

Bifunctional Bis(2-carboxyethyl)isocyanurate Crystal for High-Performance Photocatalytic Degradation of Rose Bengal Dye and Luminescent Sensing of PO_4^{3-} , NO_3^- , Cl^- , $\text{Cr}_2\text{O}_7^{2-}$ and F^- ions

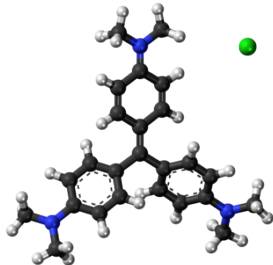
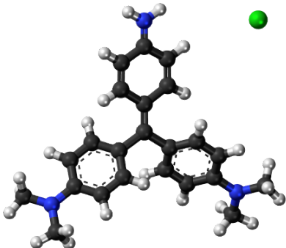
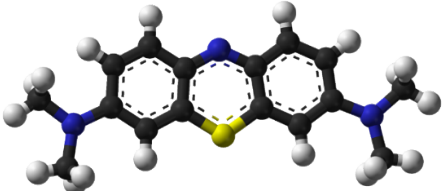
Priyanka Singh^a, Musheer Ahmad^b, Kafeel Ahmad Siddiqui^a

^aDepartment of Chemistry, National Institute of Technology Raipur,
G E Road Raipur – 492010, Chhattisgarh, India

^bDepartment of Applied Chemistry, Faculty of Engineering and Technology, Aligarh Muslim University,
Aligarh, UP (India) - 202002

^a e-mail: kasiddiqui.chy@nitrr.ac.in

Table S1. Structure and electrical property of used dyes.

S.No.	Dye	Dye Structure	λ_{max} (nm)
Cationic			
1.	Crystal Violet		590.67
2.	Methyl Violet		589.49
3.	Methylene Blue		662.63


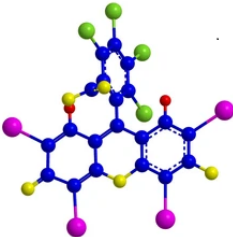
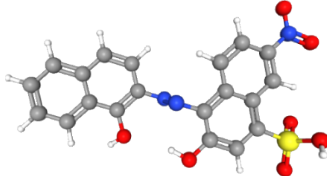
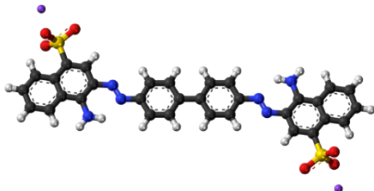
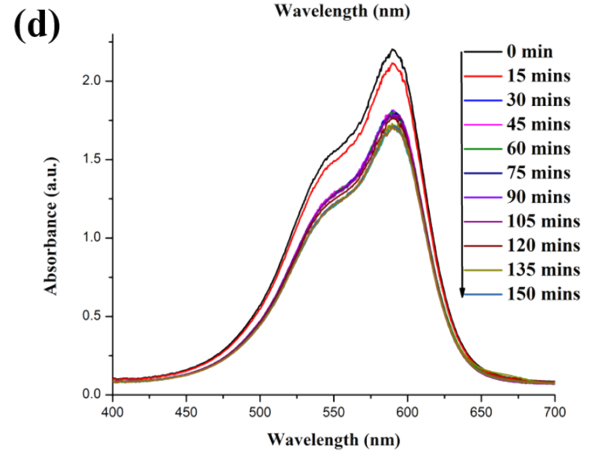
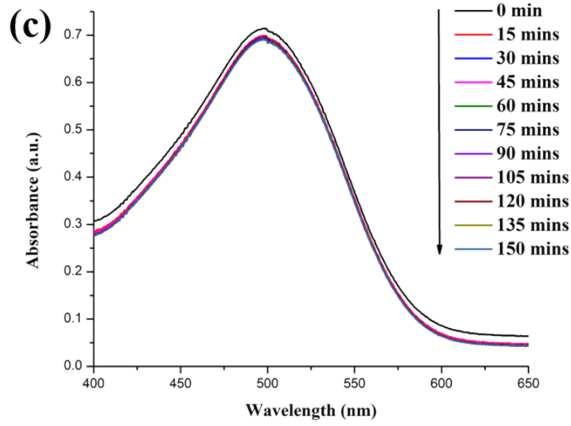
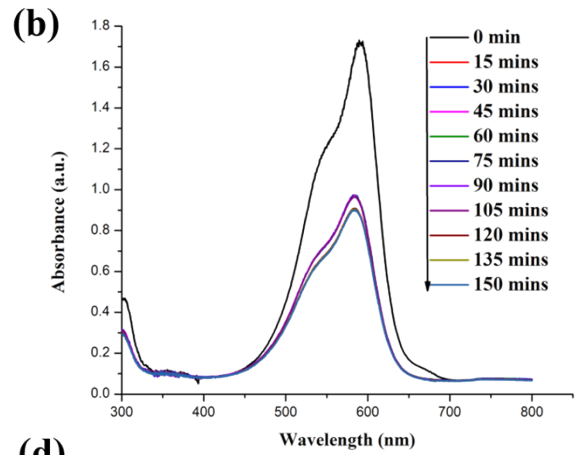
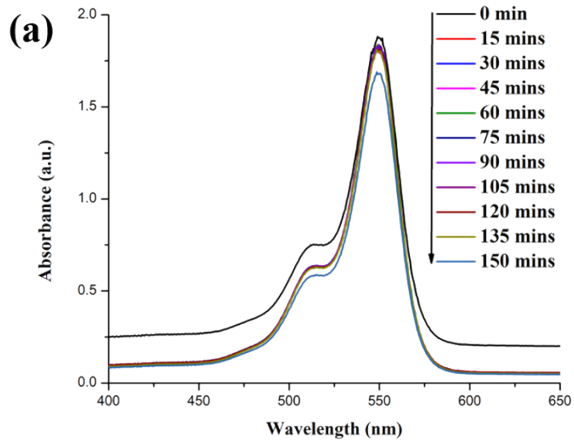
4.	Rhodamine 6G		525.31
Anionic			
2.	Rose Bengal		549.44
3.	Eriochrome Black T		529.23
4.	Congo Red		497.82

