Supplementary Information (SI) for ChemComm.

Supporting Information

4

Contents

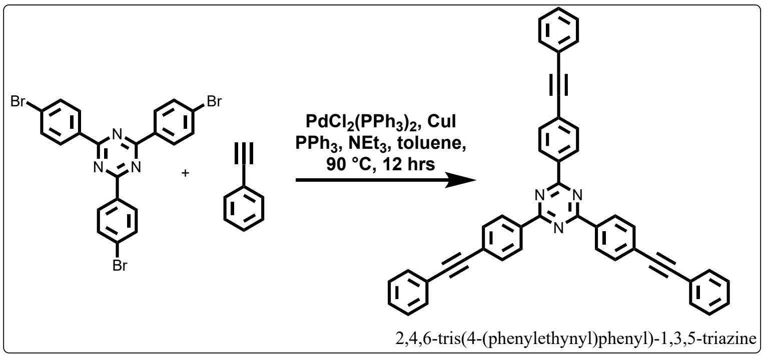
List of figures:

1. General Information

All the chemicals and solvents were used as purchased without any further purification. 4-bromobenzonitrile, trifluoromethane sulfonic acid, iodine, phenylacetylene, dimethylsulfoxide, triethylamine, $PdCl_2(PPh_3)_2$, CuI, PPh_3, toluene, ammoniumacetace, aceticacid, terepthaldehyde, *p*-tolualdehyde, benzil, dichloromethane, petroleumether, ethylacetate, diethylether, chloroform, potassiunferricyanide, NaOH, benzene, were purchased from Sigma-Aldrich, Tokyo Chemical Industry (TCI), Finar and Spectrochem. ^{1}H-NMR and ^{13}C-NMR were recorded in JEOL ECZS 400MHz and 100MHz respectively. ^{13}C CPMAS NMR experiment was performed at 15KHz, with 3s contact time. The UV-Vis absorption studies were conducted by using Cary 5000 UV-Vis NIR spectrometer. EPR was recorded in BRUKER EPR. BET surface area analysis was done in Micro 100C/ Altamira Instruments.

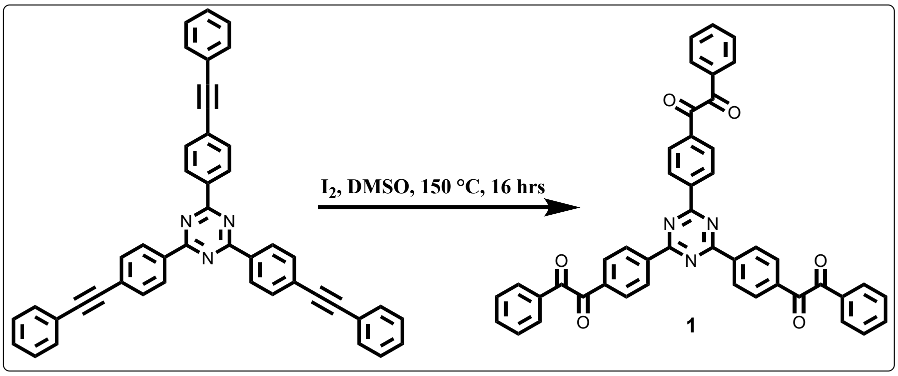
2. Experimental section:

1. Synthesis of 2,4,6-*tris*(4-(phenylethynyl)phenyl)-1,3,5-triazine:



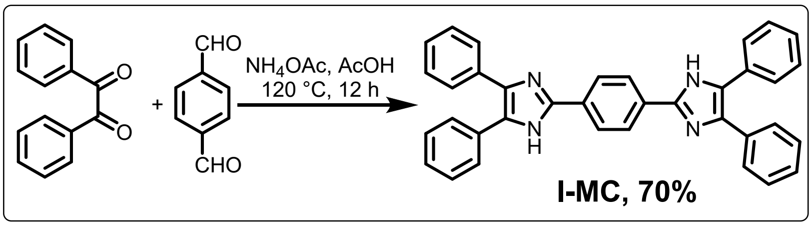
2,4,6-*tris*(4-(phenylethynyl)phenyl)-1,3,5-triazine (1g, 1.83 mmol) was charged into a 2 neck RB under inert atmosphere and then added by 5mol% of $Pd(PPh_3)_2Cl_2$, 7 mol% of CuI and triphenylphosphine (20.7 mg, 0.109 mmol) and 50 ml of triethylamine and 50 ml of toluene. The mixture was purged with N_2 gas for 20 minutes and then added by phenylacetylene (748 mg, 7.33 mmol). The mixture was heated at 90 ̊C till the completion of the reaction, analysed by TLC. After the completion of reaction triethylamine was removed by rotary evaporator and the residue was dissolved in DCM and washed with water for about three times. The obtained organic layer was dried by using sodium sulphate anhydrous and the solvent was removed by rotary evaporator. The obtained crude product was purified by running column chromatography in 100% hexane. The pure product was obtained in 80% yields. ^{1}H NMR (400 MHz, $CDCl_3$, in ppm): 8.77 (d, 6H), 7.75 (d, 6H), 7.59(d, 6H), 7.29-7.46 (m, 9H).

2. Synthesis of **1**.



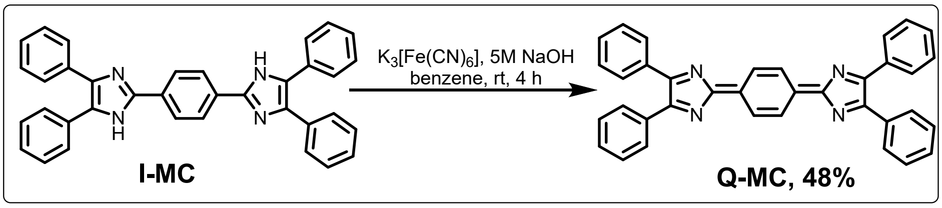
Take 2,2',2''-((1,3,5-triazine-2,4,6-triyl)*tris*(benzene-4,1-diyl))tris(1-phenylethane-1,2-dione) (900mg, 1.47 mmol) into RB and added by 30 ml of DMSO and iodine (393 mg, 3.09 mmol). The mixture was heated at 150 ˚C for about 12 hrs. After the completion of the reaction, the reaction mixture was cooled to room temperature and then poured into an ice. The solid formed was filtered off and the solid washed with diethyl ether. The product came along with the diethyl ether and residue was left behind. The diethyl ether was evaporated by using rotary evaporator to obtain pure product in 90% yields. ^{1}H NMR (400 MHz, CH_2Cl_2, δ in ppm): 8.88 (d, 6H), 8.17 (d, 6H), 8.02 (d, 6H), 7.70 (t, 3H), 7.55(t, 6H); ^{13}C NMR (100 MHz, $CDCl_3$): 193, 171, 140, 136, 135, 132, 130, 129.

3. Synthesis of **I-MC**:[1]



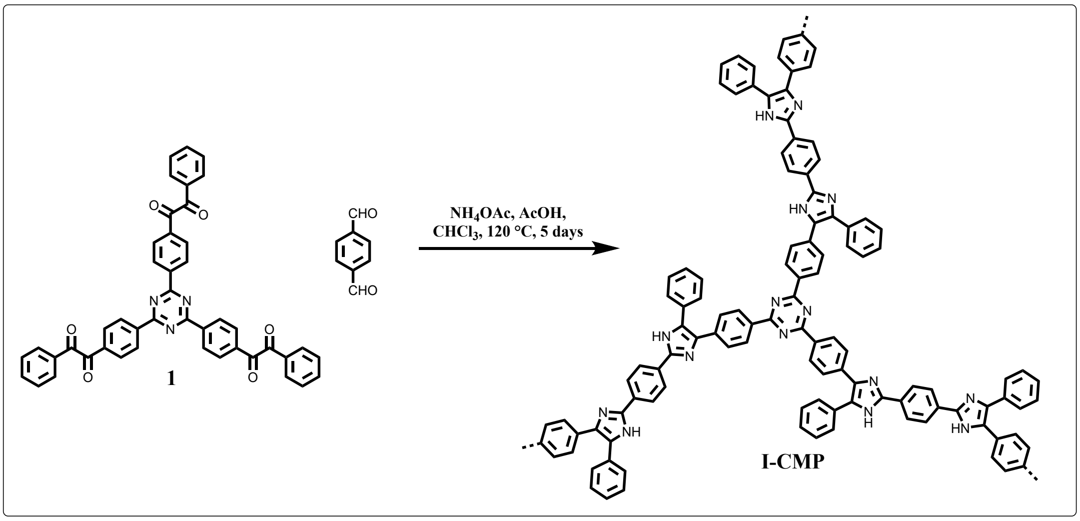
I-MC was synthesized as per the reported procedure, in brief by cooking the mixture of benzil(1.49 mmol, 2 eq), terepthaldehyde(0.745 mmol, 1 eq) and ammoniumacetate(29.8 mmol, 40 eq) in 50 ml of acetic acid at 120 ^{o}C for about 12 hrs. obtaind the yellow coloured compound **I-MC** in 70 % yields.

4. Synthesis of **Q-MC**:



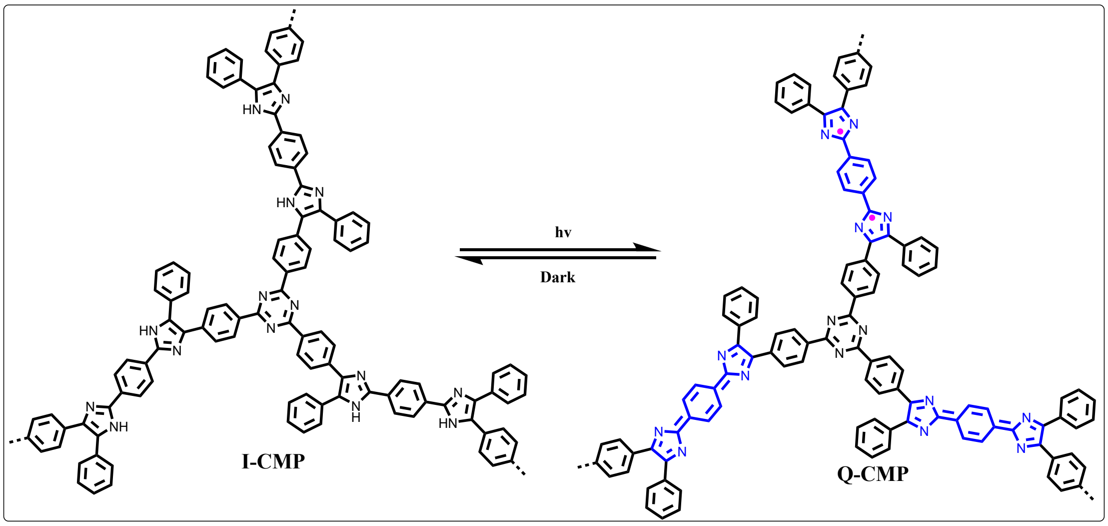
To the solution of **I-MC** (0.19 mmol, 1 eq) in 20 ml of benzene was added by 1 ml of 5M NaOH solution followed by $K_3[Fe(CN)_6]$ (1.94 mmol, 20 eq) and the mixture was stirred at room temperature for about 4 hrs. The organic layer was extracted by benzene to yield greenish blue microcrystal of **Q-MC** in 50% yields.

5. Synthesis of **I-CMP**:



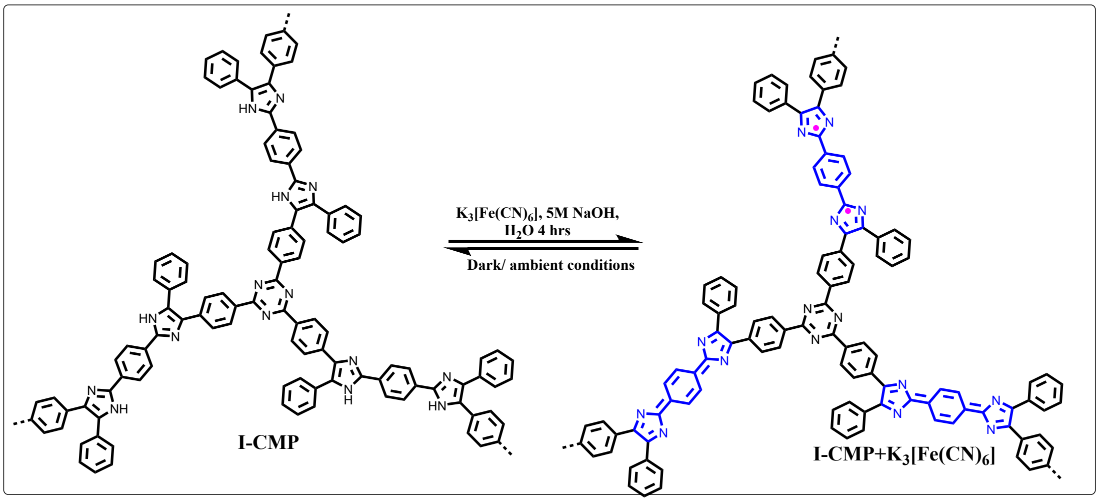
15 ml pressure vessel was charged with 200mg of 1 (0.28 m moles) and 57 mg of terepthaldehyde (0.42 m moles) was added by 0.5 ml of acetic acid and 437 mg of NH_4OAc (5.66 m moles) and 10 ml of chloroform solvent. The mixture was purged with N_2 gas for about 15 minutes and sealed with the lid. The reaction mixture was heated at 120 ˚C for 5 days to yield the insoluble yellow solid. The solid was filtered off and washed with excess of water followed by methanol and DMF to remove the unreactive monomers and the oligomers. Further polymer was purified by Soxhlet extraction with THF solvent and dried for 24 hrs. to yield **I-CMP** in 90% yields.

6. Synthesis of **Q-CMP**:



Q-CMP was obtained by shining sunlight on **I-CMP** for 15 minutes for the complete conversion to **Q-CMP**.

