Electronic Supplementary Material (ESI) for RSC Advances.

Substitution effect on chalcone based materials for corrosion and photocrosslinking applications

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SUPPLEMENTARY DETAILS

The additional information's are given as supporting file.

1) Details of data collection, solution and refinement, fractional coordinate with anisotropic thermal parameters and lists of bond lengths and angles. The CIF data of crystal **III**, Cambridge Crystallographic Data Centre (CCDC) deposition number is 909642.

2) Video on HOPM frames of crystal **III** with the isotropic to crystalline phase.

3) **Figure S 1**. Harvested single crystal images of chalcone **III**.

4) **Figure S 2.** FT-IR spectra of the intermediate and the final product of chalcone **III**.

5). **Figure S 3**. ORTEP Diagram of materials **I**, **II** and **III**.

6) **Table S 1.** Hydrogen bonding coordinates data of crystal **III**.

7) Output file of Gaussian package is an evident for DFT calculation.

Figure S 1. Harvested single crystal images of chalcone **III**.

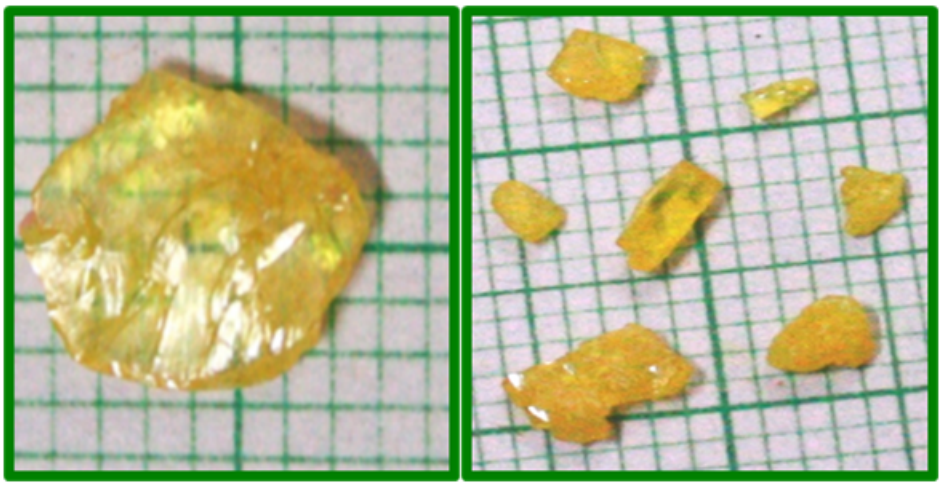
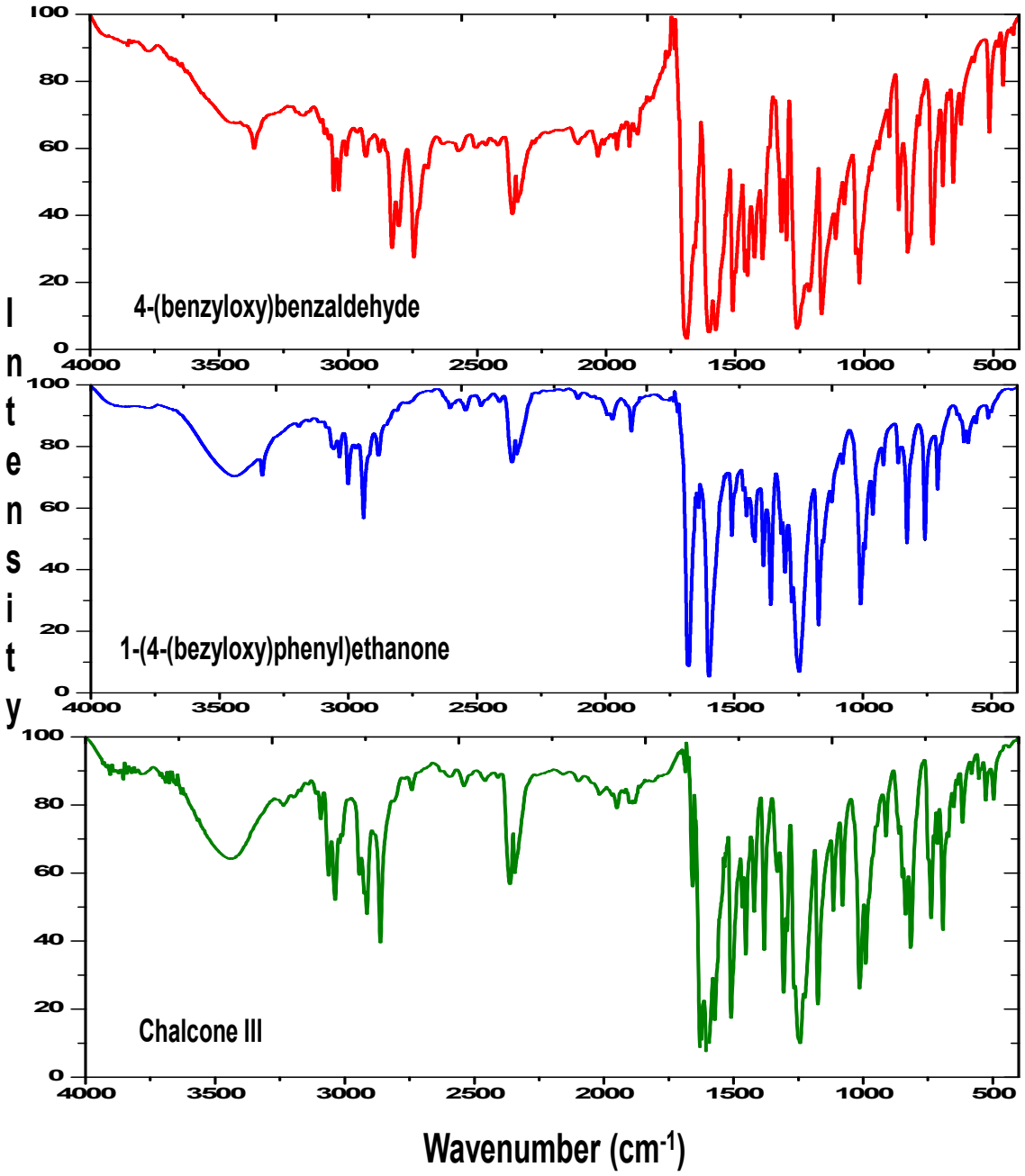


