Template effect of innocent and coordinating anions on the formation of interpenetrated 2D and 3D networks: methyl orange and iodine sorption studies

Fayaz Baig[a], Krishnan Rangan[b], Shibu M Eappen[c], Sanjay K. Mandal[d]* and Madhushree Sarkar[a]*

[a.] *Department of Chemistry, BITS Pilani, Pilani Campus, Rajasthan 333031, India. Email: msarkar@pilani.bits-pilani.ac.in*

[b.] *Department of Chemistry, BITS Pilani, Hyderabad Campus, Jawahar Nagar Shameerpet Mandal Ranga Reddy District Hyderabad 500078, India.*

[c.] *Sophiscated Test and Instrumentation Centre, Cochin University of Science and Technology Campus, Cochin 682022, India .*

[d.] *Department of Chemical Sciences, Indian Institute of Science Education and Research Mohali, Sector 81, S.A.S. Nagar, Punjab 140 306, India. E-mail: sanjaymandal@iisermohali.ac.in*

Supporting Information:

- IR, ^{1}H NMR, ^{13}C NMR, Powder XRD and ORTEP of **L1** (Fig. S1-S5)
- IR, Powder XRD and ORTEP of **CP1** (Fig. S6-S8), **[HL1][ClO$_4$]** (Fig. S9-S11), **CP2** (Fig. S12-S14) and **CP2_BN** (Fig. S15, S16 and S18)
- UV-Visible spectra for the dye degradation studies of **CP2** (Fig. S17)
- Crystallographic data and refinement parameters of **CP2_BN** (Table S1)