Table S2.Hydrogen bonding parameters for KA@PS (Å) and (°)

D–H···A	d(D···H)	d(H···A)	<(D–H···A)
N(2)–H(2)···O(1)#1	0.860	1.912	180
O(3)–H(3)···O(4)#2	0.820	1.858	159.56

Symmetry transformations used to generate equivalent atoms: #1 $x, -1+y, z$; #2 $\frac{1}{2}-x, -1/2-y, 1-z$.



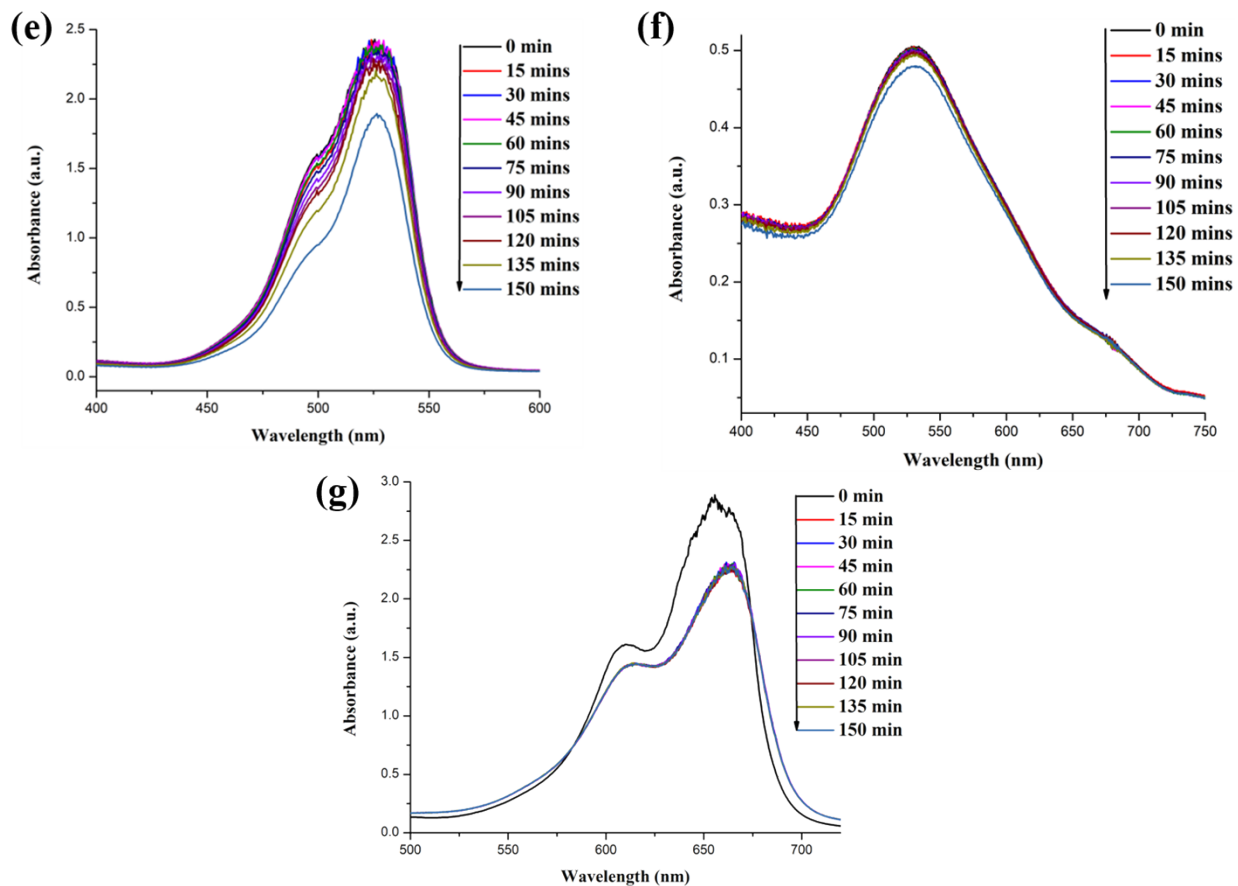


Figure S1: UV-visible spectra of the blank RB (a), MV (b), CR (c), CV (d), Rh6G (e), EBT (f) and MB (g) from aqueous solution at several time intervals.