Figure S 2. FT-IR spectra of the intermediates and the final product of chalcone **III**.



The FT-IR shows the following groups are present in the chalcone intermediate and the final product.

Wave number (cm^{-1})	**Assignment**
~ 3058	Aromatic proton stretching
~ 2933	Aliphatic protons stretching
~ 1660	C=O (carbonyl) stretching
~ 1602	C=C stretching
~ 1465	CH_3 bending (C-H-deformation)
~ 1257	C-O stretching
~ 829, 777, 661	Out of plane, C-H bending

The ^{1}H-NMR spectral data of before photo-crosslinking were mentioned in manuscript.

^{1}H-NMR of after photocrosslinking material **I**

^{1}H-NMR (500 MHz,$CDCl_3$) (δ/ppm): 3.75 (s, 2H, –OH); 4.25 (m, 4H, cyclobutane–CH); 5.2 (d, 4H, Ar–CH_2); 6.78 (d, 4H, Ar–CH); 6.96 (d, 4H, Ar–CH); 7.23 (m, 10H, Ar–CH); 7.39 (d, 4H, Ar–H); 7.67 (d, 4H, Ar–CH).

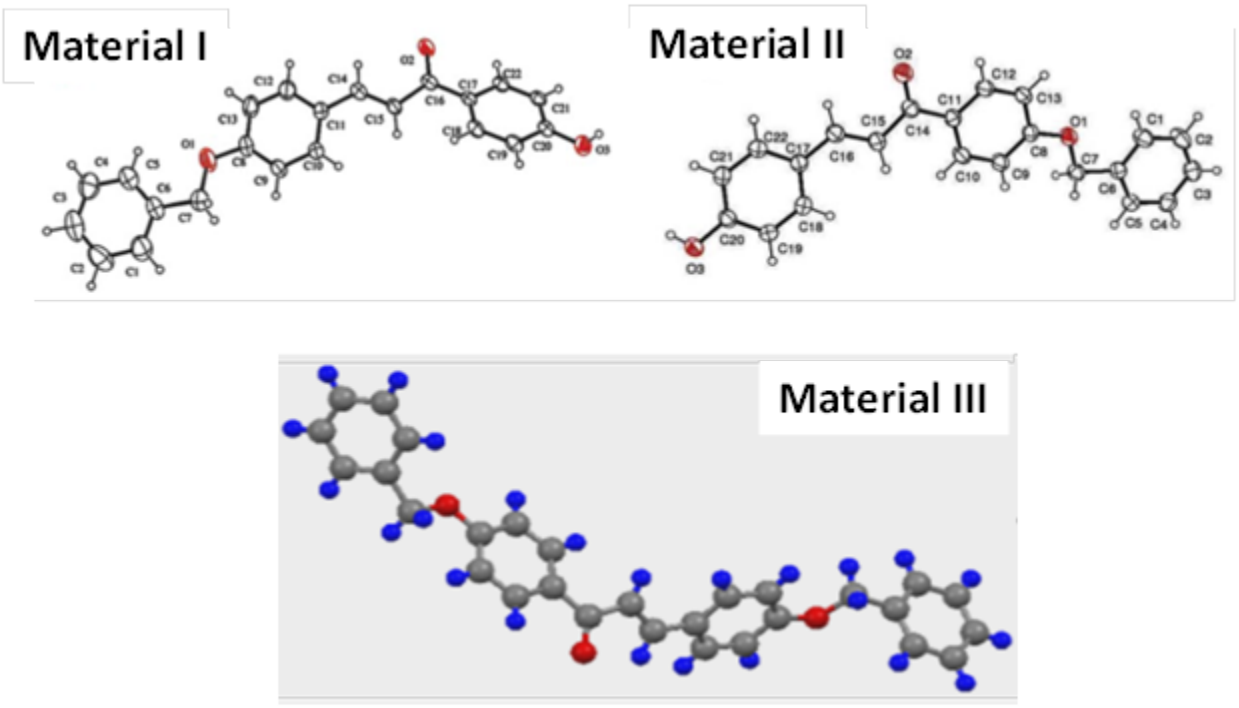
^{1}H-NMR of after photocrosslinking material **II**

^{1}H-NMR (500 MHz,$CDCl_3$) (δ/ppm): 3.51 (s, 2H, –OH); 4.25 (m, 4H, cyclobutane–CH); 5.2 (d, 4H, Ar–CH_2); 6.81 (d, 4H, Ar–CH); 7.01 (d, 4H, Ar–CH); 7.16 (d, 4H, Ar–CH) 7.25 (m, 10H, Ar–CH); 7.71 (m, 4H, Ar–H).

^{1}H-NMR of after photocrosslinking of material **III**

^{1}H-NMR (500 MHz,$CDCl_3$) (δ/ppm): 4.22 (m, 4H, cyclobutane–CH); 5.21 (d, 8H, Ar–CH_2); 6.92 (d, 4H, Ar–CH); 7.07 (d, 4H, Ar–CH); 7.18 (m, 10H, Ar–CH); 7.23 (d, 4H, Ar–H); 7.82 (d, 4H, Ar–CH)

5). **Figure S 3**. ORTEP Diagram of materials **I**, **II** and **III**.



6) **Table S 1.** Hydrogen bonding coordinates data of crystal **III**.

CRYSTAL III				
	x	**y**	**z**	**U(eq)**
H(1)	-216	2496	-1057	65
H(2)	-1182	13328	-1959	70
H(3)	-1647	10784	-2983	71
H(4)	-1160	7354	-3090	73
H(5)	-196	6541	-2181	64
H(7A)	799	8471	-1311	67
H(7B)	723	10295	-682	67
H(9)	583	3557	359	61
H(10)	1426	1357	1044	62
H(12)	2540	5874	486	65
H(13)	1691	8036	-245	65
H(14)	2502	254	1264	58
H(15)	3305	3944	1598	59
H(18)	4657	-1772	2701	56
H(19)	5477	-1036	3846	62
H(21)	4705	5035	4094	69
H(22)	3905	4323	2930	65
H(23A)	6340	963	4593	71
H(23B)	6098	-111	5260	71
H(25)	6677	752	6619	67
H(26)	7378	2969	7585	76
H(27)	7782	6252	7224	77
H(28)	7510	7296	5898	89
H(29)	6810	5103	4925	82