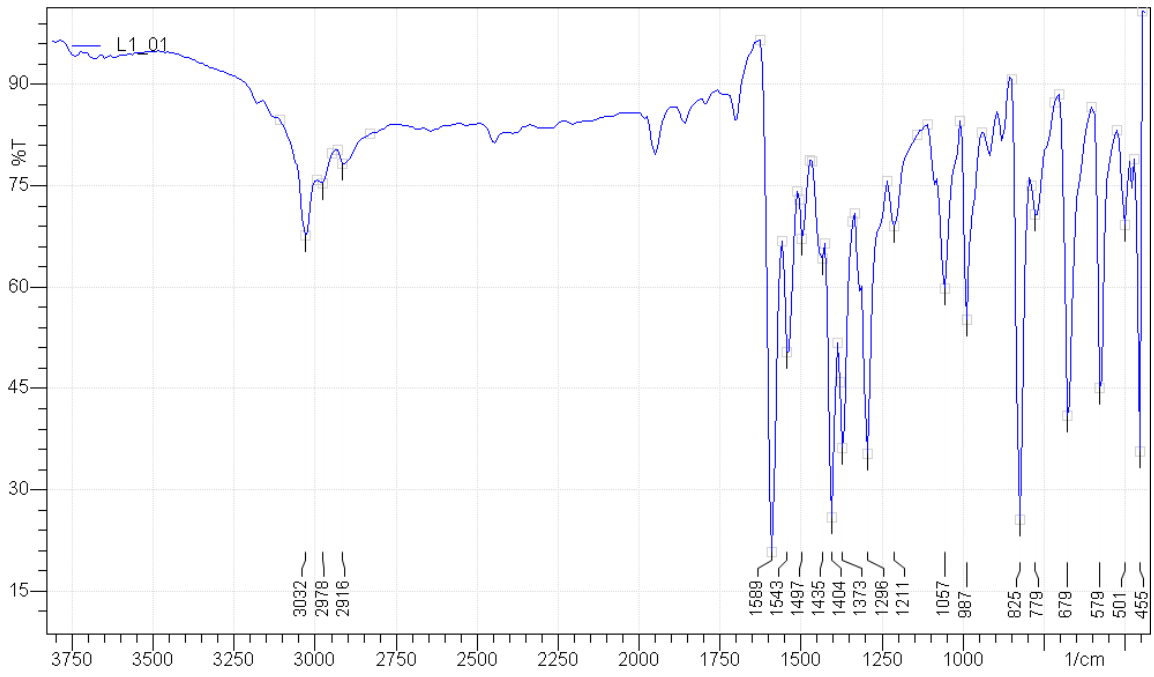


Fig. S1 IR spectra of **L1**

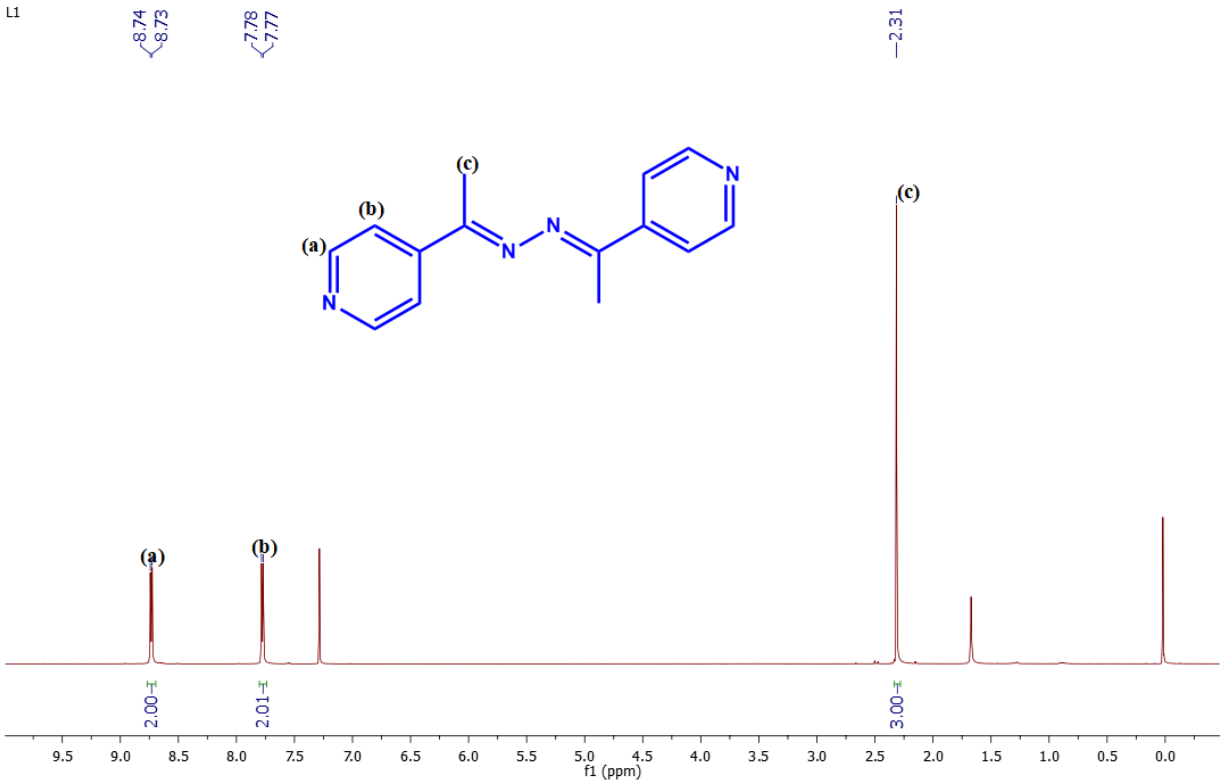


Fig. S2 ^{1}H NMR of **L1**