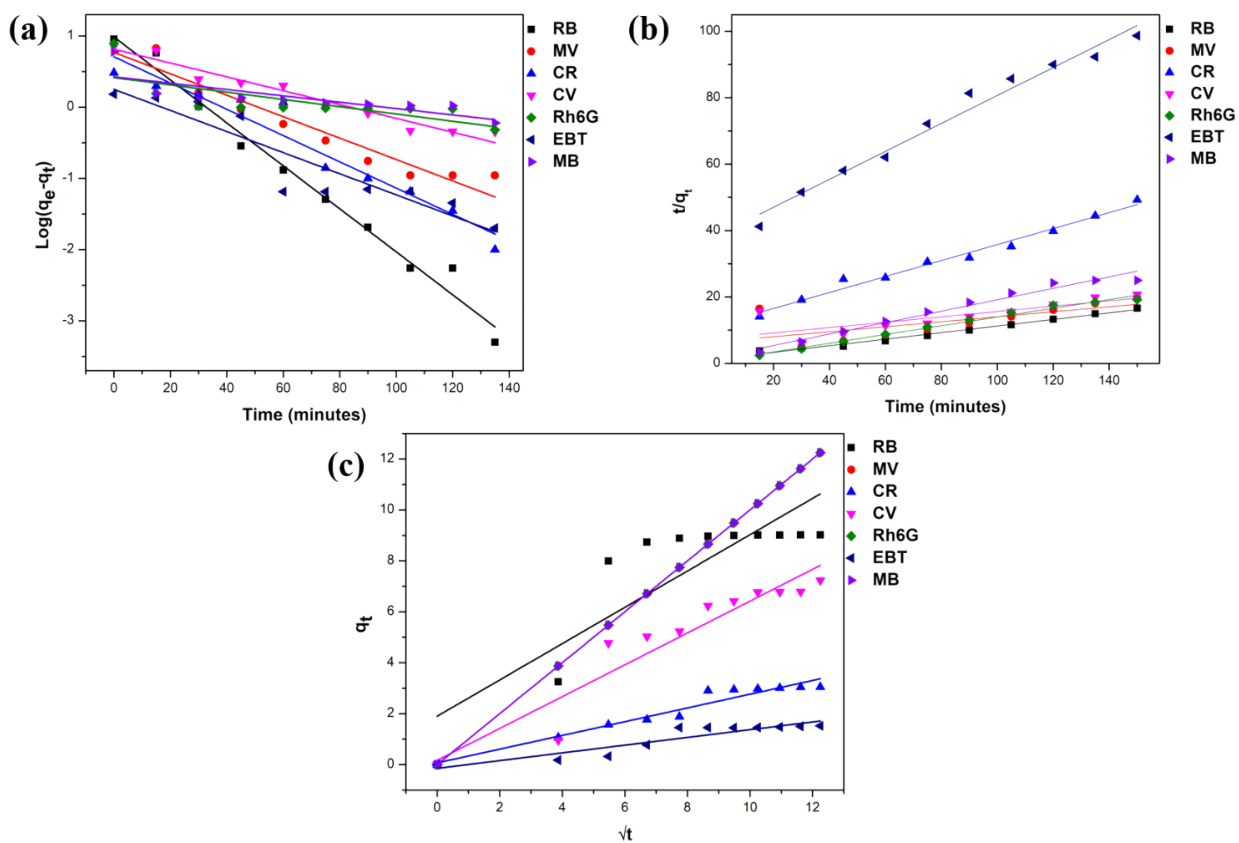
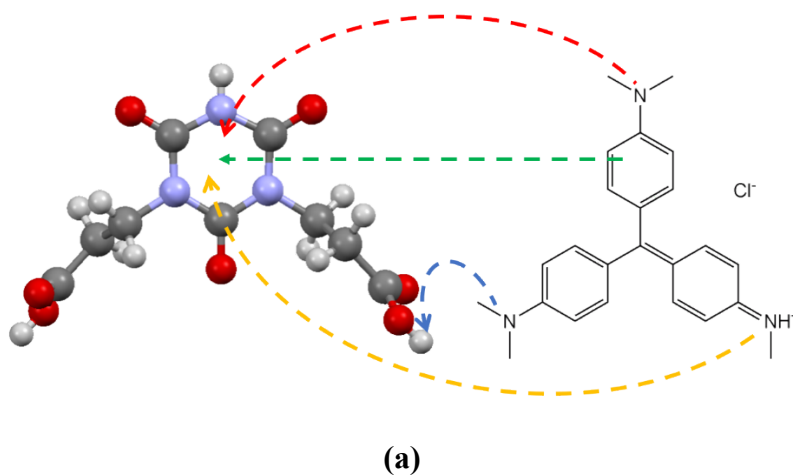
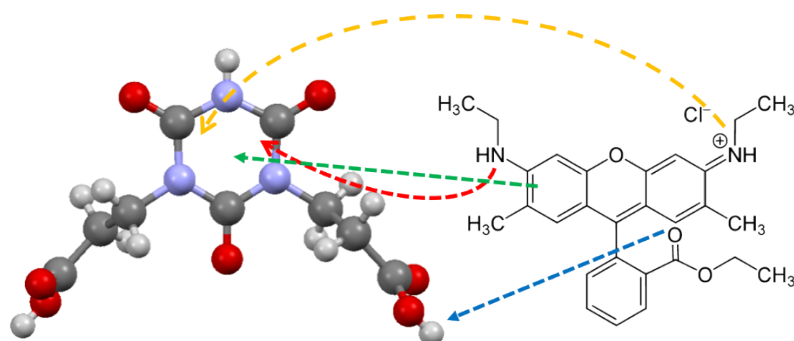
