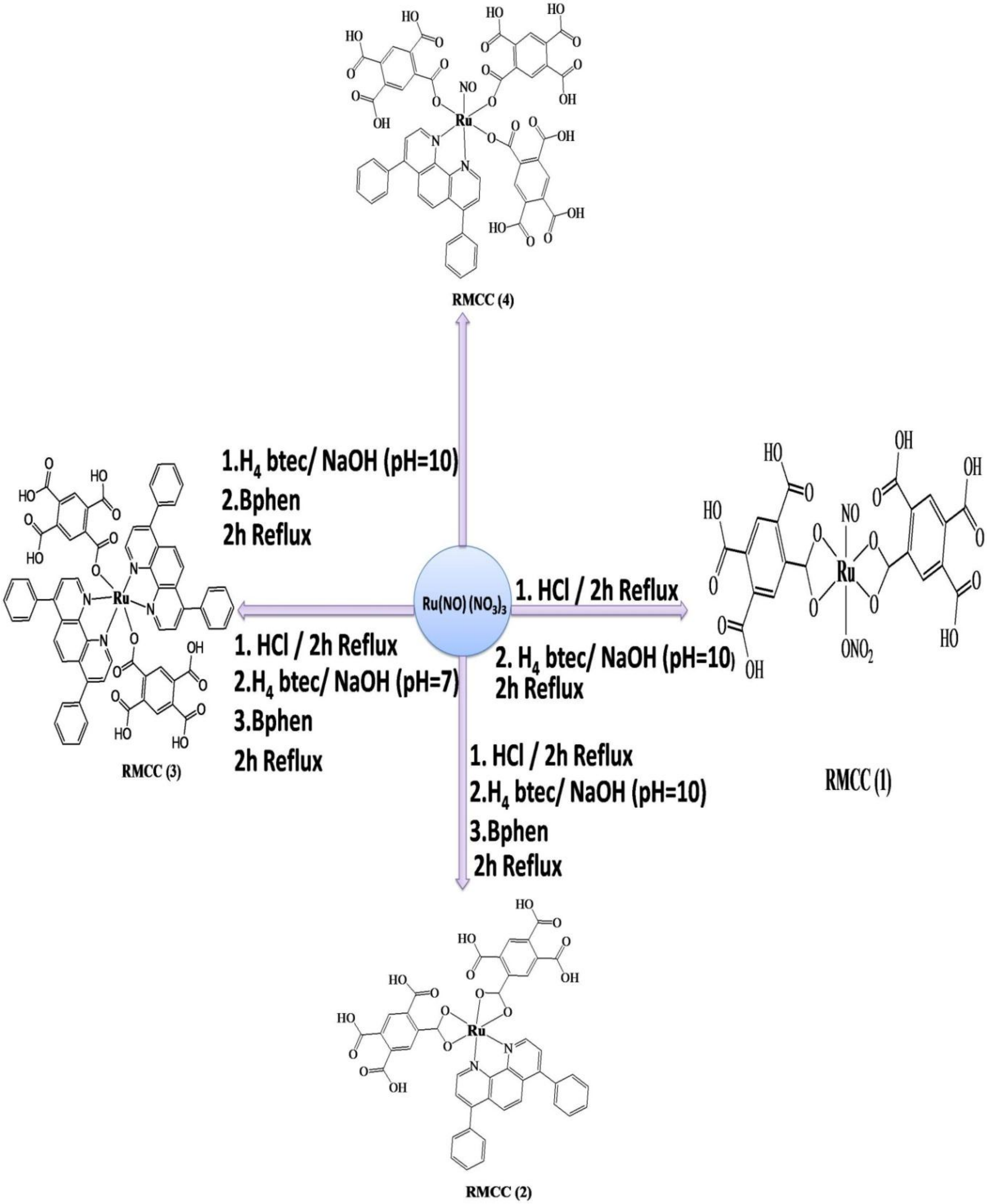

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Figure S2. FT-IR spectra of RMCCs(1-4).