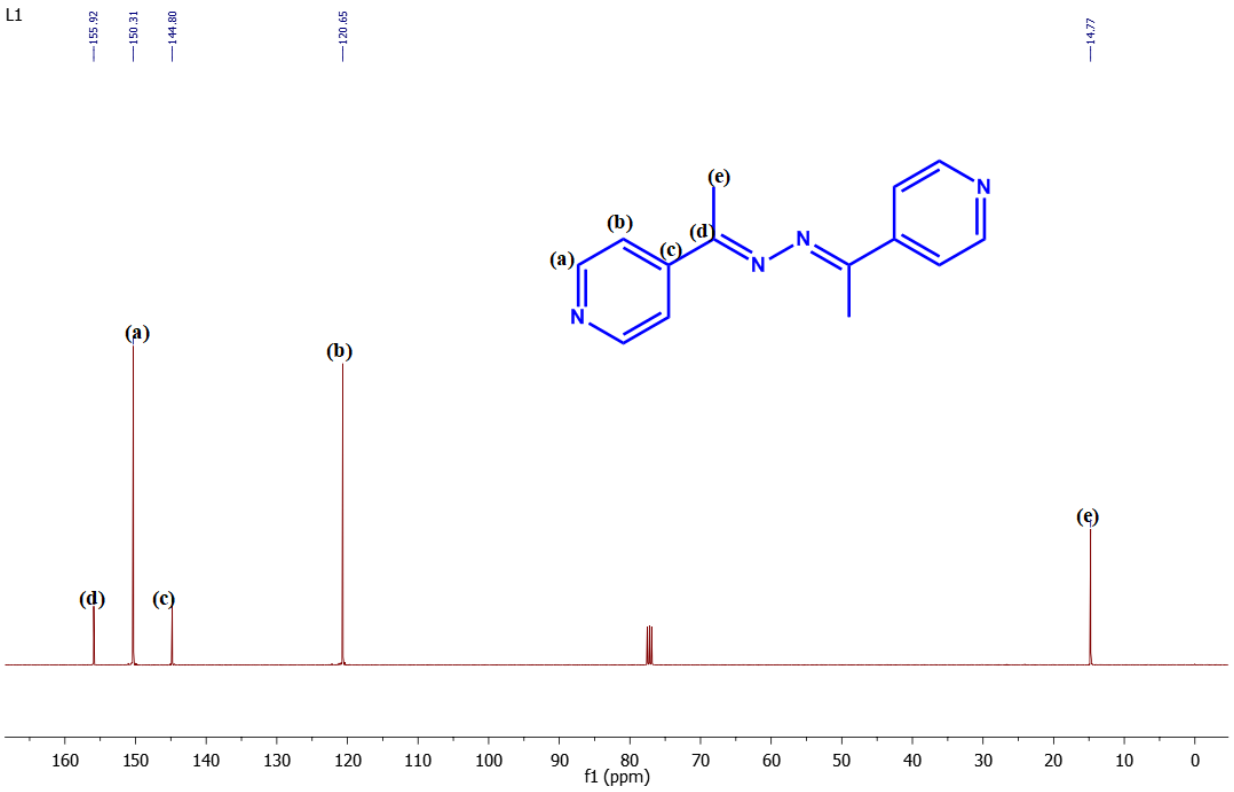


Fig. S3 ^{13}C NMR of **L1**

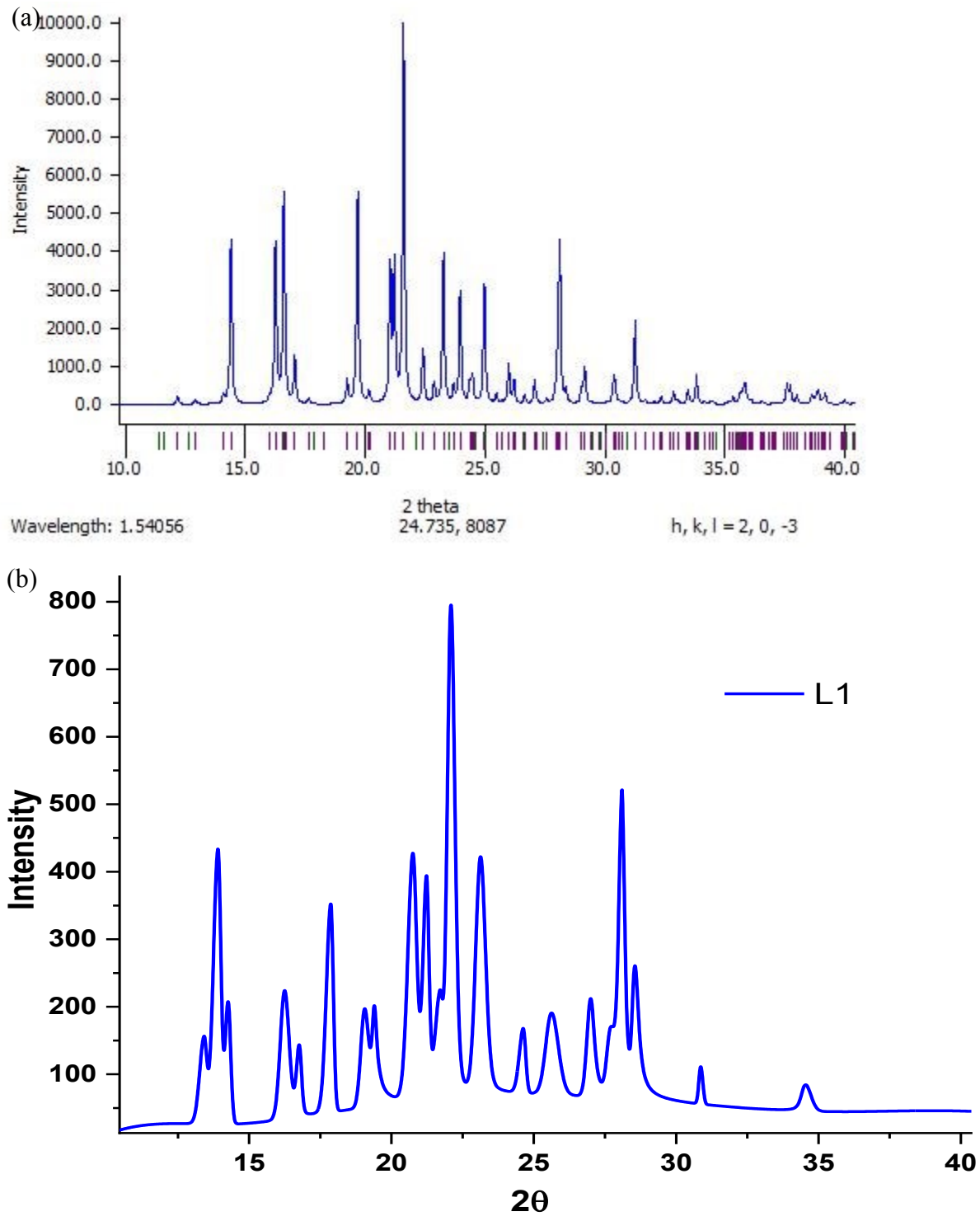