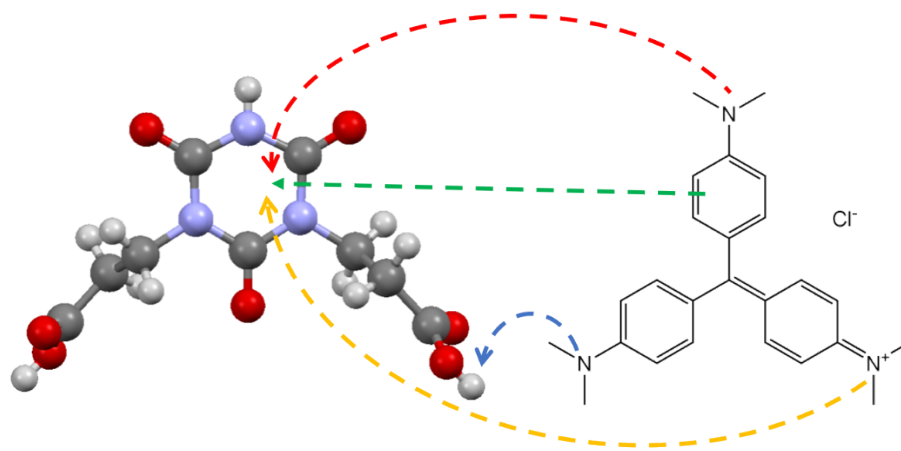
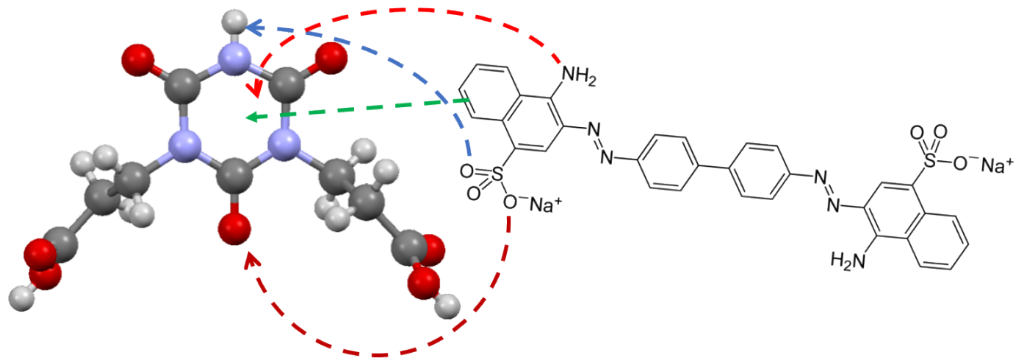
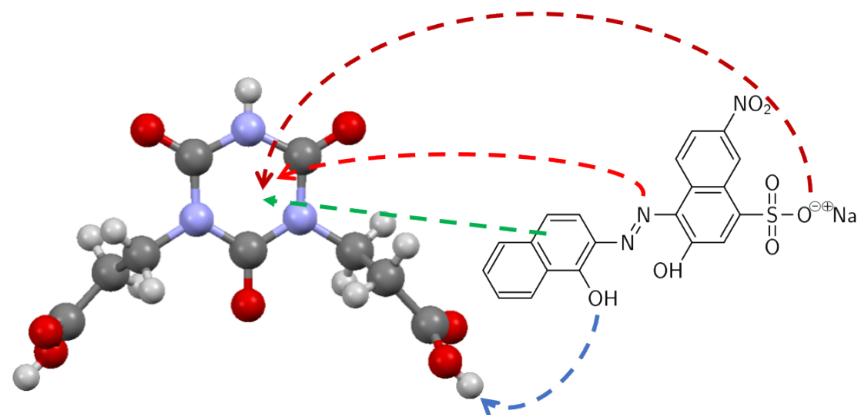