7. Synthesis of **Q-CMP** by chemical treatment:

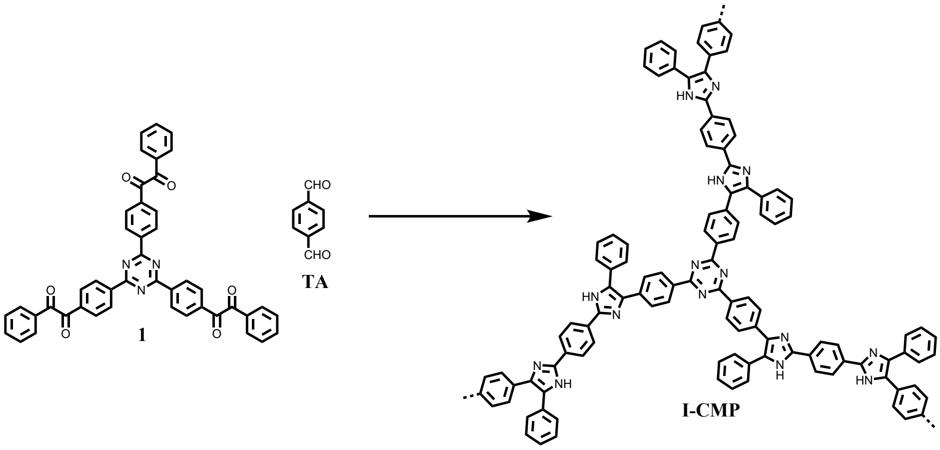


60 mg of **I-CMP** (0.104 mmol) was taken into an RB and added by 1ml of 5M NaOH solution followed by 20 mil of distilled water. The mixture was stirred at RT for about 10 minutes and then added by 348 mg of $K_3[Fe(CN)_6]$ (1.052 mmol). The mixture was stirred at rt for about 4 hrs. The solid was filtered off and washed with excess water to remove NaOH and $K_3[Fe(CN)_6]$ and finally washed with acetone and dried for about 24 hrs. to yield **Q-CMP** in 90% yields.

8. **Photochromic experiment details**: The 2 mg of the polymer was dispersed in 2 ml of a 10 mM solution of KI, $AgNO_3$, NaN_3, Benzoquinone and isopropanol in water. The dispersed solution was kept under light for 15 minutes to see the photochromic changes.

3.Polymer yield calculations:

<u>Percentage yield of I-CMP:</u>



Theoretical yield of ICM= no. of moles of limiting reagent (**1**) * molar mass of one repeating unit.

Theoretical yield = 0.42 m moles*745.89g/mol

Theoretical yield= 313.27 mg

$$\%yield = \frac{Experimental\ yield}{Theoretical\ yield} * 100$$

$$\%yield = \frac{282}{313.27} * 100 = 90\%$$

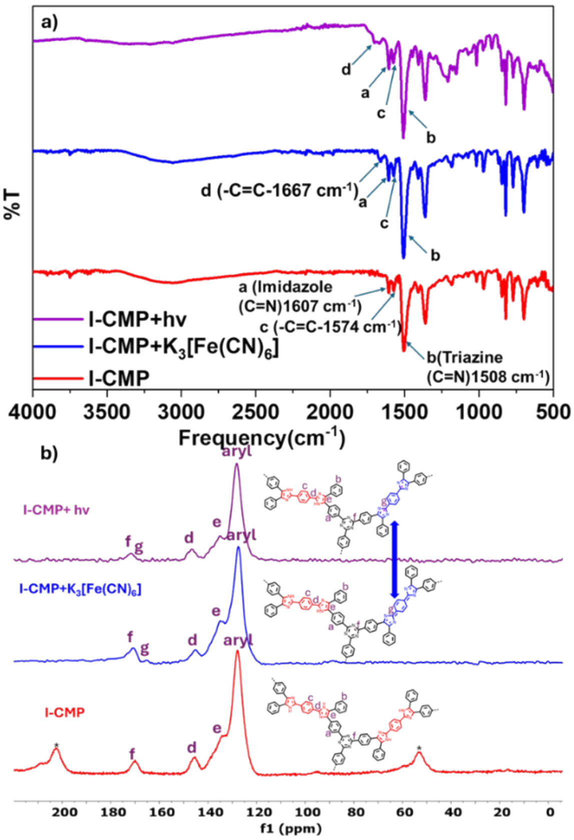


Figure S 1: (a) FT-IR and (b) ^{13}C-CPMAS NMR spectra of **I-CMP**, **I-CMP**+$K_3[Fe(CN)_6]$ and **I-CMP**+hv. *Signal is an artefact from the magic angle spinning.

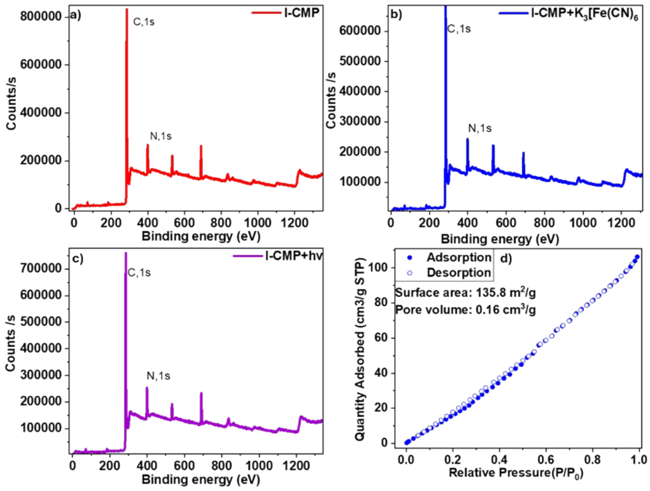


Figure S 2: XPS survey scan spectra of **I-CMP** (a), **I-CMP**+$K_3[Fe(CN)_6]$ (b) and **I-CMP**+hv (c), and the adsorption isotherm of **I-CMP** (d).

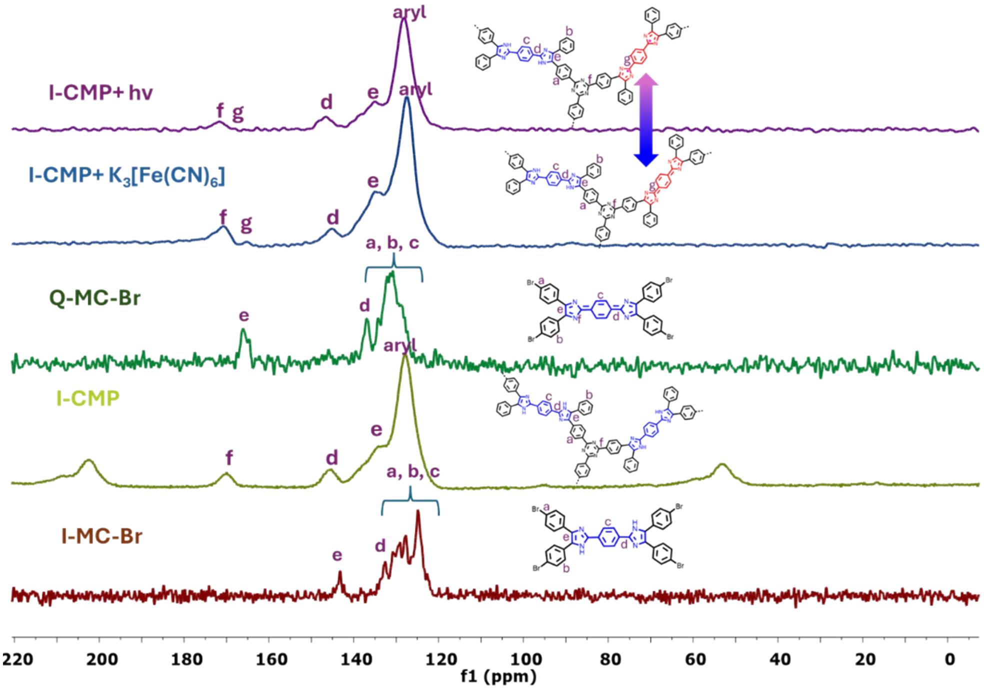


Figure S 3: ^{13}C-CPMAS NMR of **I-MC-Br**, **Q-MC-Br**, **I-CMP**, **I-CMP+K$_3$[Fe(CN)$_6$** and **I-CMP+hv**.

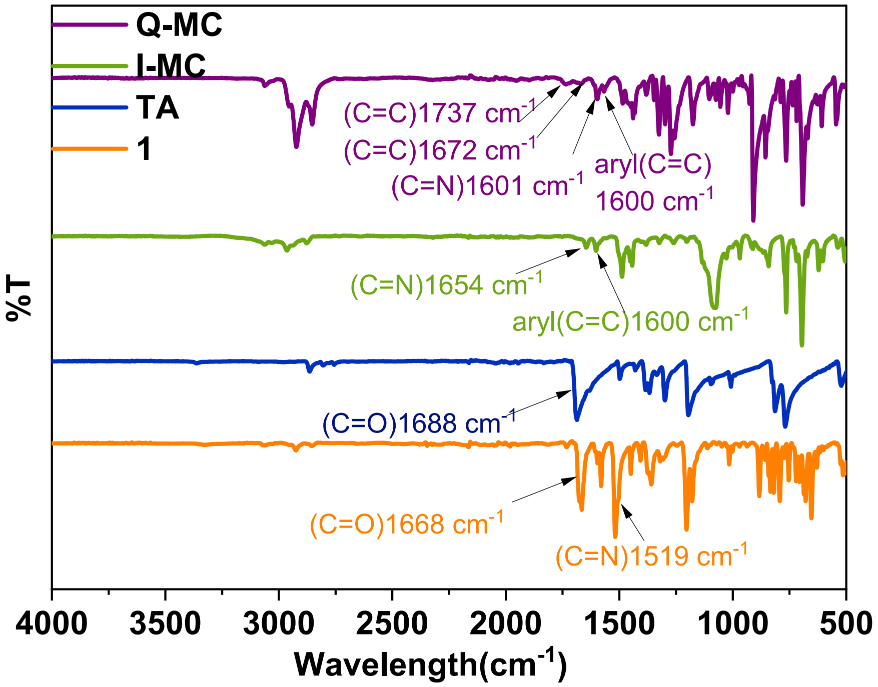


Figure S 4: FTIR spectra of **1**, **TA**, **I-MC**, and **Q-MC**.

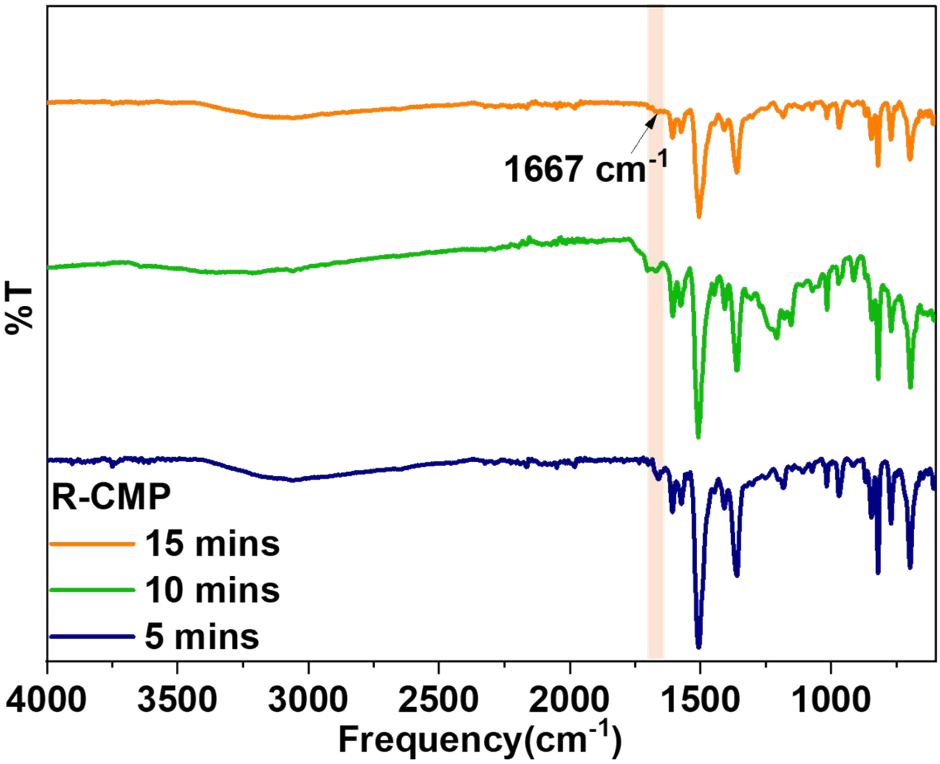


Figure S 5: FTIR spectra of **Q-CMP** at different time interval of light shining.

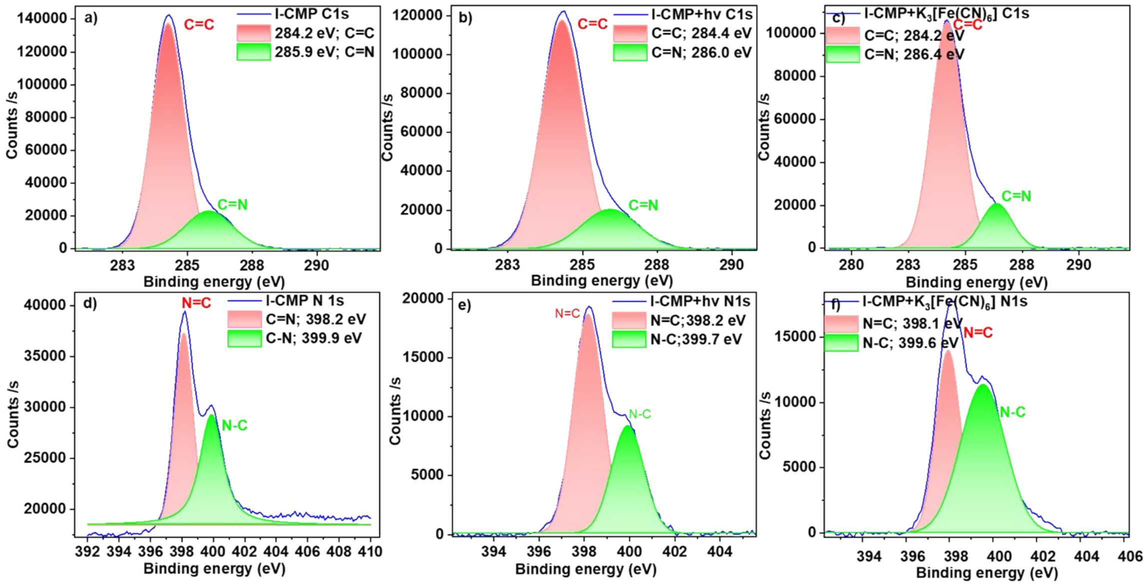


Figure S 6: High resolution XPS spectra of **I-CMP**, **I-CMP+hv** and **I-CMP+K$_3$[Fe(CN)$_6$]**.