Fig. S4 Simulated and experimental powder XRD of **L1**

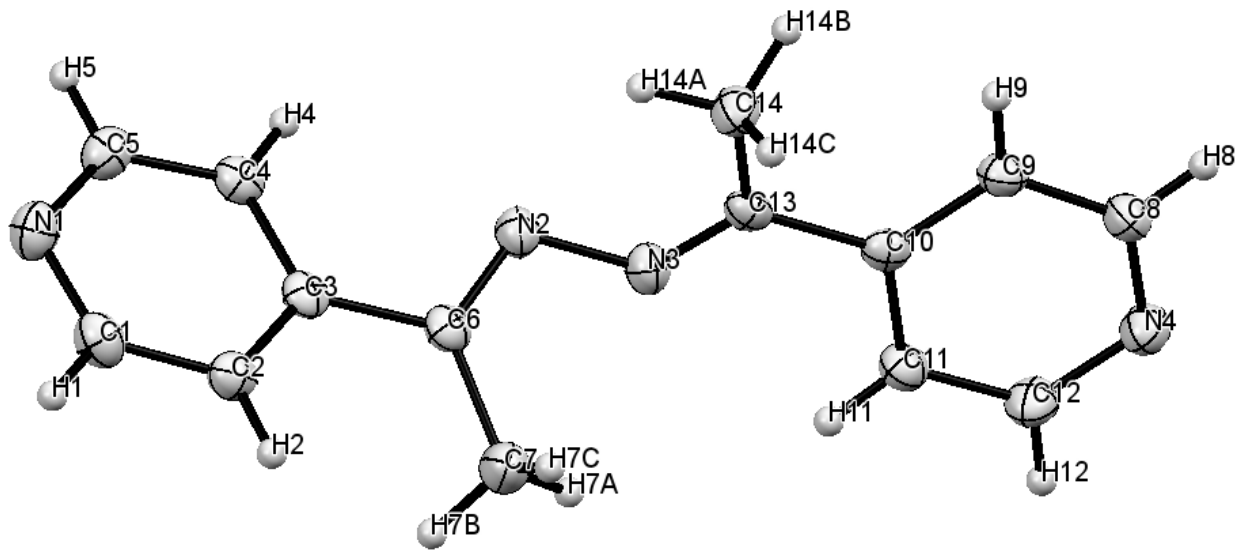


Fig. S5 ORTEP drawing of **L1** showing