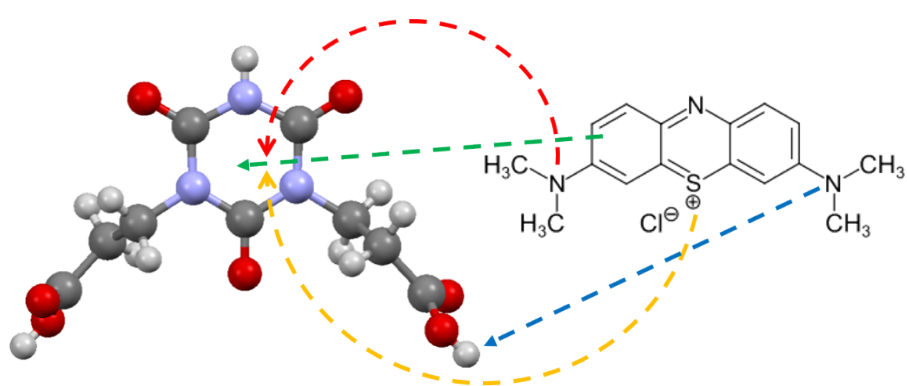
Figure S2. Adsorption kinetic plots of RB, MV, CR, CV, Rh6G, EBT and MB on KA@PS representing pseudo-first order kinetics (a); pseudo-second order kinetics (b) and intraparticle diffusion (c).