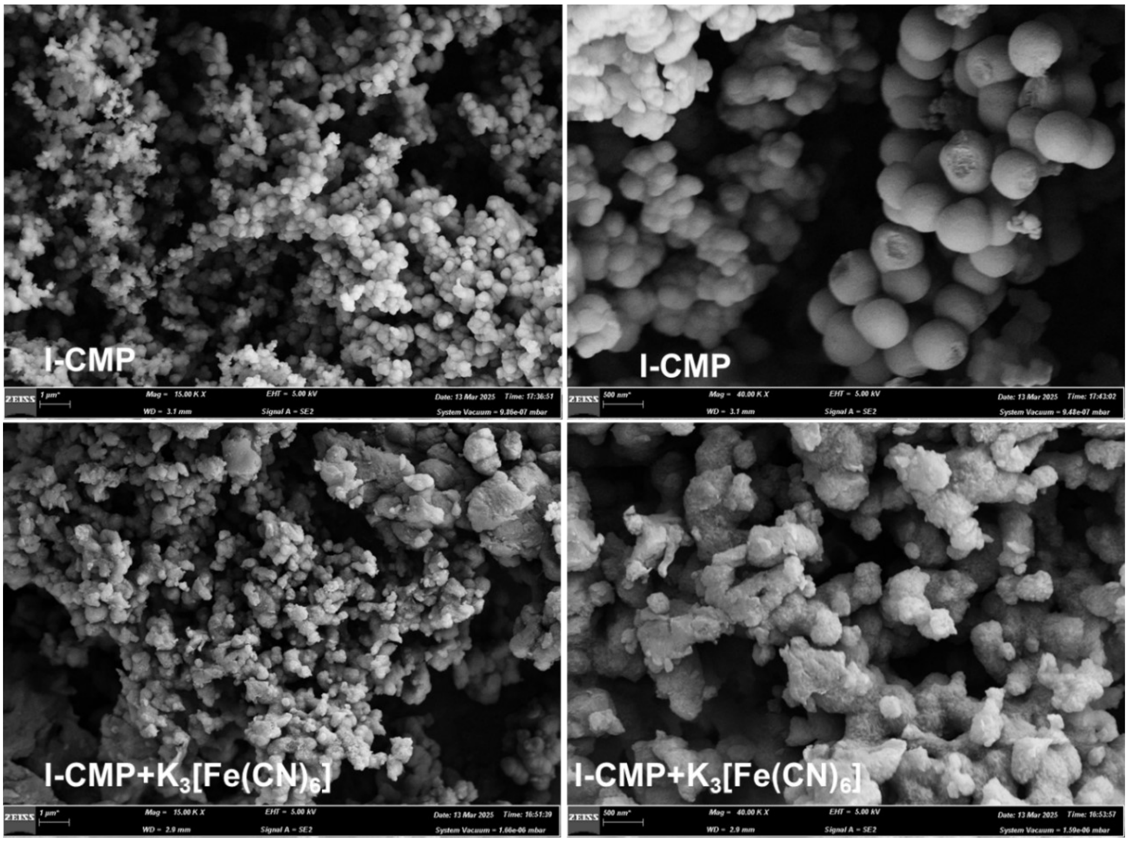


Figure S 7: FE-SEM images of **I-CMP** and **I-CMP+K$_3$[Fe(CN)$_6$]** at 1μm and 500 nm magnification scale.

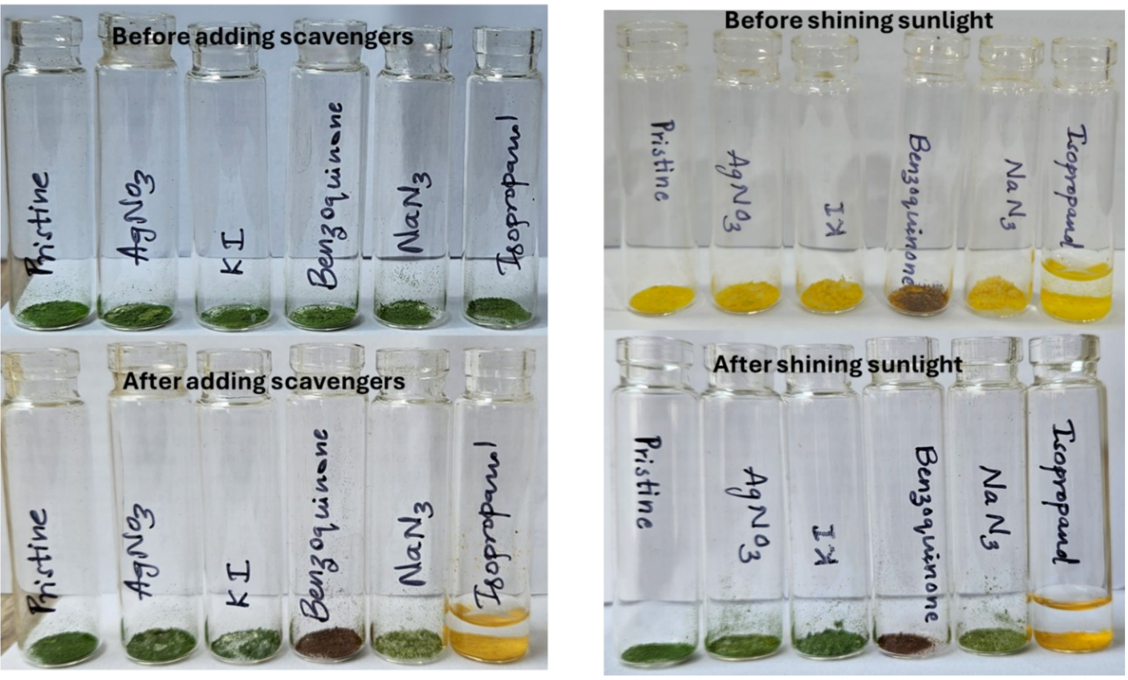


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Figure S 8: Images of **Q-CMP** before and after adding scavengers (left side) and mages of **I-CMP** before and after shining the light with scavengers (right side).

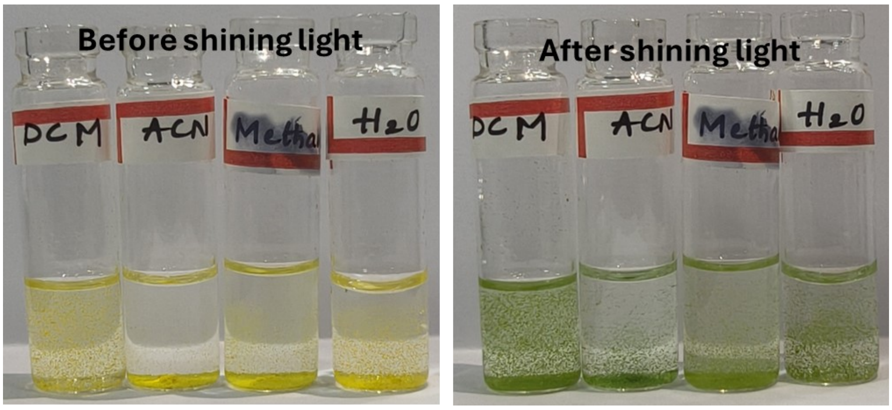


Figure S 9: Photochromic studies of **I-CMP** in dichloromethane, acetonitrile, methanol and water.

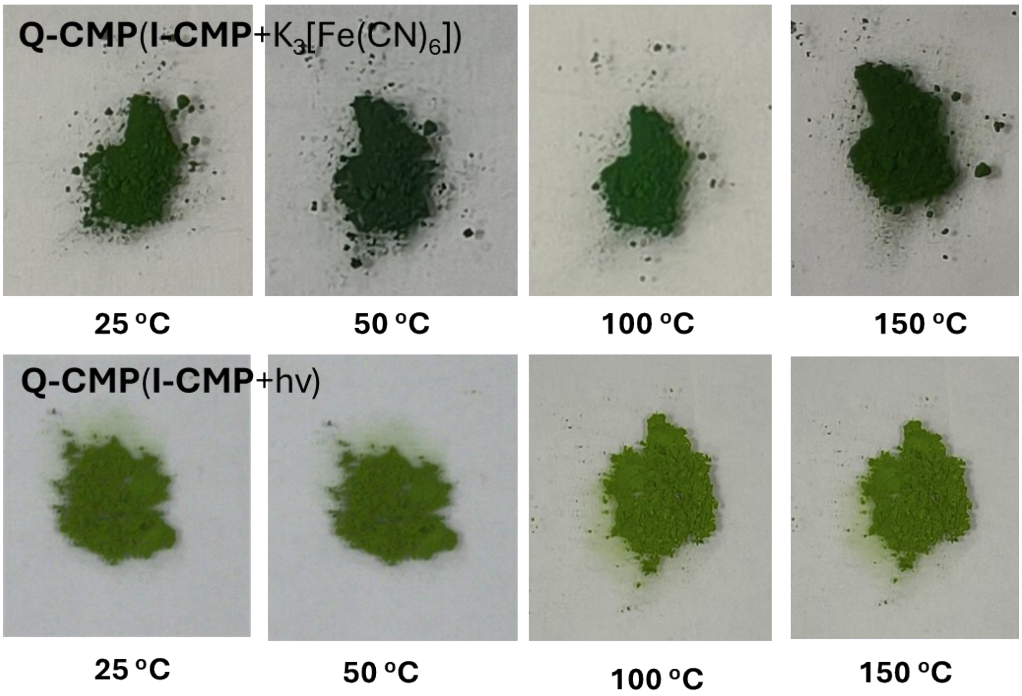
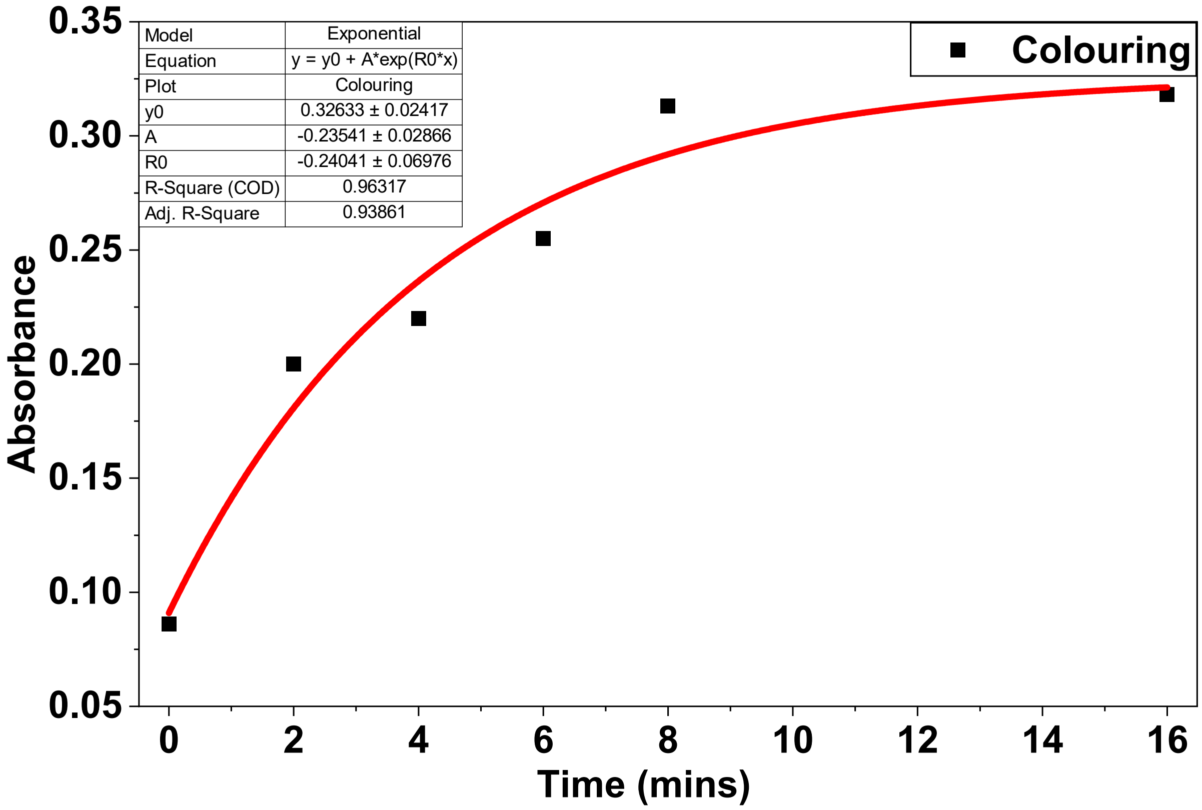


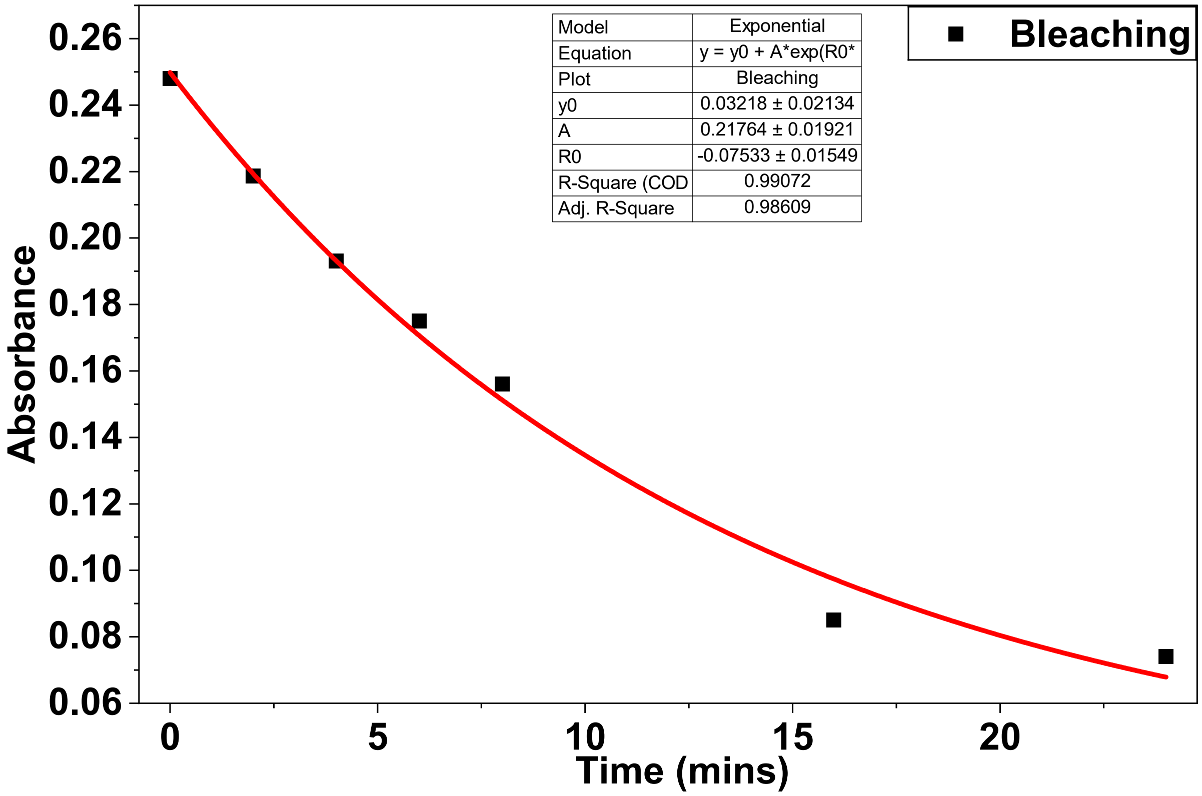
Figure S 10: The images of photochromic reversibility test of **Q-CMPs** at different temperatures.