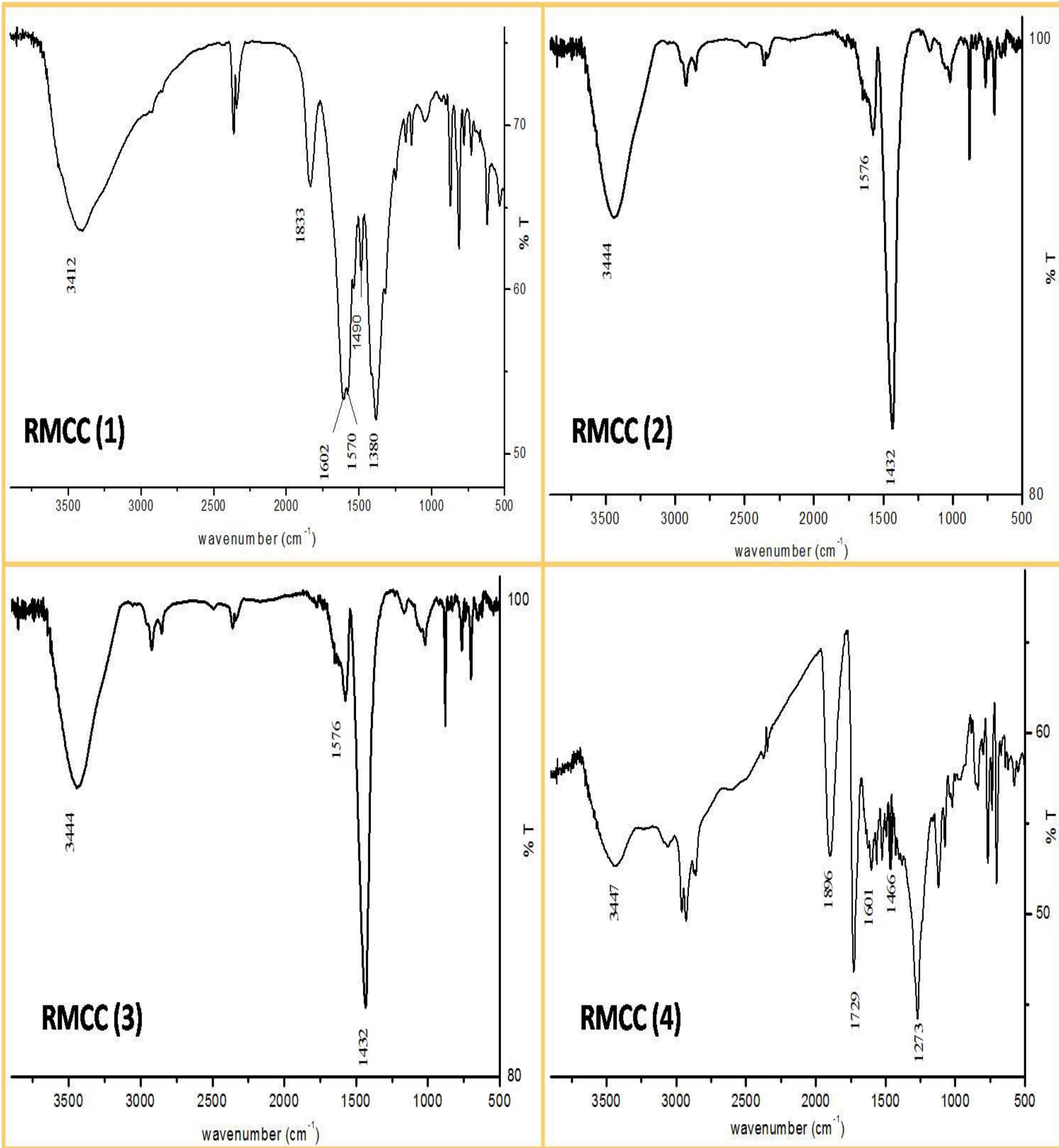

Table S3.Selected excitation energies (E, nm), oscillator strength (f), and relative orbital contributions for the visible region optical transitions of calculated at the B3LYP/LanL2DZ level.