(e)



(f)

- - - - - Hydrogen bonding
- - - - - n- π bonding
- - - - - π - π bonding
- - - - - Electrostatic repulsion
- - - - - Electrostatic attraction

Figure S3: The possible mechanism of dye adsorption among (a)MV,(b) CR,(c) CV,(d)Rh6G,(e) EBT, (f)MB andKA@PS .

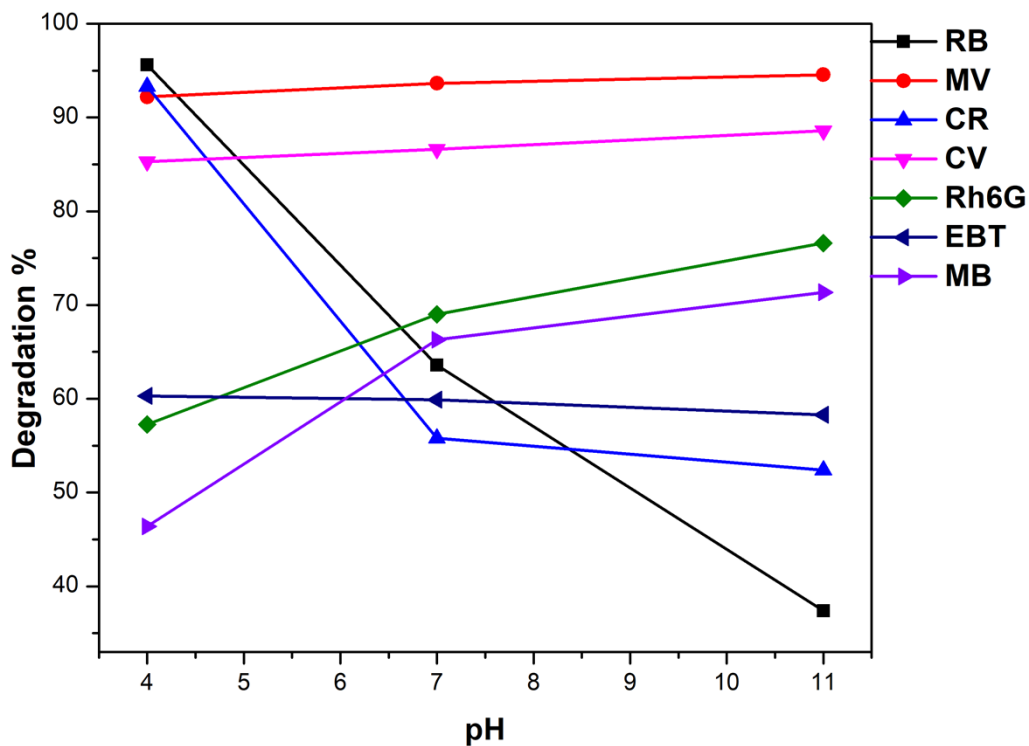


Figure S4. pH effect of KA@PS on RB, CV, CR, CV, Rh6G, EBT and MB.