Rate constant of colouring and bleaching is 2.04 X10^{-1} min^{-1} and 7.5 X 10^{-2} min^{-1}with half-life of 3.39 min and 9.20 min respectively.



Model	Exponential
Equation	y = y0 + A*exp(R0*x)
Plot	Colouring
y0	0.32633 ± 0.02417
A	-0.23541 ± 0.02866
R0	-0.24041 ± 0.06976
R-Square (COD)	0.96317
Adj. R-Square	0.93861

Figure S 11: Kinetic study of photochromic colouring state of **I-CMP** at ambient conditions.



Model	Exponential
Equation	y = y0 + A*exp(R0*
Plot	Bleaching
y0	0.03218 ± 0.02134
A	0.21764 ± 0.01921
R0	-0.07533 ± 0.01549
R-Square (COD	0.99072
Adj. R-Square	0.98609

Figure S 12: Kinetic study of photochromic bleaching state of **Q-CMP** by keeping it under dark.

The photochromism under inert and dry atmosphere were performed by taking 5 mg of oven dried polymer, **I-CMP** before the experiment was added by dry dichloromethane solvent and exposed to sunlight.

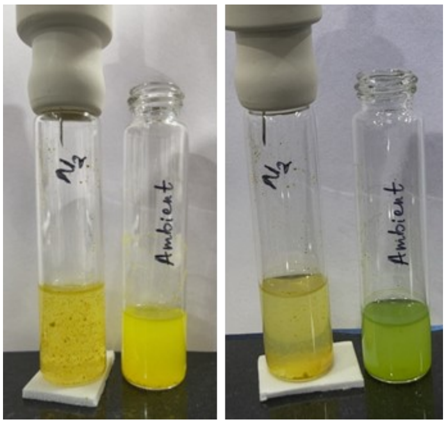


Figure S 13: Photochromism of **I-CMP** in dry dichloromethane solvent under inert and ambient conditions, left photo before shining the light right one is after shining the light.

The photochromism under inert and dry atmosphere were performed by taking 5 mg of oven dried polymer, **I-CMP** before the experiment and exposed to sunlight.

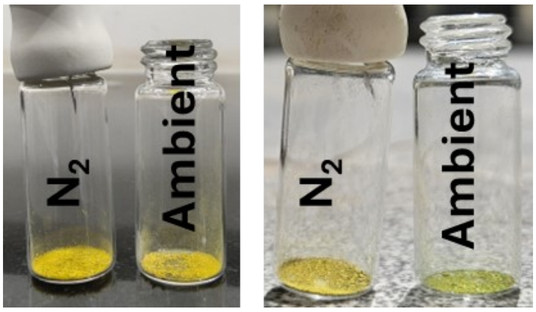


Figure S 14: Photochromism of **I-CMP** in the dry and ambient conditions, left side (before shining the light) right side (after shining the light).

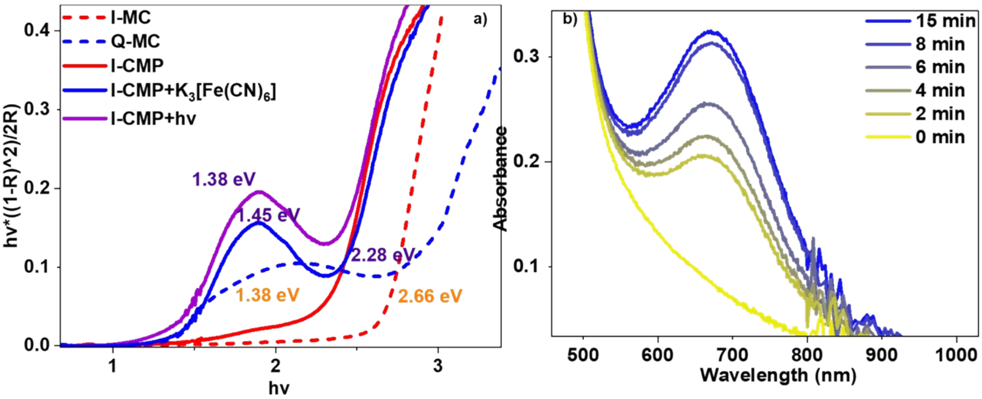


Figure S 15: Diffused reflectance absorption spectra of **I-MC**, **Q-MC**, **I-CMP**, **I-CMP+K_3[Fe(CN)$_6$]** and **I-CMP+hv** (a) and time-dependent photochromic changes of **I-CMP** (b).

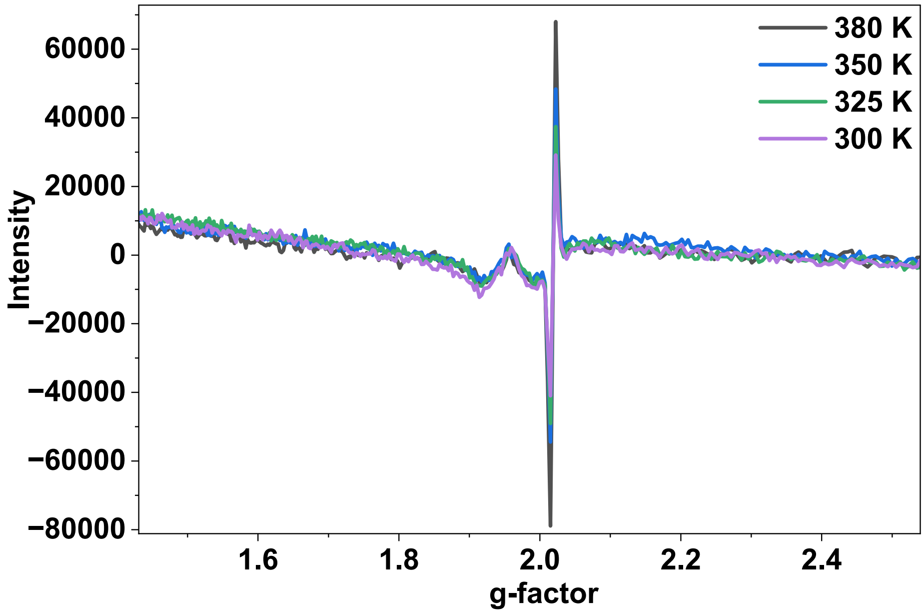


Figure S 16 : EPR spectra of powder **Q-CMP** (**I-CMP**+ $K_3[Fe\ (CN)_6]$ measured at variable temperatures.

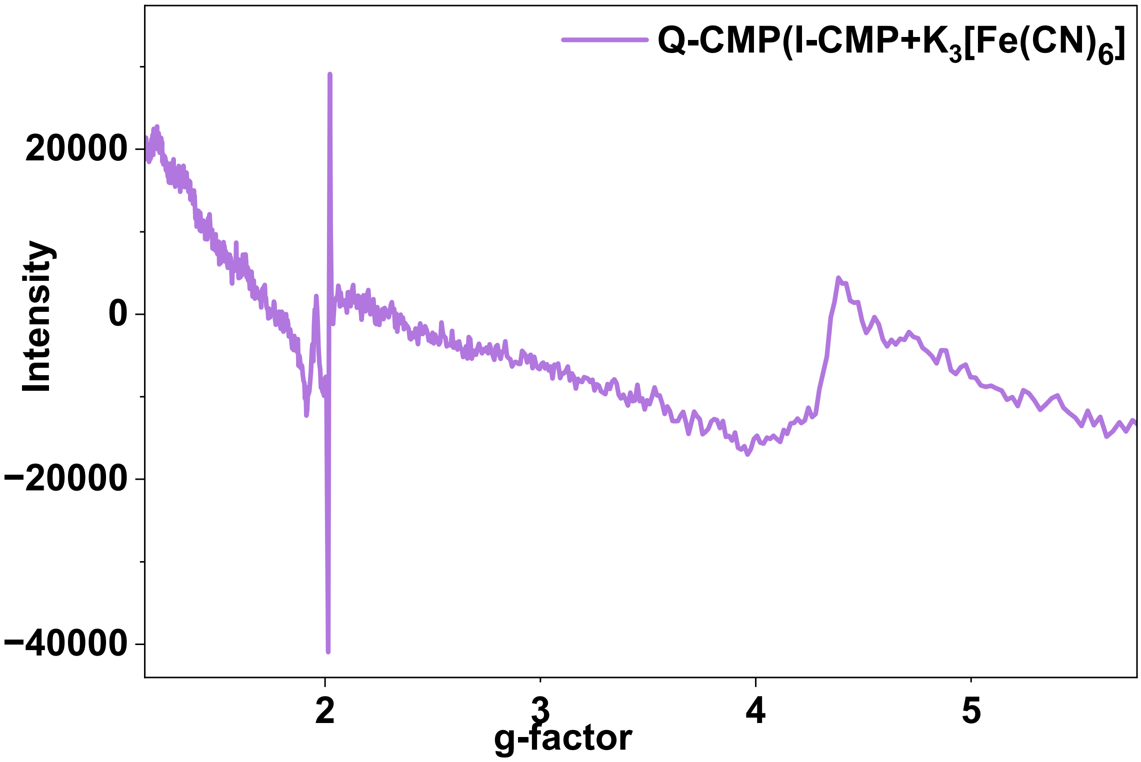
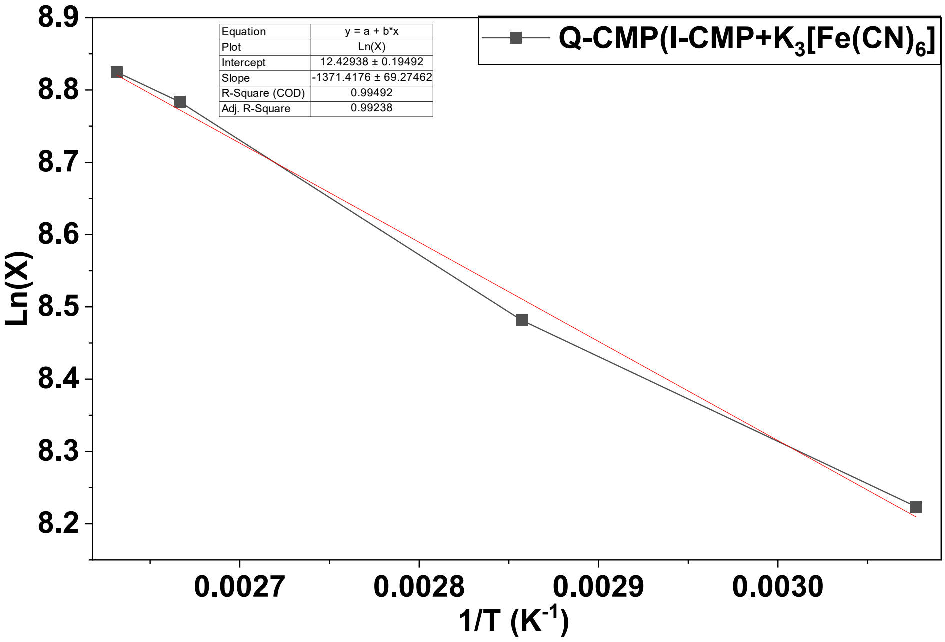


Figure S 17: Wide field EPR spectra of powder **Q-CMP** (**I-CMP**+ $K_3[Fe\ (CN)_6]$ measured at 300K.



Equation	y = a + b*x
Plot	Ln(X)
Intercept	12.42938 ± 0.19492
Slope	-1371.4176 ± 69.27462
R-Square (COD)	0.99492
Adj. R-Square	0.99238

Figure S 18: Double-integrated intensity analysis of EPR signals versus 1/T using a van't Hoff analysis

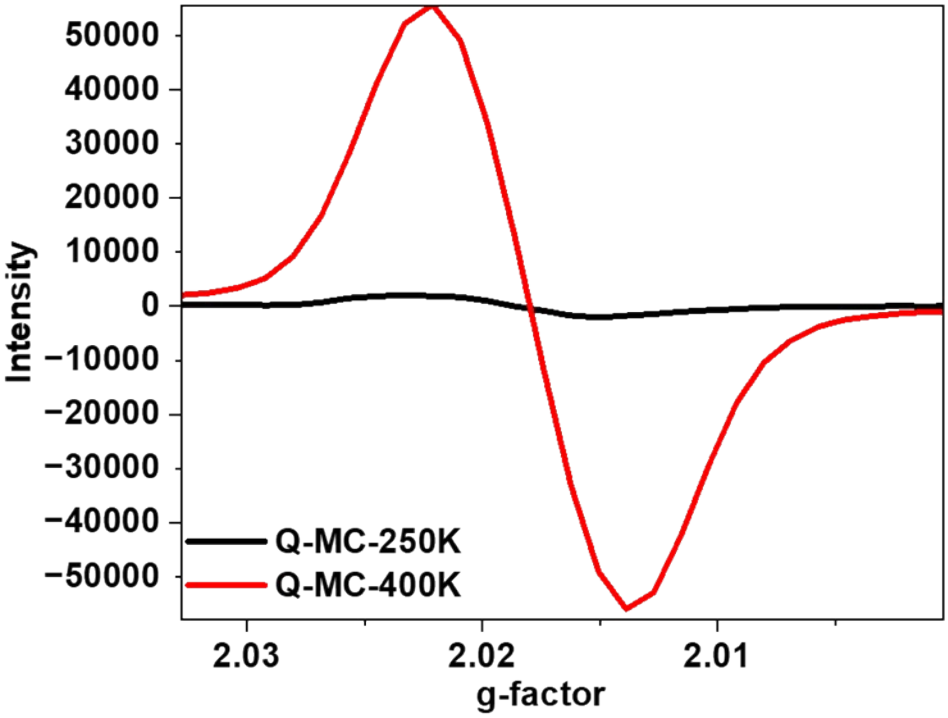


Figure S 19 : VT-EPR spectra of **Q-MC** in powder form.