Dye	TD-DFT excitation energy/nm	Oscillator Strength (*f*)	Assignment
RMCC (1)	620	0.01	H-1 → L %19 H → L %67
	527	0.06	H-1 → L %21
	496	0.28	H-1 → L %64 H → L %18
RMCC (2)	643	0.72	H-2 → L+3 %12 H → L %32 H → L+1 %27 H → L+3 %46 H → L+4 %21
	547	0.38	H-2→L %17 H-2→L+1 %15 H-2→L+3 %30 H-2→L+4 %14 H-1→L %25 H-1→L+1 %21 H-1→ L+3 %35 H-1→L+4 %16 H → L %13 H → L+1 %11 H → L+3 %11
	510	0.1	H-2 →L %23 H-2 →L+1 %18 H-2→L+3 %38 H-2L→+4 %17 H-1→L %22 H-1→L+1 %20 H-1 →L+3 %24 H-1→L+4 %11 H→ L %11 H → L+3 %16
	712	0.02	H-5 →L %12 H-4→ L %13 H-3 → L %27 H-2 → L %27
	557	0.3	H-5→L %13 H-1→L %26 H-1→L+1 %11 H→ L %46 H → L+1 %18

RMCC (3)			H→ L+3	%11
			H-5→ L+1	%13
			H-3→ L+1	%10
			H-2 → L	%10
			H-2→L+1	%13
		0.17	H-1→L	%11
			H-1→L+1	%23
			H-1→L+2	%11
	517		H-1→L+4	%11
			H →L	%20
			H → L+1	%39
			H → L+3	%17
			H → L+4	%17
			H-1 →L+2	%10
			H → L	%35
	737	0.12	H → L+1	%25
			H → L+3	%40
			H → L+4	%7
			H-2→L	%11
			H-2→L+1	%15
			H-2→L+3	%33
	568	0.43	H-1→L	%27
RMCC (4)			H-1→L+1	% 19
			H-1→ L+3	%33
			H → L	%15
			H → L+1	%14
			H → L+3	%18
	547	0.28	H-2 →L	%20
			H-2 →L+1	%15
			H-2→L+3	%40
			H-1→L	%25
			H-1→L+1	%23
			H-1 →L+3	%25
			H → L	%16
			H → L+3	%17

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Figure S4. UV-Visible absorption spectra for RMCC(4) solution, 10^{-5} (M) in DMF (red line) and after sensitization onto TiO_2 film (black line).

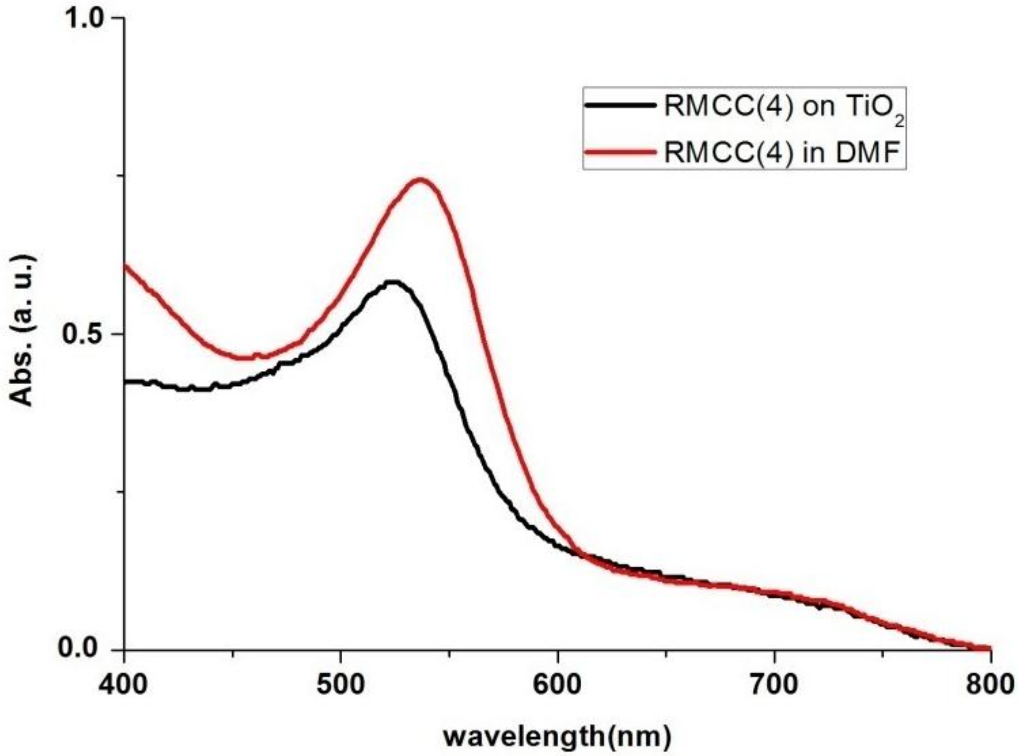

Figure S5. The 250 MHz ^{1}H-NMR spectra of RMCC (1) and RMCC(4), recorded at 25^{o}C in d-DMSO solvent.