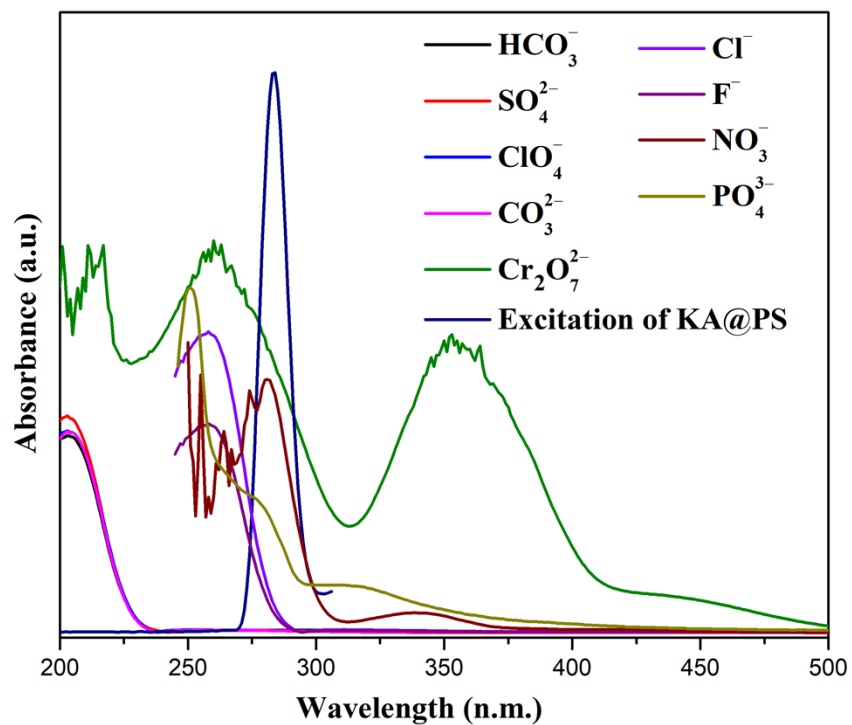


Figure S5: Spectral overlap between the UV-Vis absorption spectra of various anions and the excitation spectra of KA@PS

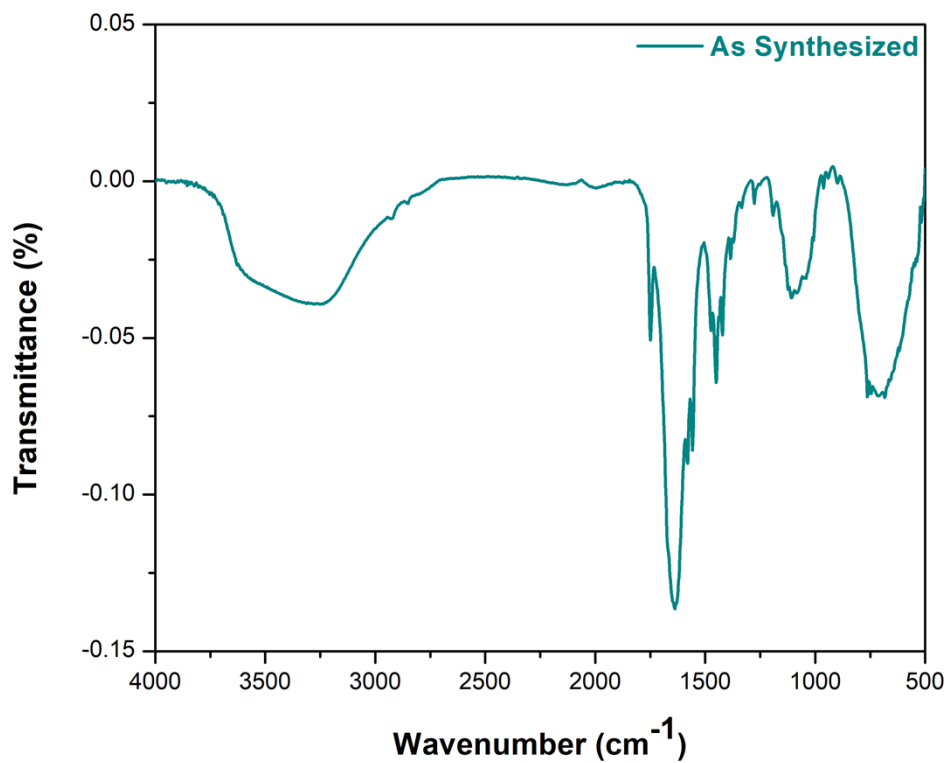


Figure S6. FT-IR of KA@PS.