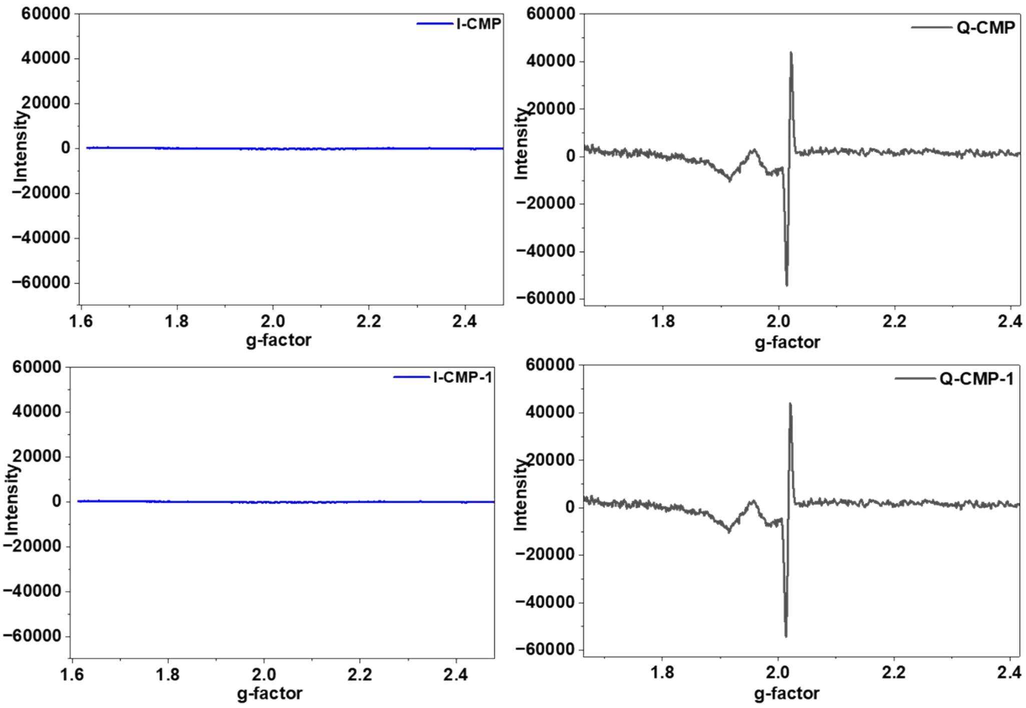
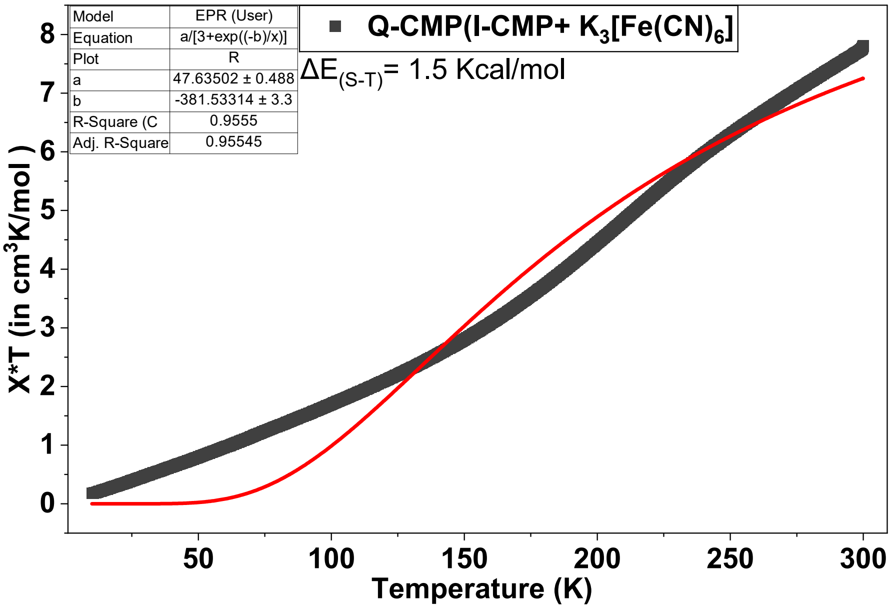


Figure S 20: EPR spectra of **I-CMP** photochromic cycle in powder form.



Model	EPR (User)
Equation	a/[3+exp((-b)/x)]
Plot	R
a	47.63502 ± 0.488
b	-381.53314 ± 3.3
R-Square (C	0.9555
Adj. R-Square	0.95545

Figure S 21: SQUID magnetometry data of **Q-CMP[I-CMP+$K_3Fe(CN)_6$]** obtained in the powder form at constant field of 5000 Oe and varying the temperature from 2-300 K. Magnetic moment data is converted to magnetic susceptibility as a function of temperature and fitted by using Bleaney-Bowers equation (Red line).

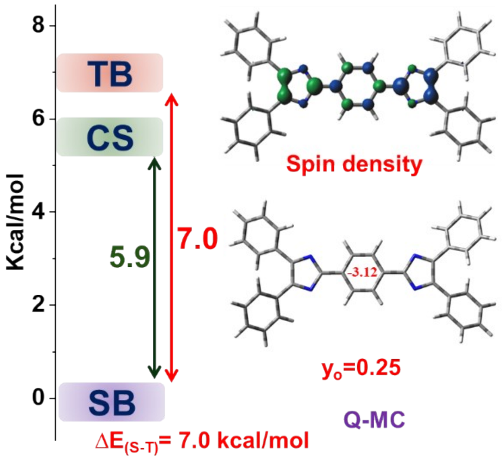
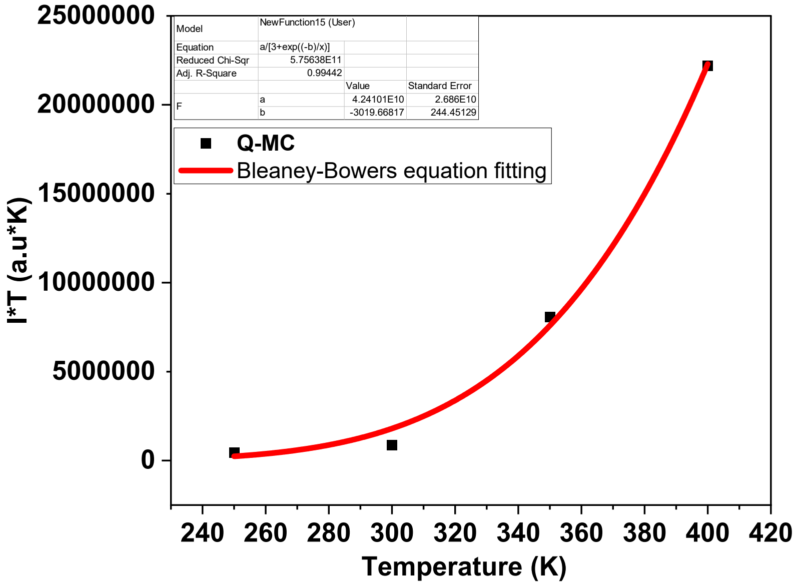


Figure S 22: DFT computed $\Delta E_{(S\text{-}T)}$, spin density, biradical character (y_0) and aromaticity of the central phenyl ring by NICS(0) (Nucleus independent chemical shift method) of **Q-MC**.



Model	NewFunction15 (User)		
Equation	a/[3+exp((-b)/x)]		
Reduced Chi-Sqr	5.75638E11		
Adj. R-Square	0.99442		
		Value	Standard Error
F	a	4.24101E10	2.686E10
	b	-3019.66817	244.45129

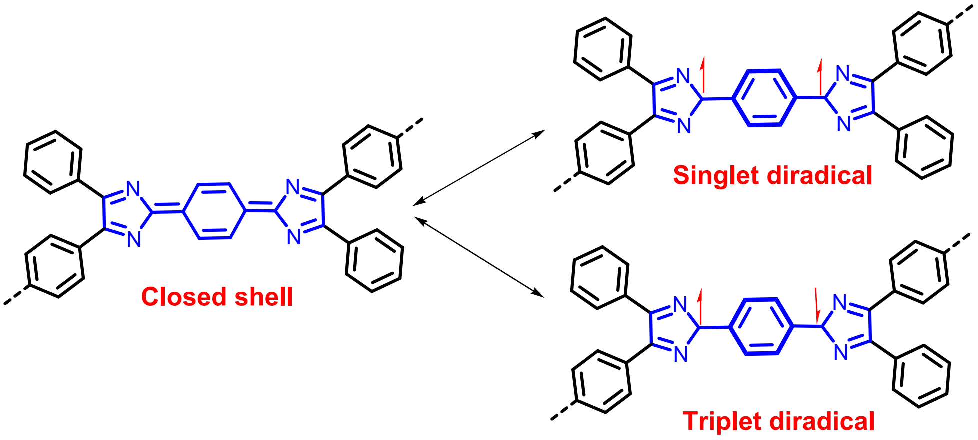
Figure S 23: I*T vs T from EPR data of **Q-MC** in toluene solvent at different temperatures under ambient atmosphere. Red line is fitted data by using Bleaney-Bowers equation.

4. DFT calculations:

CS stands for closed shell, indicating all the electrons are paired.

SD (earlier SB) stands for singlet diradical, indicating the electrons are not paired but present in degenerate orbitals with opposite spins.

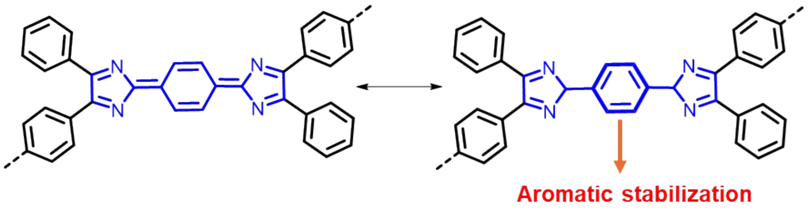
TD (earlier TB) stands for triplet diradical, indicating the electrons are not paired but present in degenerate orbitals with the same spins.



Generally, the pro-aromatic quinoidal molecules having extended π-electron delocalisation will undergo a transformation towards an open-shell system to attain aromatic stabilisation. For such systems, the ground state would most probably be the SD state with an accessible TD state. The lower the energy gap ($\Delta E_{(S-T)}$) between singlet and triplet states, the higher the open-shell diradical character, due to the thermally accessible paramagnetic triplet state.

DFT calculations on TIT revealed that the ground state is the SD state with an energy gap between the singlet and triplet states of $\Delta E_{(S-T)}$ = 5.9 kcal/mol. This energy is sufficient to thermally access the triplet state at room temperature, forming a diradicaloid. In addition, the natural orbital occupation number (NOON) calculations compute the diradical character value (y_0) of the fragment to be 25%.

Since the pro-aromatic molecules transform to an open-shell system to attain aromatic stabilisation by generating benzenoid structures, Nucleus Independent Chemical Shift (NICS (0)) calculations were carried out by GIAO-UCAMB3LYP/6311G (d, p) method, to evaluate the aromaticity of the central benzene ring. Typically, the higher the negative NICS value, the more aromatic the benzene ring would be, which in turn supports its open-shell nature. The polymeric fragment (**TIT**) has been found to have -4.35 ppm, indicating that the central phenyl unit possesses benzene-like character and will have aromatic stabilisation energy.



The biradical character value (y_0) has been evaluated by using the Natural orbital occupation number (NOON) calculations. Generally, y_0 value ranges from 0 to 1; zero indicates an absolute closed shell, and one indicates a complete open-shell nature. The TIT fragment showed a y_0 value of 0.25, indicating that this unit consists of a diradicaloid nature.

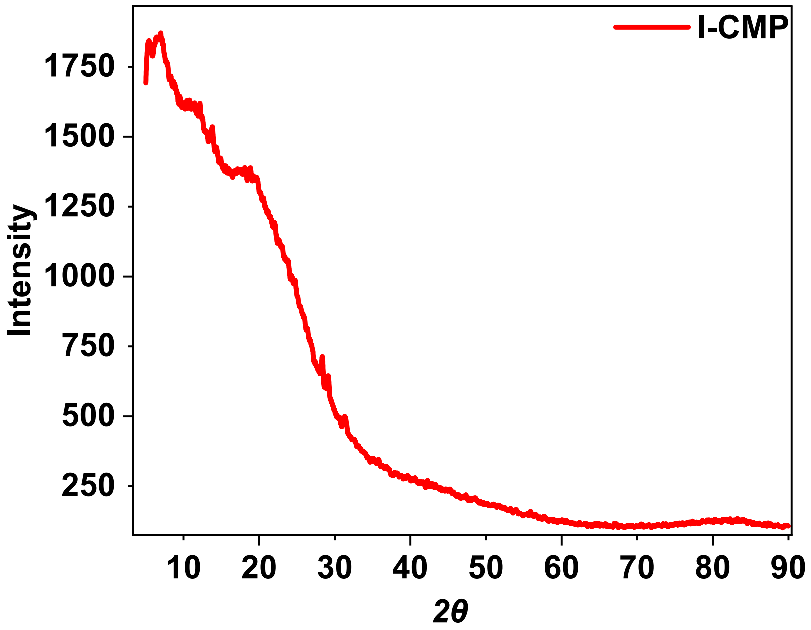


Figure S 24: Powder XRD spectra of **I-CMP**.