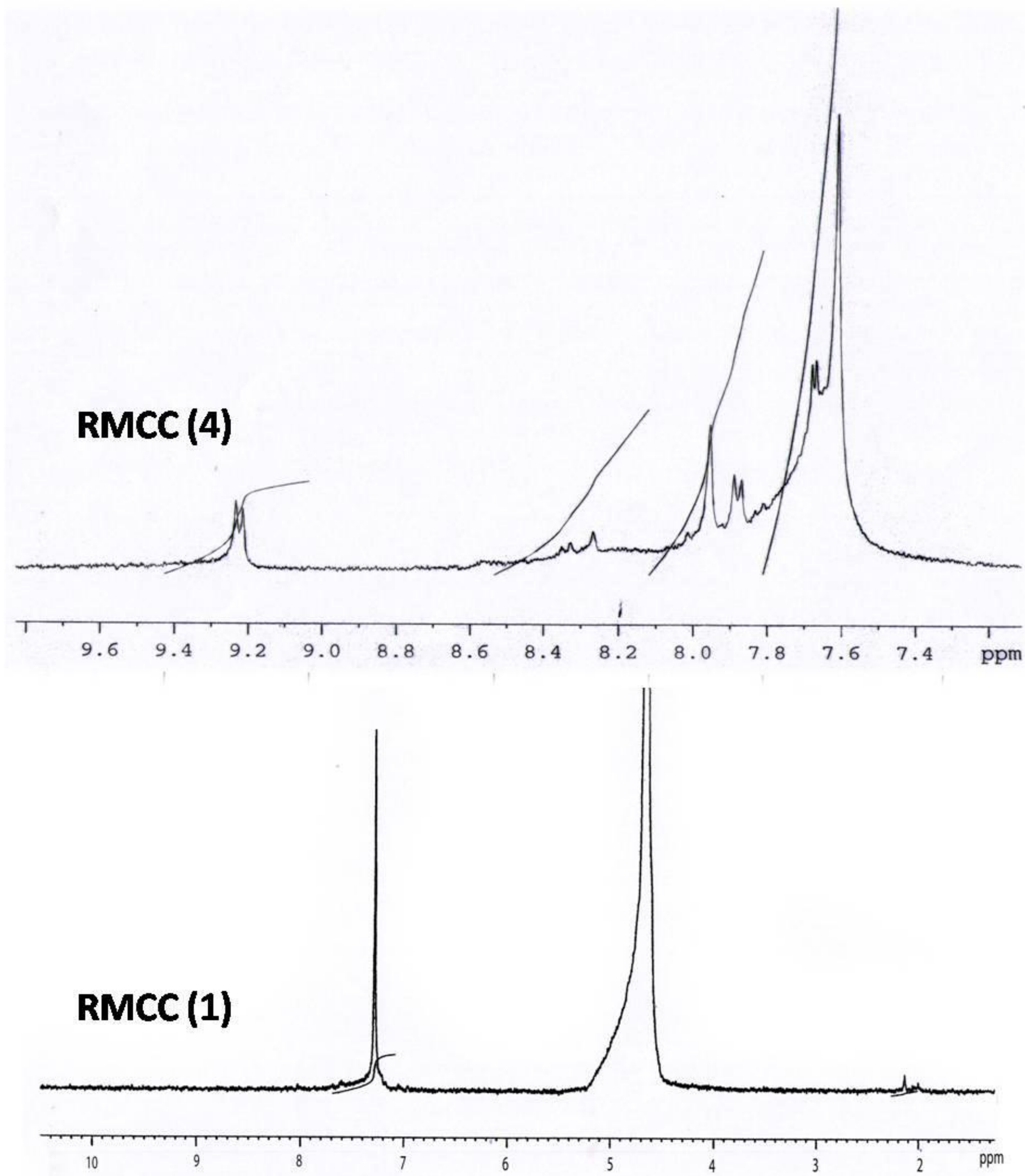

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Figure S6. Plot comparing the I-V behavior of TiO_2 electrode films sensitized in RMCC (4) concentrations of 4×10 $^{-2}$, 4×10 $^{-3}$, 4×10 $^{-4}$ (|m) and RMCC (4) with 4×10 $^{-4}$ (M) and 13, 15 and 23 (μm) of TiO_2 film thickness.

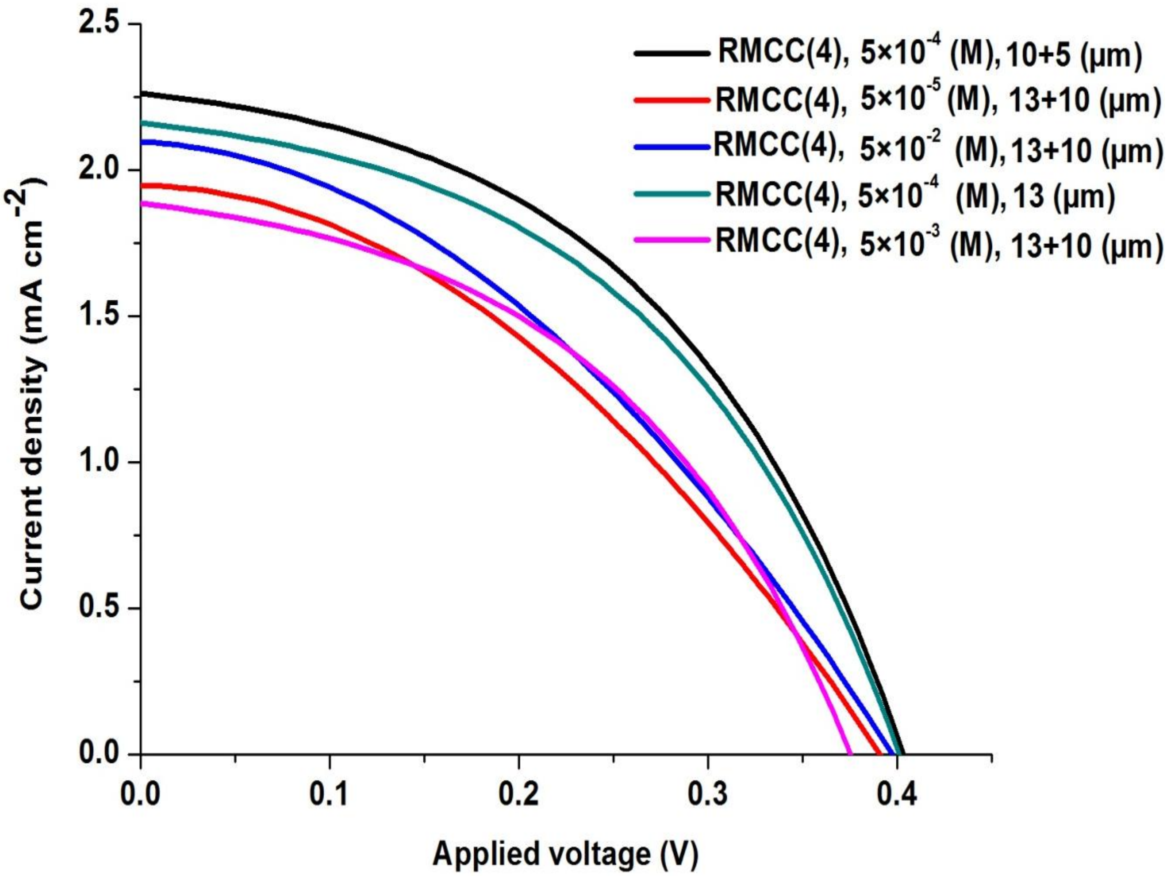

Figure S7. Diagram of five highest occupied and five lowest unoccupied molecular orbital levels of novel RMCC (1-4).