thermal ellipsoids at the 50% probability level

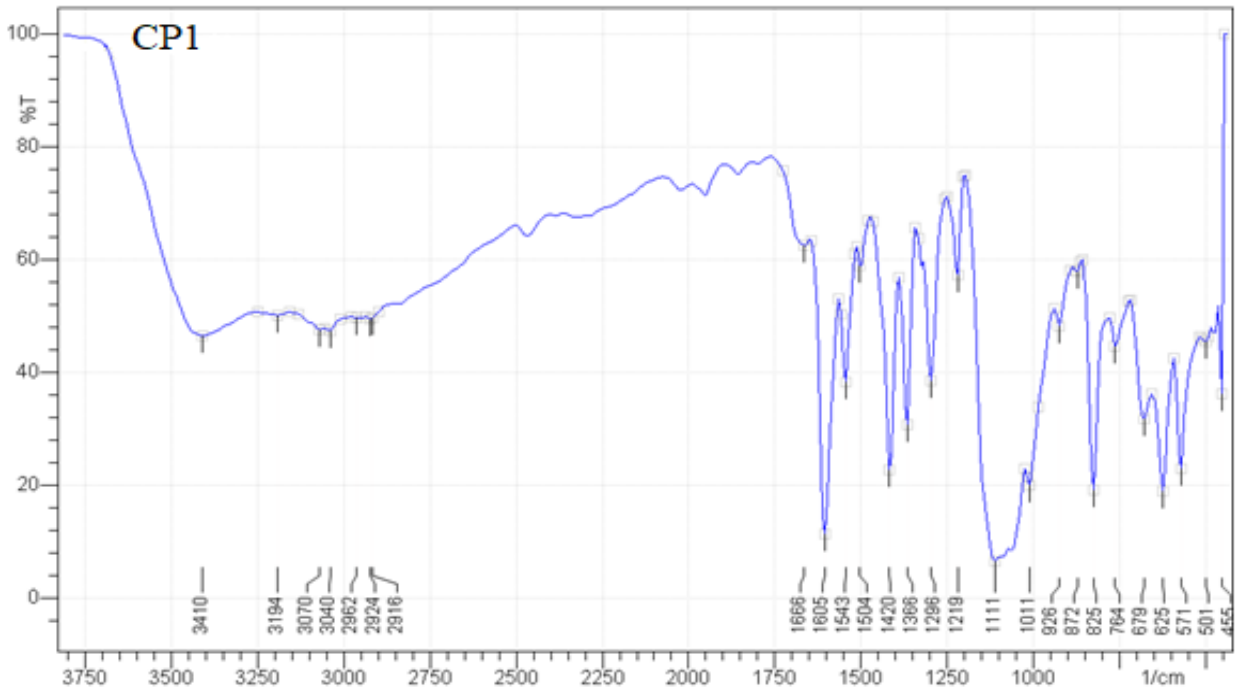
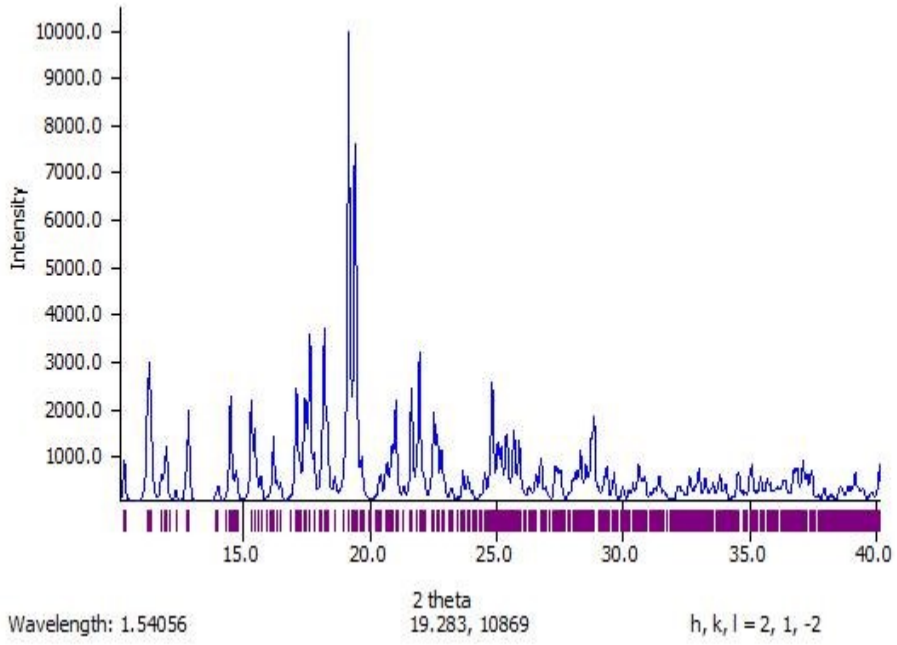