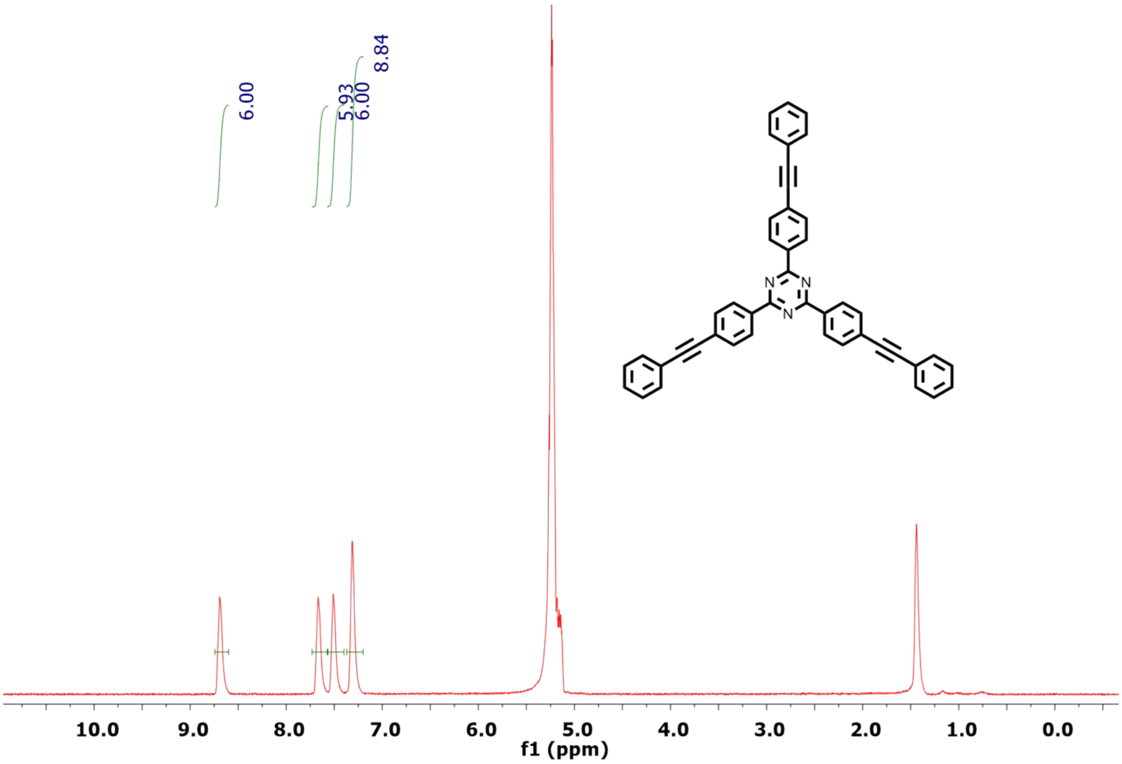


Figure S 25: ^{1}H NMR of 2,4,6-tris(4-(phenylethynyl)phenyl)-1,3,5-triazine recorded in CH_2Cl_2.

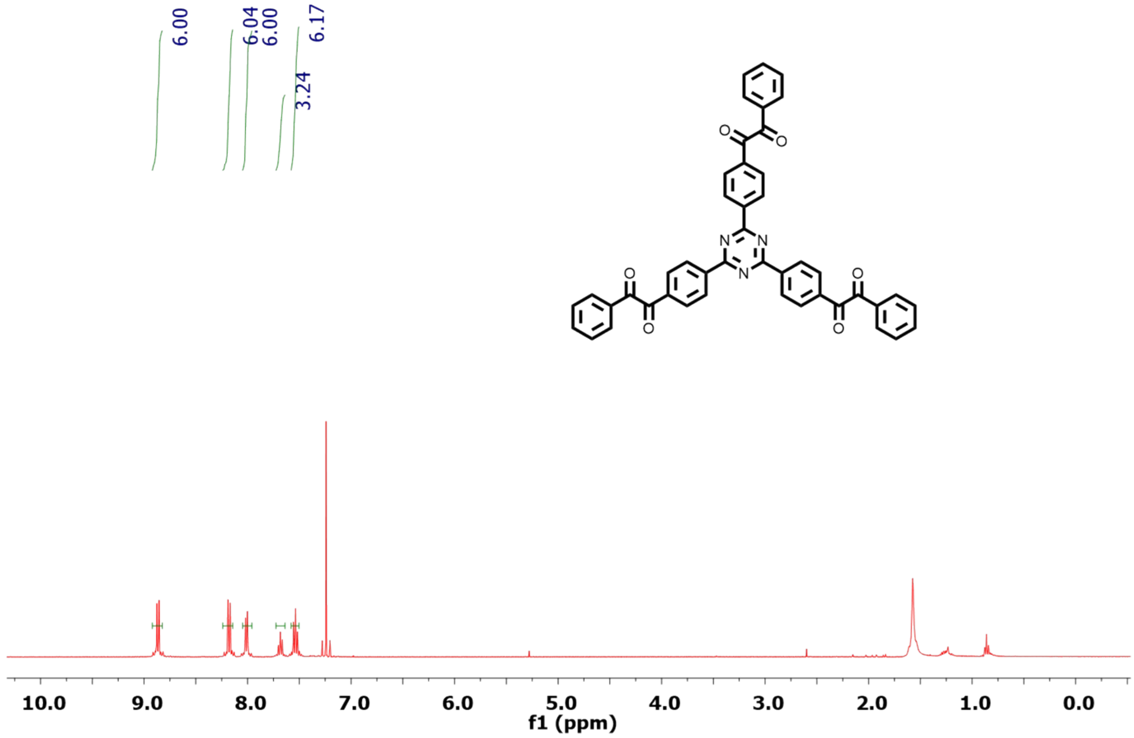


Figure S 26: ^{1}H NMR of **1** recorded in $CDCl_3$.

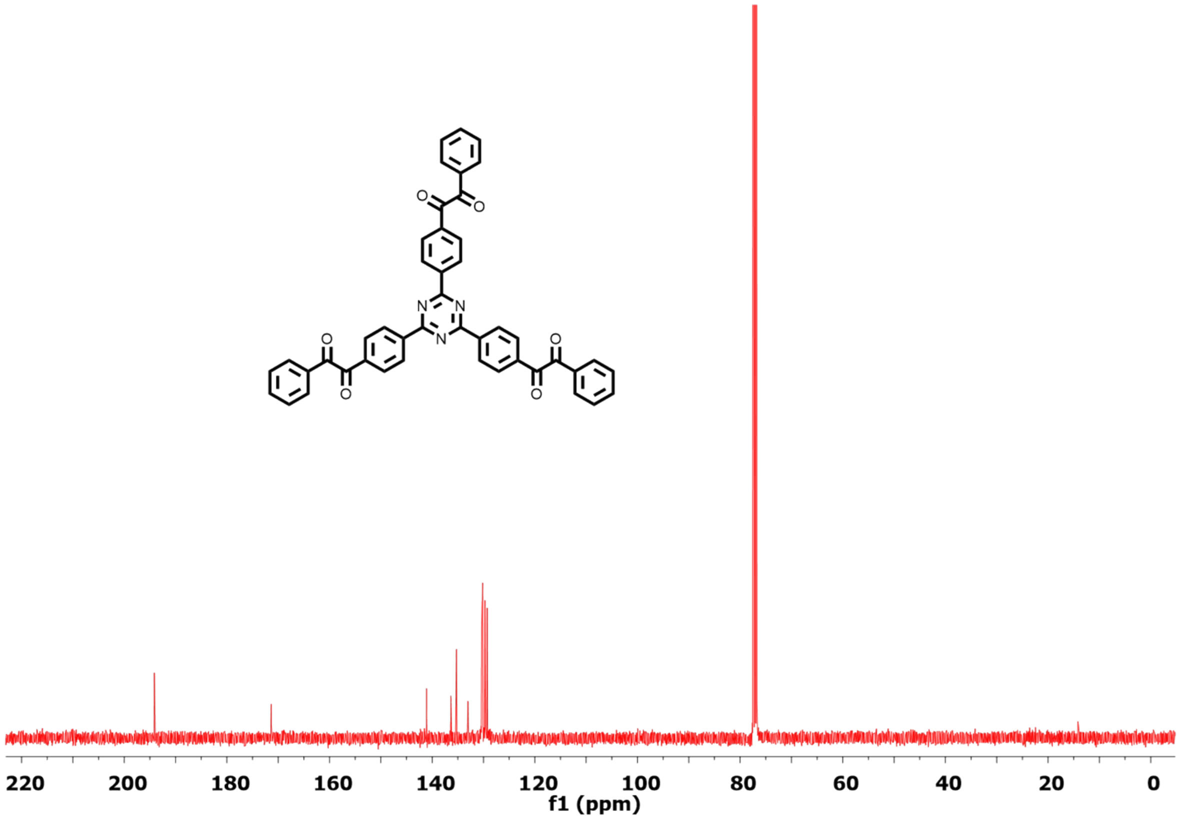


Figure S 27: ^{13}C NMR of **1** recorded in $CDCl_3$.

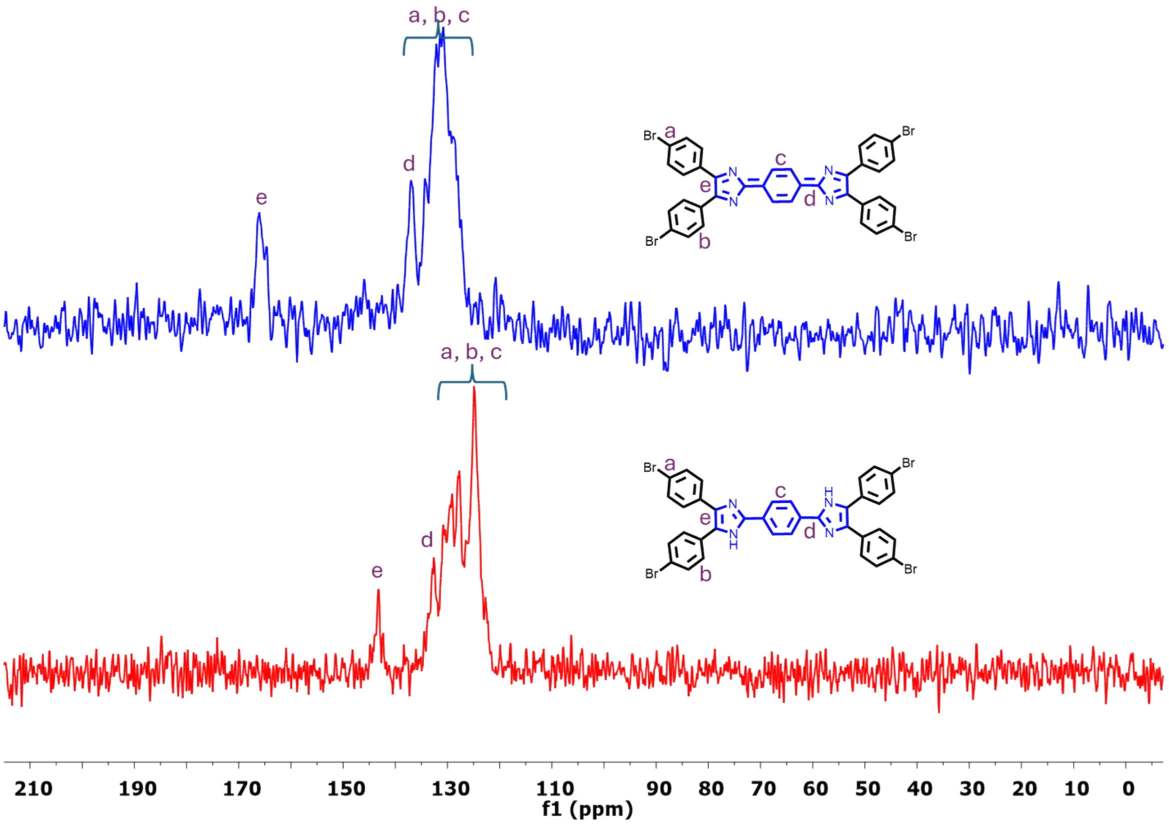


Figure S 28: ^{13}C-CPMAS NMR of **I-MC-Br** and **Q-MC-Br**.

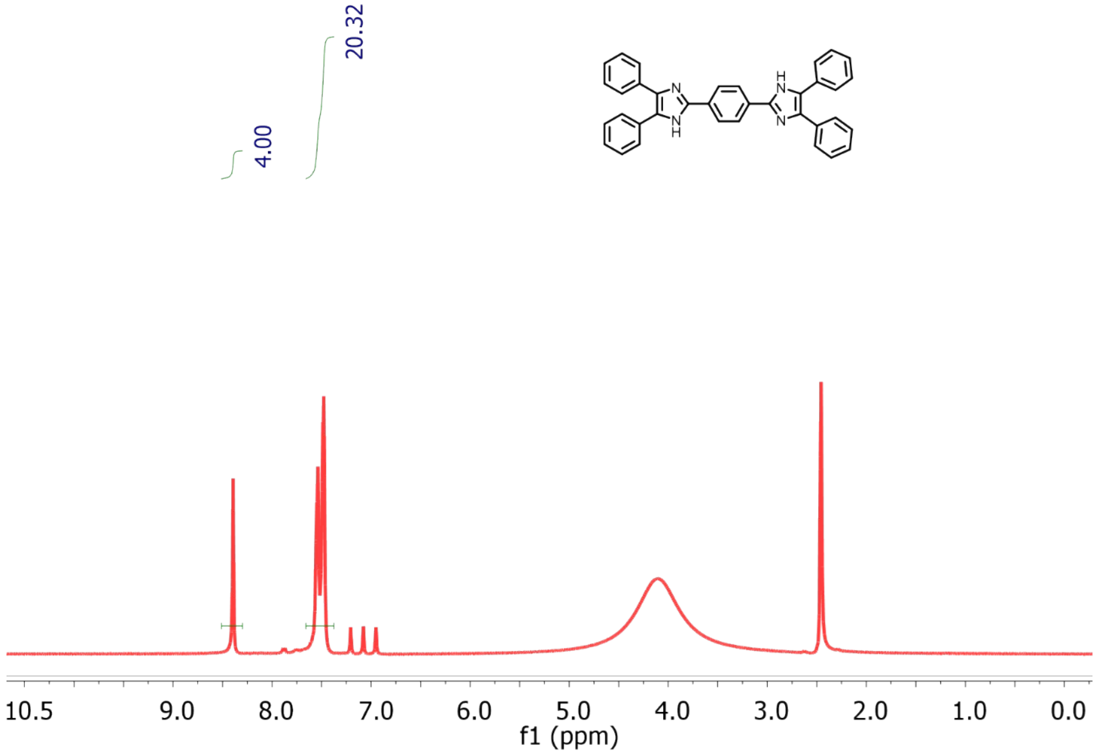


Figure S 29: ^{1}H NMR of **I-MC** recorded in DMSO-d6.