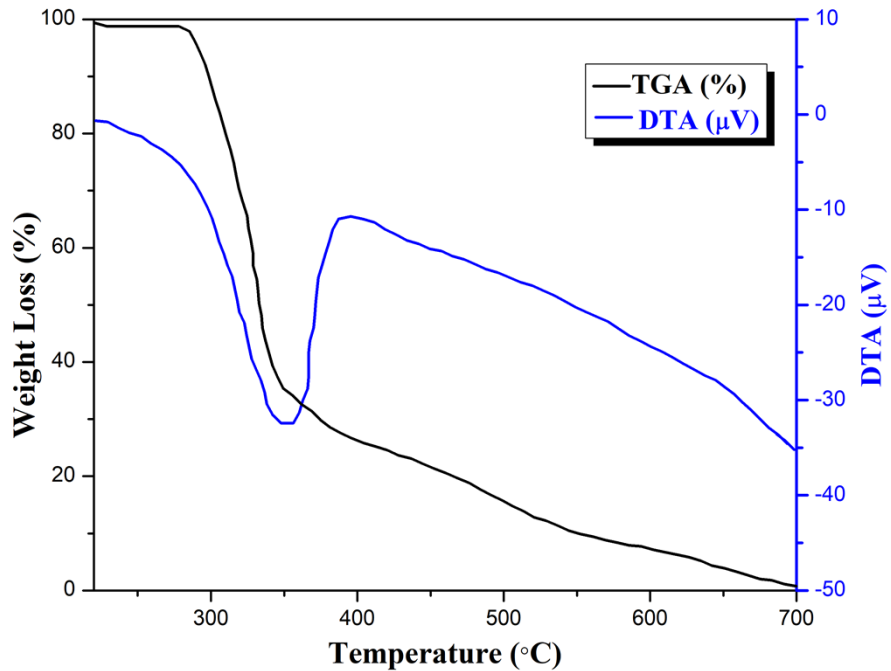


Figure S7. TG/DTA of KA@PS .

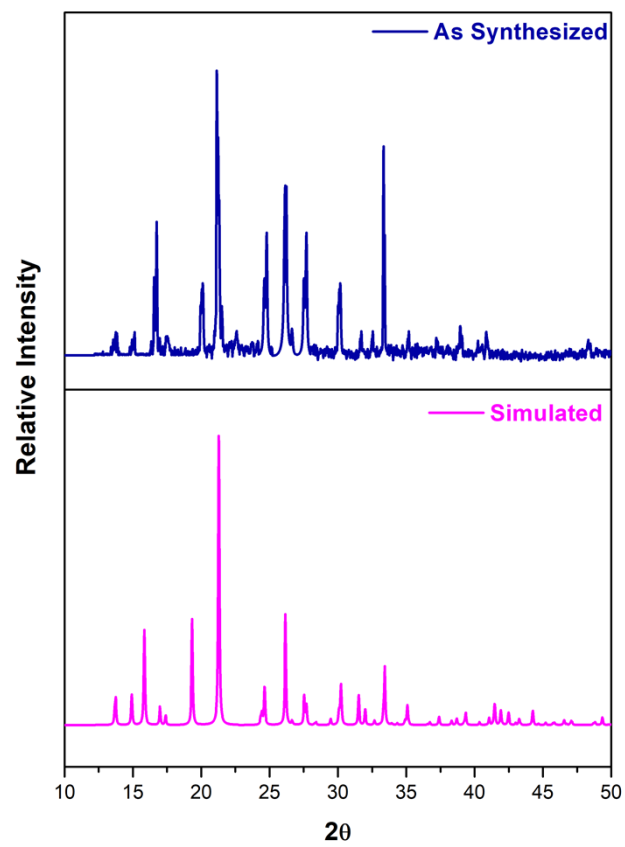


Figure S8. PXR D of KA@PS .