Fig. S6 IR spectra of **CP1**

(a)



(b)

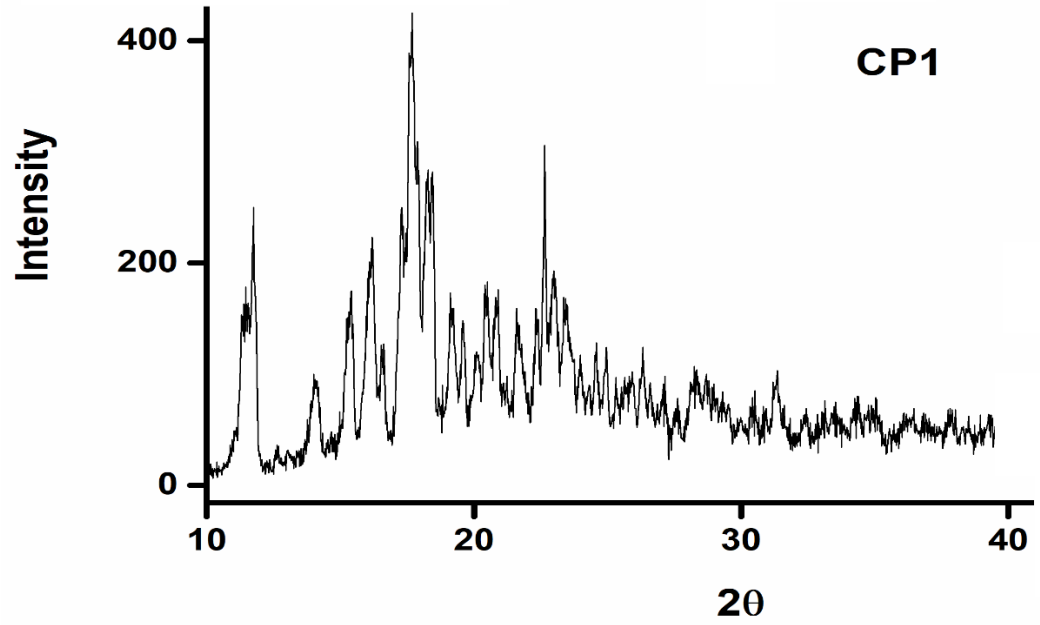


Fig. S7 (a) Simulated and (b) experimental powder XRD of **CP1**

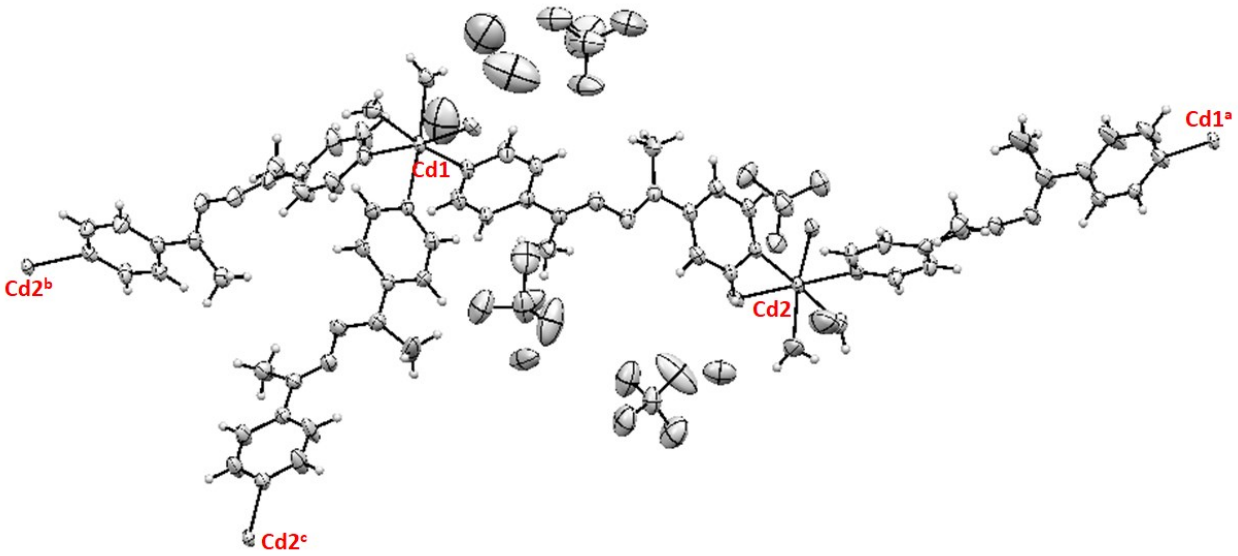


Fig. S8 ORTEP drawing of **CP1** showing thermal ellipsoids at the 50% probability level; Symmetry codes: a: –x, 1-y, 1-z, b: 2-x, 1-y, -z; c: -1+x, +y, -1+z