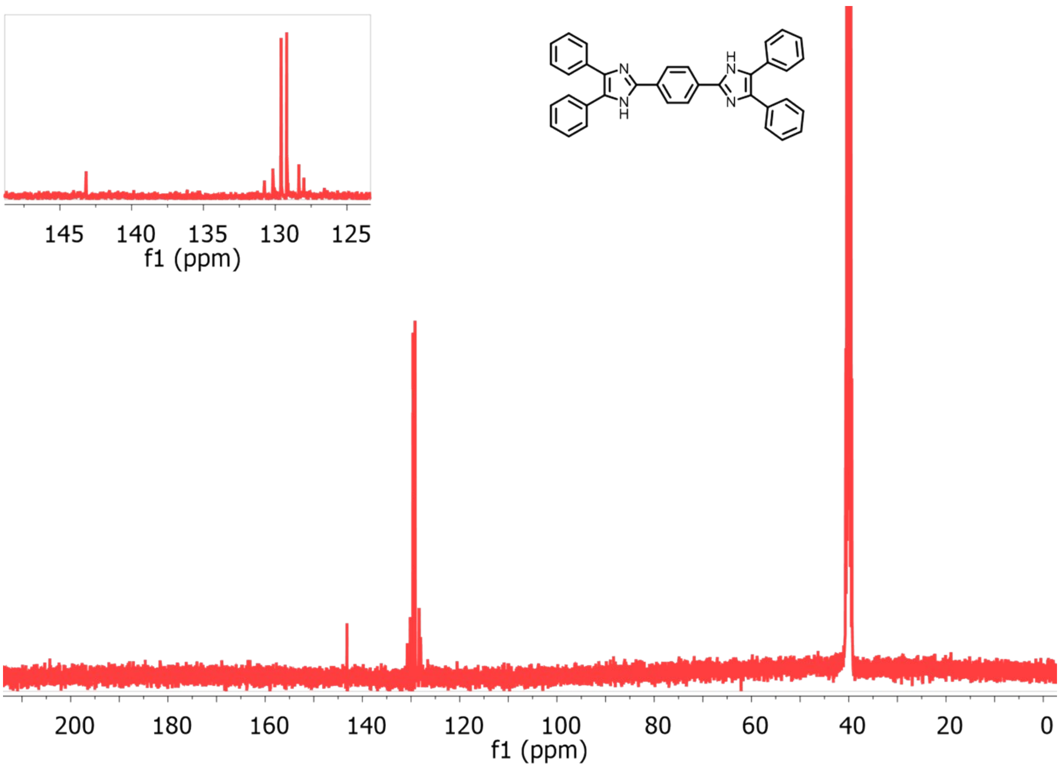


Figure S 30: ^{13}C NMR of **I-MC** recorded in DMSO-d6.

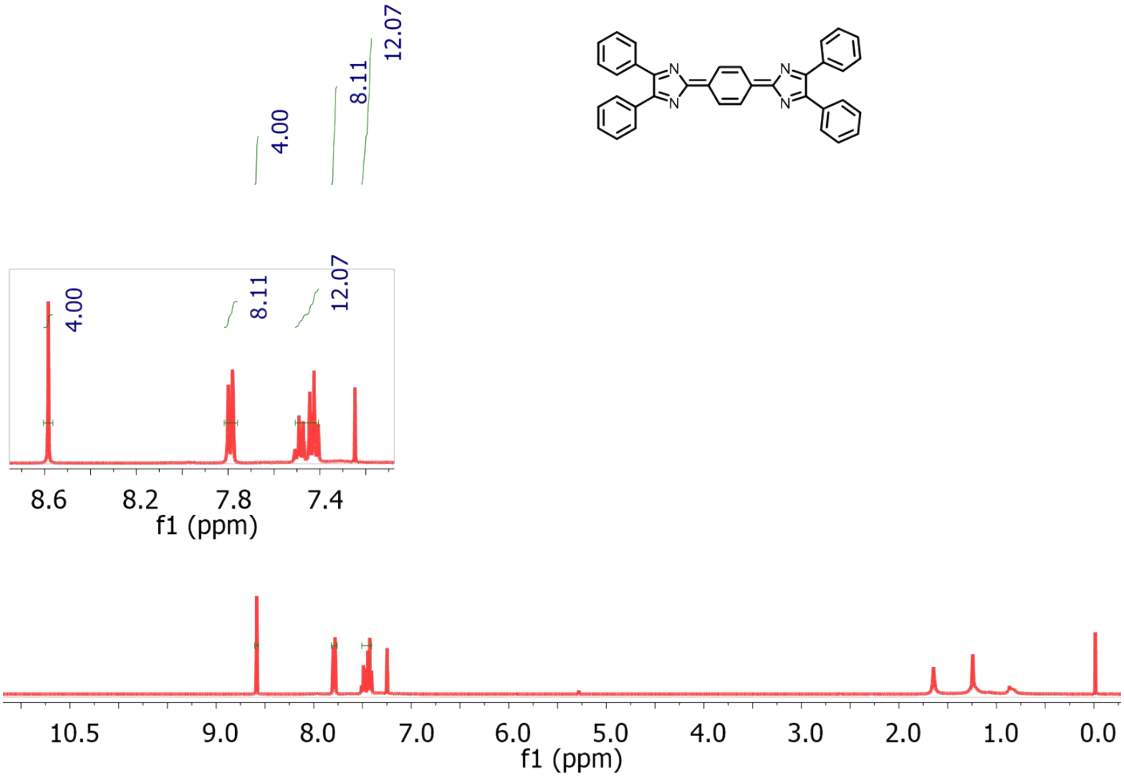


Figure S 31: ^{1}H NMR of **Q-MC** recorded in $CDCl_3$.

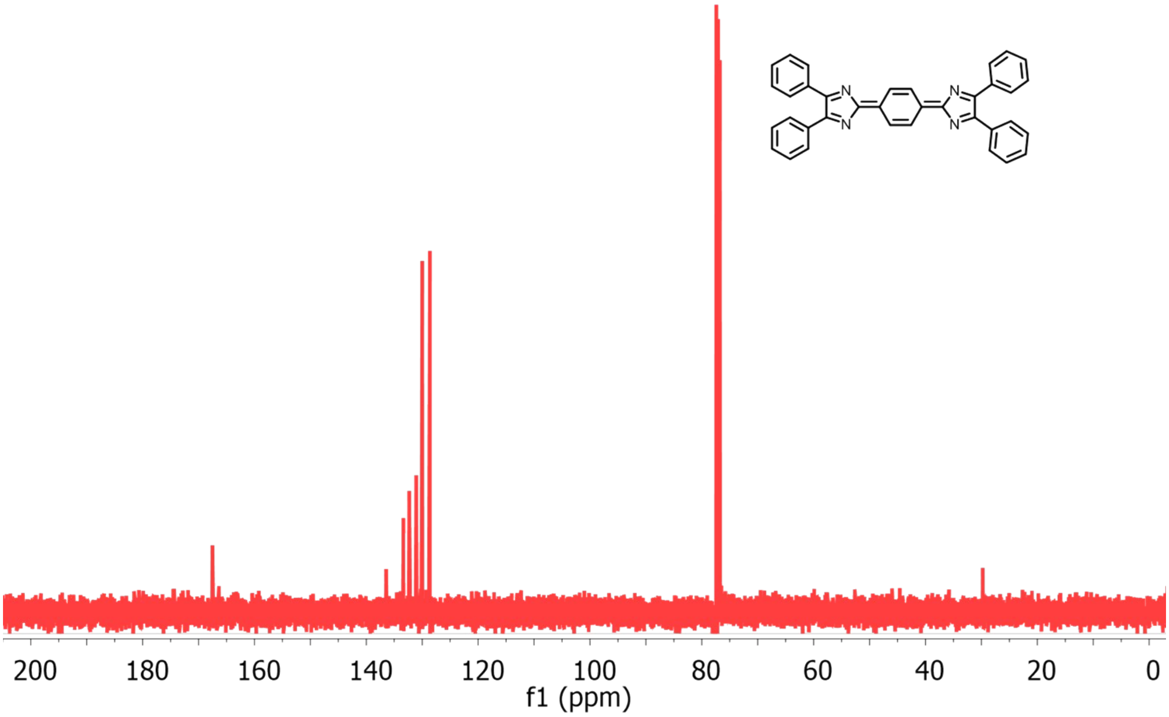


Figure S 32: ^{13}C NMR of **Q-MC** recorded in CDCl$_3$.

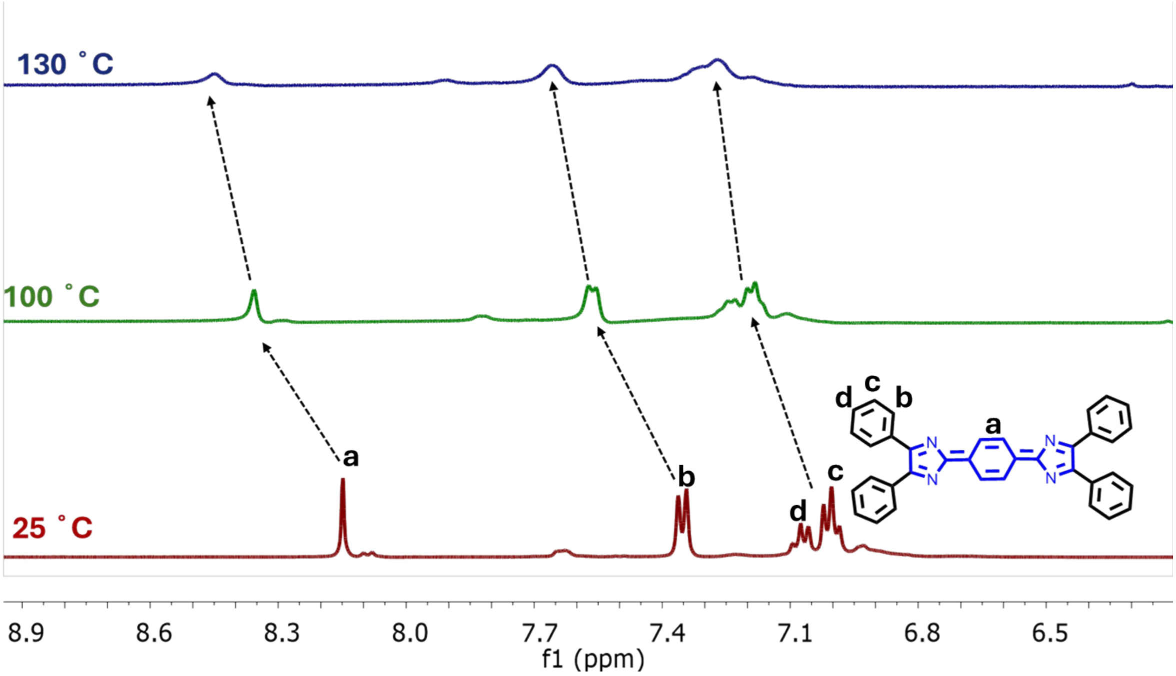


Figure S 33: Variable temperature ^{1}H NMR of **Q-MC** recorded in tetrachloroethane solvent.

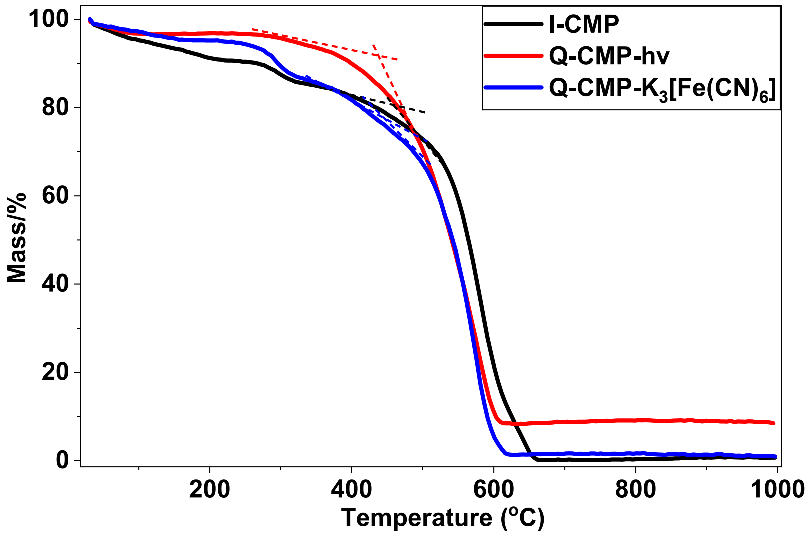


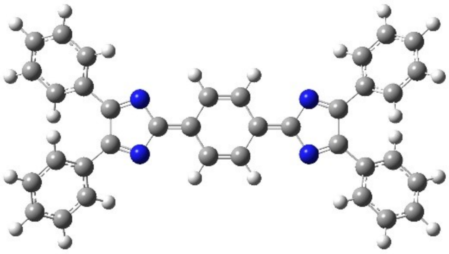
Figure S 34: Thermal gravimetric analysis of **I-CMP**, **Q-CMP(I-CMP+hv)** and **Q-CMP(I-CMP+K$_3$[Fe(CN)$_6$])**.

Cartesian co-ordinates used for the DFT calculations:

1. **Q0 DFT calculation coordinates:**

   Zero imaginary frequencies in all the calculations.

Closed shell:



rcam-b3lyp/6-311g(d,p)

Charge = 0 Multiplicity = 1

Sum of electronic and thermal energies= -1604.212169

Sum of electronic and thermal enthalpies= -1604.211224

Sum of electronic and thermal free energies= -1604.308225

C	0.67536	-1.23821	0.00055
C	-0.67532	-1.23821	-0.00047
C	-1.41174	0.00001	0.
C	-0.67532	1.23823	0.00049
C	0.67537	1.23822	-0.00053
C	1.41178	0.	0.00002
H	1.24459	-2.15957	-0.00052
H	-1.24456	-2.15956	0.00065
H	-1.24455	2.15958	-0.00064

H	1.2446	2.15958	0.00055
C	2.79166	0.	0.00002
C	4.7893	-0.74291	-0.0177
C	4.7893	0.74291	0.01775
C	-2.79162	0.00001	0.
C	-4.78925	-0.74289	0.01772
C	-4.78925	0.74293	-0.01774
N	3.55113	-1.15724	-0.01
N	3.55113	1.15724	0.01005
N	-3.55109	-1.15722	0.01009
N	-3.55108	1.15725	-0.0101
C	5.90904	-1.6907	-0.09615
C	7.08479	-1.39406	-0.79303
C	5.76713	-2.95543	0.48626
C	8.09867	-2.33765	-0.89284
H	7.19912	-0.429	-1.2724
C	6.7851	-3.89159	0.39219
H	4.84567	-3.18553	1.00849
C	7.95507	-3.58495	-0.2964
H	9.0023	-2.09808	-1.44362
H	6.66608	-4.86553	0.85558
H	8.75095	-4.31882	-0.37144
C	5.90904	1.6907	0.09622
C	7.08478	1.39406	0.79314
C	5.76716	2.95541	-0.48622
C	8.09865	2.33764	0.89297
H	7.19908	0.429	1.27253
C	6.78513	3.89157	-0.39213
H	4.84571	3.18551	-1.00848
C	7.95508	3.58494	0.2965
H	9.00226	2.09808	1.44377
H	6.66613	4.8655	-0.85554
H	8.75096	4.3188	0.37155
C	-5.90902	-1.69065	0.09612
C	-7.08485	-1.39392	0.79283
C	-5.76709	-2.95542	-0.48619
C	-8.09877	-2.33747	0.89259
H	-7.19921	-0.42881	1.2721
C	-6.7851	-3.89155	-0.39217
H	-4.84557	-3.18559	-1.0083
C	-7.95514	-3.58482	0.29626
H	-9.00246	-2.09782	1.44324
H	-6.66605	-4.86552	-0.85548
H	-8.75105	-4.31865	0.37126
C	-5.90901	1.69069	-0.09614
C	-5.7671	2.95544	0.48621

C	-7.08482	1.39398	-0.79291
C	-6.7851	3.89157	0.39217
H	-4.8456	3.18559	1.00836
C	-8.09873	2.33753	-0.89268
H	-7.19916	0.42888	-1.27221
C	-7.95512	3.58487	-0.29631
H	-6.66607	4.86553	0.85552
H	-9.0024	2.0979	-1.44336
H	-8.75103	4.31871	-0.37131

Singlet diradical:

ucam-b3lyp/6-311g(d,p)

Charge = 0 Multiplicity = 1

Sum of electronic and thermal energies= -1604.212360
Sum of electronic and thermal enthalpies= -1604.211415
Sum of electronic and thermal free energies= -1604.310041

C	0.67536	-1.23821	0.00055
C	-0.67532	-1.23821	-0.00047
C	-1.41174	0.00001	0.
C	-0.67532	1.23823	0.00049
C	0.67537	1.23822	-0.00053
C	1.41178	0.	0.00002
H	1.24459	-2.15957	-0.00052
H	-1.24456	-2.15956	0.00065
H	-1.24455	2.15958	-0.00064
H	1.2446	2.15958	0.00055
C	2.79166	0.	0.00002
C	4.7893	-0.74291	-0.0177
C	4.7893	0.74291	0.01775
C	-2.79162	0.00001	0.