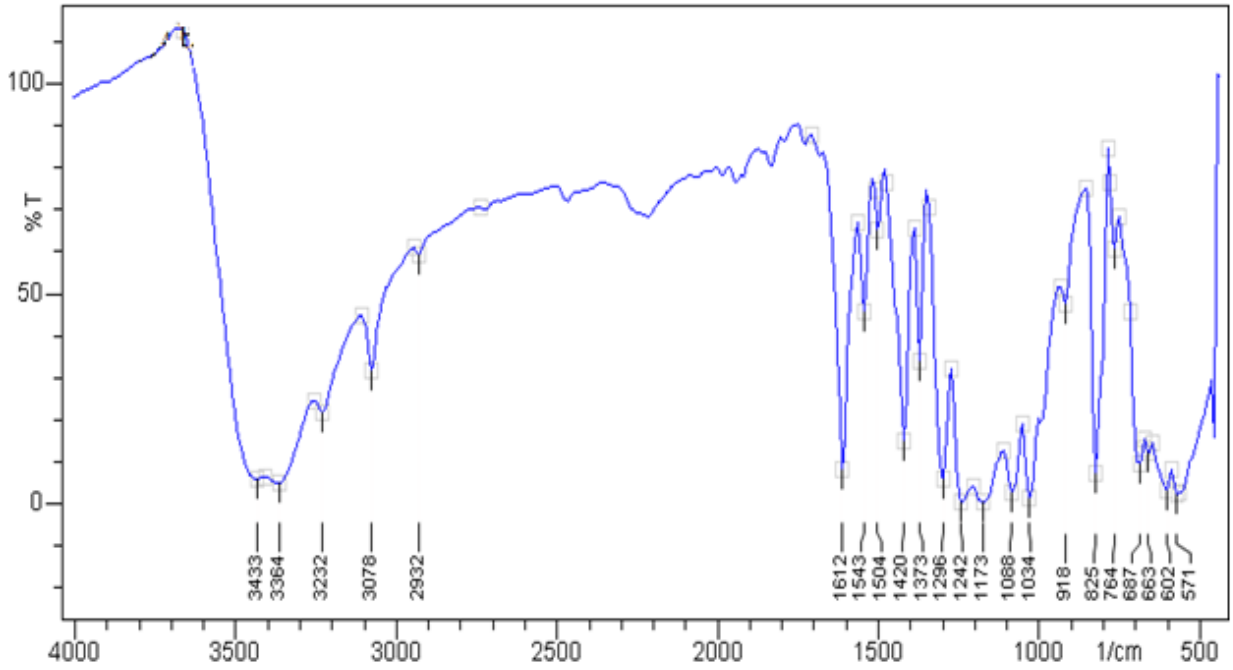


Fig. S9 IR spectra of **[HL1][ClO$_4$]**

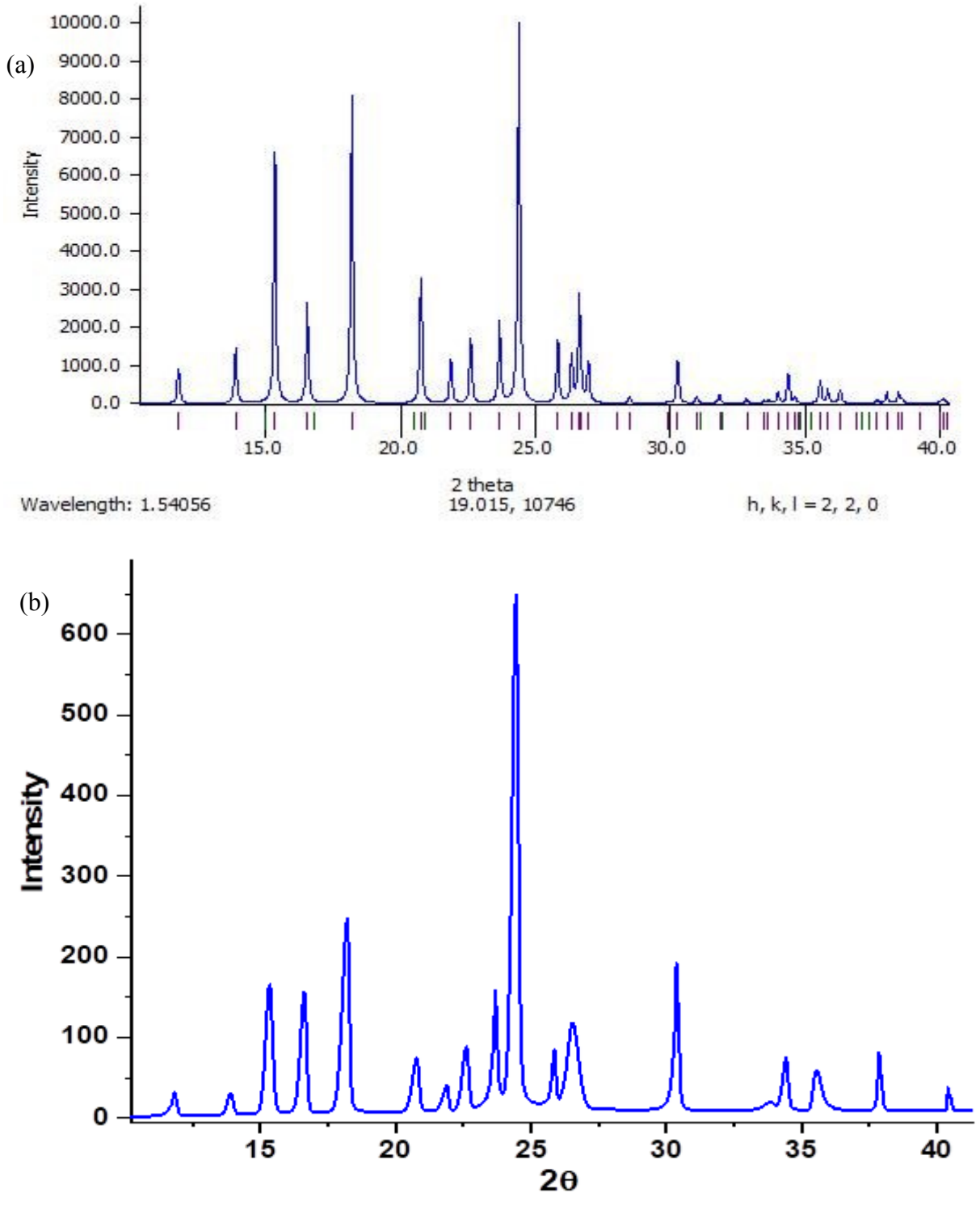


Fig. S10 Simulated and experimental powder XRD of **[HL1][ClO$_4$]**

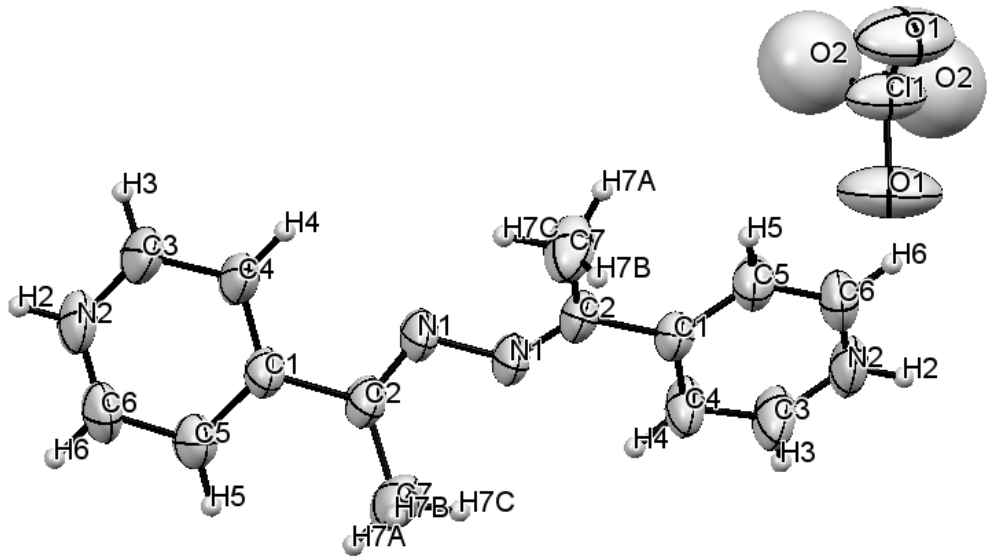


Fig. S11 ORTEP drawing of **[HL1][ClO4]** showing thermal ellipsoids at the 50% probability level