C	-4.78925	-0.74289	0.01772
C	-4.78925	0.74293	-0.01774
N	3.55113	-1.15724	-0.01
N	3.55113	1.15724	0.01005
N	-3.55109	-1.15722	0.01009
N	-3.55108	1.15725	-0.0101
C	5.90904	-1.6907	-0.09615
C	7.08479	-1.39406	-0.79303
C	5.76713	-2.95543	0.48626
C	8.09867	-2.33765	-0.89284
H	7.19912	-0.429	-1.2724
C	6.7851	-3.89159	0.39219
H	4.84567	-3.18553	1.00849
C	7.95507	-3.58495	-0.2964
H	9.0023	-2.09808	-1.44362
H	6.66608	-4.86553	0.85558
H	8.75095	-4.31882	-0.37144
C	5.90904	1.6907	0.09622
C	7.08478	1.39406	0.79314
C	5.76716	2.95541	-0.48622
C	8.09865	2.33764	0.89297
H	7.19908	0.429	1.27253
C	6.78513	3.89157	-0.39213
H	4.84571	3.18551	-1.00848
C	7.95508	3.58494	0.2965
H	9.00226	2.09808	1.44377
H	6.66613	4.8655	-0.85554
H	8.75096	4.3188	0.37155
C	-5.90902	-1.69065	0.09612
C	-7.08485	-1.39392	0.79283
C	-5.76709	-2.95542	-0.48619
C	-8.09877	-2.33747	0.89259

H	-7.19921	-0.42881	1.2721
C	-6.7851	-3.89155	-0.39217
H	-4.84557	-3.18559	-1.0083
C	-7.95514	-3.58482	0.29626
H	-9.00246	-2.09782	1.44324
H	-6.66605	-4.86552	-0.85548
H	-8.75105	-4.31865	0.37126
C	-5.90901	1.69069	-0.09614
C	-5.7671	2.95544	0.48621
C	-7.08482	1.39398	-0.79291
C	-6.7851	3.89157	0.39217
H	-4.8456	3.18559	1.00836
C	-8.09873	2.33753	-0.89268
H	-7.19916	0.42888	-1.27221
C	-7.95512	3.58487	-0.29631
H	-6.66607	4.86553	0.85552
H	-9.0024	2.0979	-1.44336
H	-8.75103	4.31871	-0.37131

$\langle S^2 \rangle = 0.886$

Triplet diradical:

ucam-b3lyp/6-311g(d,p)

Charge = 0 Multiplicity = 3

Sum of electronic and thermal energies= -1604.212360
Sum of electronic and thermal enthalpies= -1604.211415
Sum of electronic and thermal free energies= -1604.310041

C	0.67536	-1.23821	0.00055
C	-0.67532	-1.23821	-0.00047

C	-1.41174	0.00001	0.
C	-0.67532	1.23823	0.00049
C	0.67537	1.23822	-0.00053
C	1.41178	0.	0.00002
H	1.24459	-2.15957	-0.00052
H	-1.24456	-2.15956	0.00065
H	-1.24455	2.15958	-0.00064
H	1.2446	2.15958	0.00055
C	2.79166	0.	0.00002
C	4.7893	-0.74291	-0.0177
C	4.7893	0.74291	0.01775
C	-2.79162	0.00001	0.
C	-4.78925	-0.74289	0.01772
C	-4.78925	0.74293	-0.01774
N	3.55113	-1.15724	-0.01
N	3.55113	1.15724	0.01005
N	-3.55109	-1.15722	0.01009
N	-3.55108	1.15725	-0.0101
C	5.90904	-1.6907	-0.09615
C	7.08479	-1.39406	-0.79303
C	5.76713	-2.95543	0.48626
C	8.09867	-2.33765	-0.89284
H	7.19912	-0.429	-1.2724
C	6.7851	-3.89159	0.39219
H	4.84567	-3.18553	1.00849
C	7.95507	-3.58495	-0.2964
H	9.0023	-2.09808	-1.44362
H	6.66608	-4.86553	0.85558
H	8.75095	-4.31882	-0.37144
C	5.90904	1.6907	0.09622
C	7.08478	1.39406	0.79314
C	5.76716	2.95541	-0.48622

C	8.09865	2.33764	0.89297
H	7.19908	0.429	1.27253
C	6.78513	3.89157	-0.39213
H	4.84571	3.18551	-1.00848
C	7.95508	3.58494	0.2965
H	9.00226	2.09808	1.44377
H	6.66613	4.8655	-0.85554
H	8.75096	4.3188	0.37155
C	-5.90902	-1.69065	0.09612
C	-7.08485	-1.39392	0.79283
C	-5.76709	-2.95542	-0.48619
C	-8.09877	-2.33747	0.89259
H	-7.19921	-0.42881	1.2721
C	-6.7851	-3.89155	-0.39217
H	-4.84557	-3.18559	-1.0083
C	-7.95514	-3.58482	0.29626
H	-9.00246	-2.09782	1.44324
H	-6.66605	-4.86552	-0.85548
H	-8.75105	-4.31865	0.37126
C	-5.90901	1.69069	-0.09614
C	-5.7671	2.95544	0.48621
C	-7.08482	1.39398	-0.79291
C	-6.7851	3.89157	0.39217
H	-4.8456	3.18559	1.00836
C	-8.09873	2.33753	-0.89268
H	-7.19916	0.42888	-1.27221
C	-7.95512	3.58487	-0.29631
H	-6.66607	4.86553	0.85552
H	-9.0024	2.0979	-1.44336
H	-8.75103	4.31871	-0.37131

$\langle S^2 \rangle = 2.0541$

NICS(0) calculation

nmr=giao ucam-b3lyp/6-311g(d,p)

Charge = 0 Multiplicity = 1

C	0.68411400	1.21917300	-0.00036800
C	-0.68410700	1.21917300	0.00038500
C	-1.39988100	0.00000000	0.00000700
C	-0.68410700	-1.21917200	-0.00037900
C	0.68411400	-1.21917300	0.00036100
C	1.39988900	0.00000000	-0.00000700
H	1.24667300	2.14284000	0.00168900
H	-1.24666600	2.14284000	-0.00165900
H	-1.24666600	-2.14284000	0.00167100
H	1.24667300	-2.14284000	-0.00170100
C	2.82170700	0.00000000	-0.00001300
C	4.81239100	0.74126000	0.01243500
C	4.81239100	-0.74126000	-0.01248100
C	-2.82170100	0.00000000	0.00001300
C	-4.81238500	0.74125900	-0.01242200
C	-4.81238400	-0.74125900	0.01246800
N	3.56477900	1.14833900	-0.00322800
N	3.56477900	-1.14833900	0.00319400
N	-3.56477200	1.14833900	0.00324600
N	-3.56477200	-1.14833900	-0.00321200
C	5.92242000	1.69285200	0.09266800
C	7.10113900	1.40073300	0.78316200
C	5.77037600	2.95929000	-0.48006700
C	8.10740100	2.34836000	0.88465700
H	7.22296900	0.43722500	1.25978700

C	6.78225700	3.89789800	-0.38692300
H	4.84576300	3.18715400	-0.99366400
C	7.95489200	3.59496300	0.29448100
H	9.01217900	2.11302200	1.43189100
H	6.65627700	4.87213400	-0.84365200
H	8.74522700	4.33212700	0.37049800
C	5.92241900	-1.69285200	-0.09272400
C	7.10113000	-1.40073400	-0.78323300
C	5.77038100	-2.95928900	0.48001400
C	8.10739100	-2.34836100	-0.88473700
H	7.22295400	-0.43722700	-1.25986100
C	6.78226100	-3.89789800	0.38686100
H	4.84577500	-3.18715200	0.99362300
C	7.95488900	-3.59496400	-0.29455700
H	9.01216200	-2.11302500	-1.43198200
H	6.65628600	-4.87213300	0.84359300
H	8.74522300	-4.33212800	-0.37058100
C	-5.92241600	1.69284700	-0.09263200
C	-7.10115900	1.40071300	-0.78307900
C	-5.77035900	2.95929400	0.48008200
C	-8.10742800	2.34833500	-0.88455400
H	-7.22300300	0.43719600	-1.25968300
C	-6.78224500	3.89789700	0.38695800
H	-4.84573000	3.18716800	0.99364600
C	-7.95490300	3.59494800	-0.29440400
H	-9.01222400	2.11298500	-1.43175300
H	-6.65625400	4.87214100	0.84366800
H	-8.74524300	4.33210900	-0.37040400
C	-5.92241500	-1.69284700	0.09268800
C	-5.77036500	-2.95929200	-0.48003100
C	-7.10114900	-1.40071500	0.78315100
C	-6.78225100	-3.89789600	-0.38689700

H	-4.84574200	-3.18716500	-0.99360800
C	-8.10741700	-2.34833700	0.88463600
H	-7.22298700	-0.43720000	1.25975900
C	-7.95489900	-3.59494900	0.29448000
H	-6.65626500	-4.87213800	-0.84361200
H	-9.01220600	-2.11298800	1.43184700
H	-8.74523800	-4.33210900	0.37048800
Bq	3.66667E-06	1.66667E-07	1
Bq	3.9152094	0	1
Bq	6.9397475	2.649016	1.197996333
Bq	6.939745167	-2.649016333	0.801937333

NOON calculation for diradical character value:

ucam-b3lyp/6-311g(d,p) pop=no

Charge = 0 Multiplicity = 1

C	0.68411	1.21917	-0.00037
C	-0.68411	1.21917	0.00039
C	-1.39988	0.	0.00001
C	-0.68411	-1.21917	-0.00038
C	0.68411	-1.21917	0.00036
C	1.39989	0.	-0.00001
H	1.24667	2.14284	0.00169
H	-1.24667	2.14284	-0.00166
H	-1.24667	-2.14284	0.00167
H	1.24667	-2.14284	-0.0017
C	2.82171	0.	-0.00001
C	4.81239	0.74126	0.01244
C	4.81239	-0.74126	-0.01248

C	-2.8217	0.	0.00001
C	-4.81239	0.74126	-0.01242
C	-4.81238	-0.74126	0.01247
N	3.56478	1.14834	-0.00323
N	3.56478	-1.14834	0.00319
N	-3.56477	1.14834	0.00325
N	-3.56477	-1.14834	-0.00321
C	5.92242	1.69285	0.09267
C	7.10114	1.40073	0.78316
C	5.77038	2.95929	-0.48007
C	8.1074	2.34836	0.88466
H	7.22297	0.43723	1.25979
C	6.78226	3.8979	-0.38692
H	4.84576	3.18715	-0.99366
C	7.95489	3.59496	0.29448
H	9.01218	2.11302	1.43189
H	6.65628	4.87213	-0.84365
H	8.74523	4.33213	0.3705
C	5.92242	-1.69285	-0.09272
C	7.10113	-1.40073	-0.78323
C	5.77038	-2.95929	0.48001
C	8.10739	-2.34836	-0.88474
H	7.22295	-0.43723	-1.25986
C	6.78226	-3.8979	0.38686
H	4.84578	-3.18715	0.99362
C	7.95489	-3.59496	-0.29456
H	9.01216	-2.11302	-1.43198
H	6.65629	-4.87213	0.84359
H	8.74522	-4.33213	-0.37058
C	-5.92242	1.69285	-0.09263
C	-7.10116	1.40071	-0.78308
C	-5.77036	2.95929	0.48008

C	-8.10743	2.34834	-0.88455
H	-7.223	0.4372	-1.25968
C	-6.78225	3.8979	0.38696
H	-4.84573	3.18717	0.99365
C	-7.9549	3.59495	-0.2944
H	-9.01222	2.11299	-1.43175
H	-6.65625	4.87214	0.84367
H	-8.74524	4.33211	-0.3704
C	-5.92242	-1.69285	0.09269
C	-5.77037	-2.95929	-0.48003
C	-7.10115	-1.40072	0.78315
C	-6.78225	-3.8979	-0.3869
H	-4.84574	-3.18717	-0.99361
C	-8.10742	-2.34834	0.88464
H	-7.22299	-0.4372	1.25976
C	-7.9549	-3.59495	0.29448
H	-6.65627	-4.87214	-0.84361
H	-9.01221	-2.11299	1.43185
H	-8.74524	-4.33211	0.37049

References:

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2. Chen, Z.; Wannere, C. S.; Corminboeuf, C.; Puchta, R.; Schleyer, P. von R. Nucleus-Independent Chemical Shifts (NICS) as an Aromaticity Criterion. *Chem. Rev.* **2005**, *105 (10),* 3842–3888.
3. Yamaguchi, K. The Electronic Structures of Biradicals in the Unrestricted Hartree-Fock Approximation. *Chem. Phys. Lett.* **1975**, *33 (2),* 330–335.