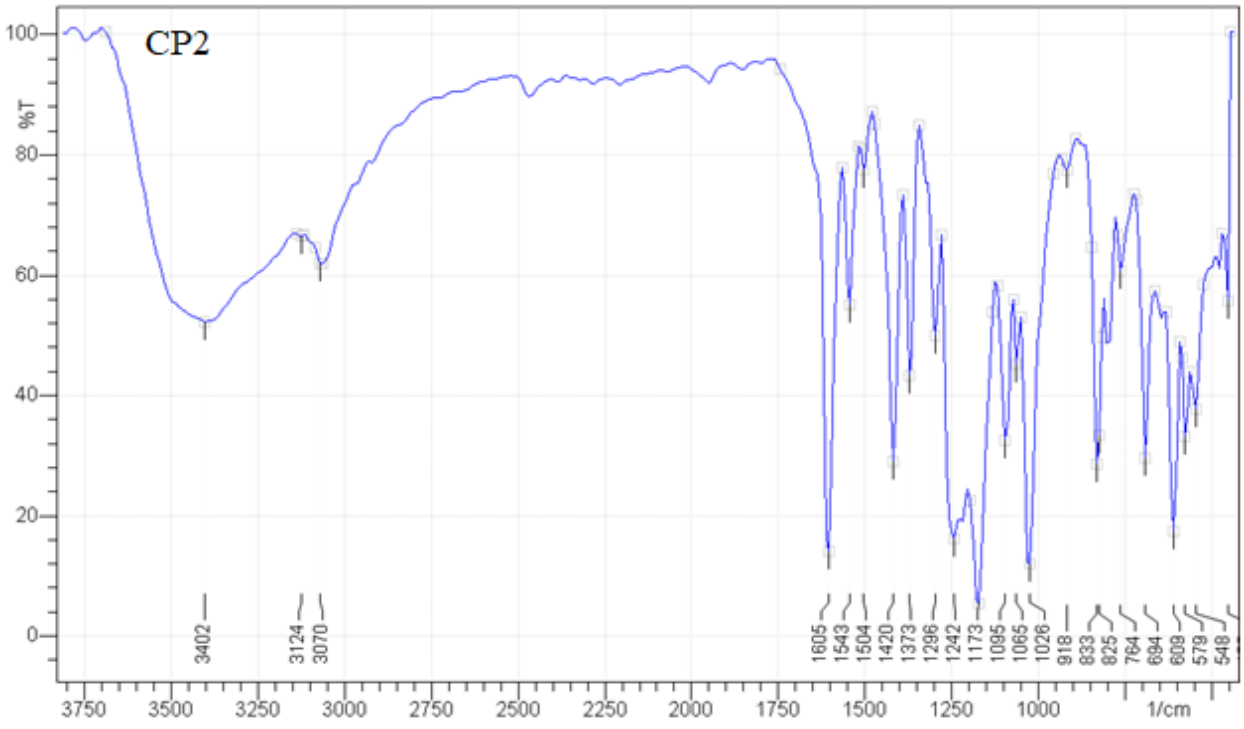


Fig. S12 IR spectra of **CP2**

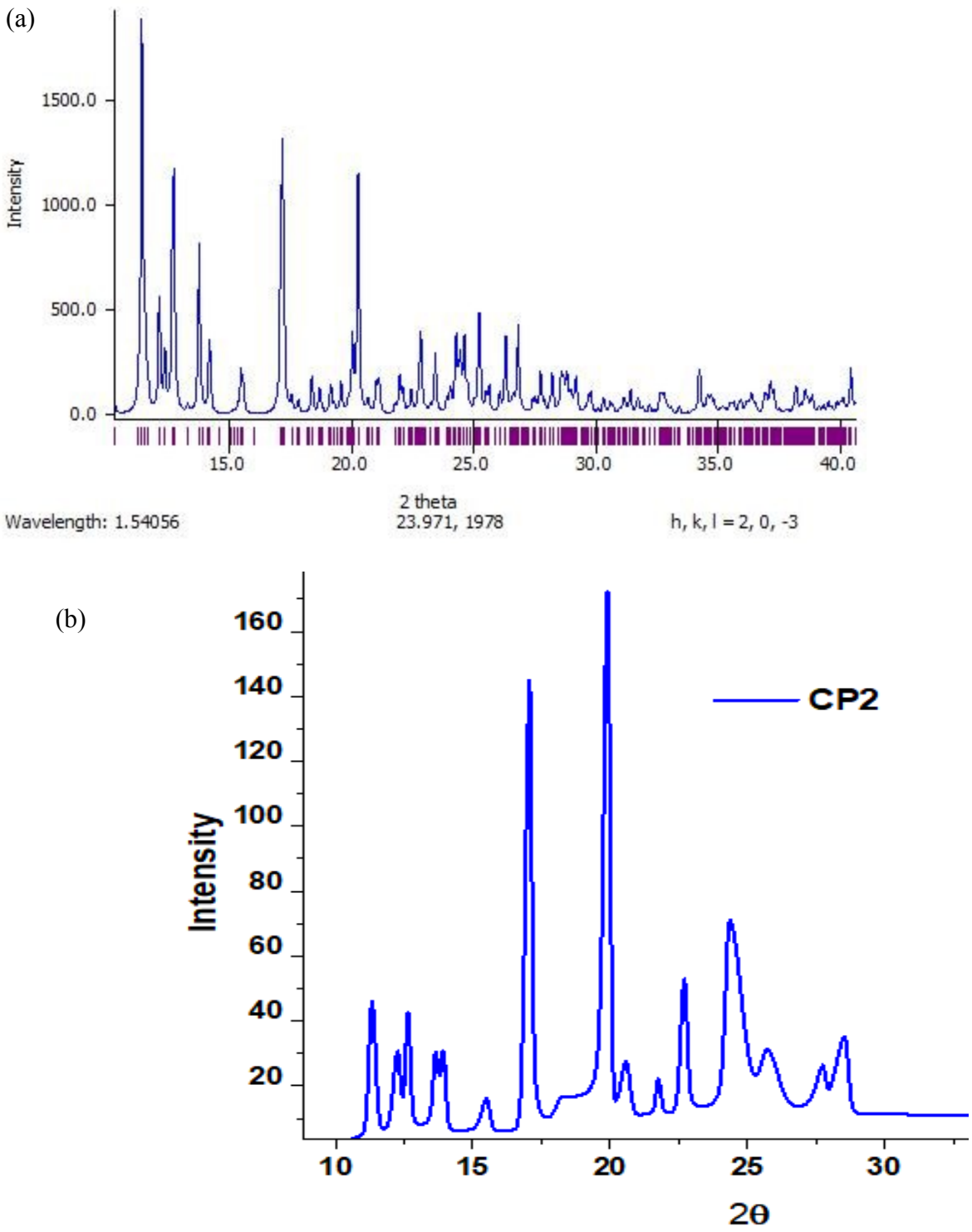


Fig. S13 (a) Simulated and (b) experimental PXRD of **CP2**

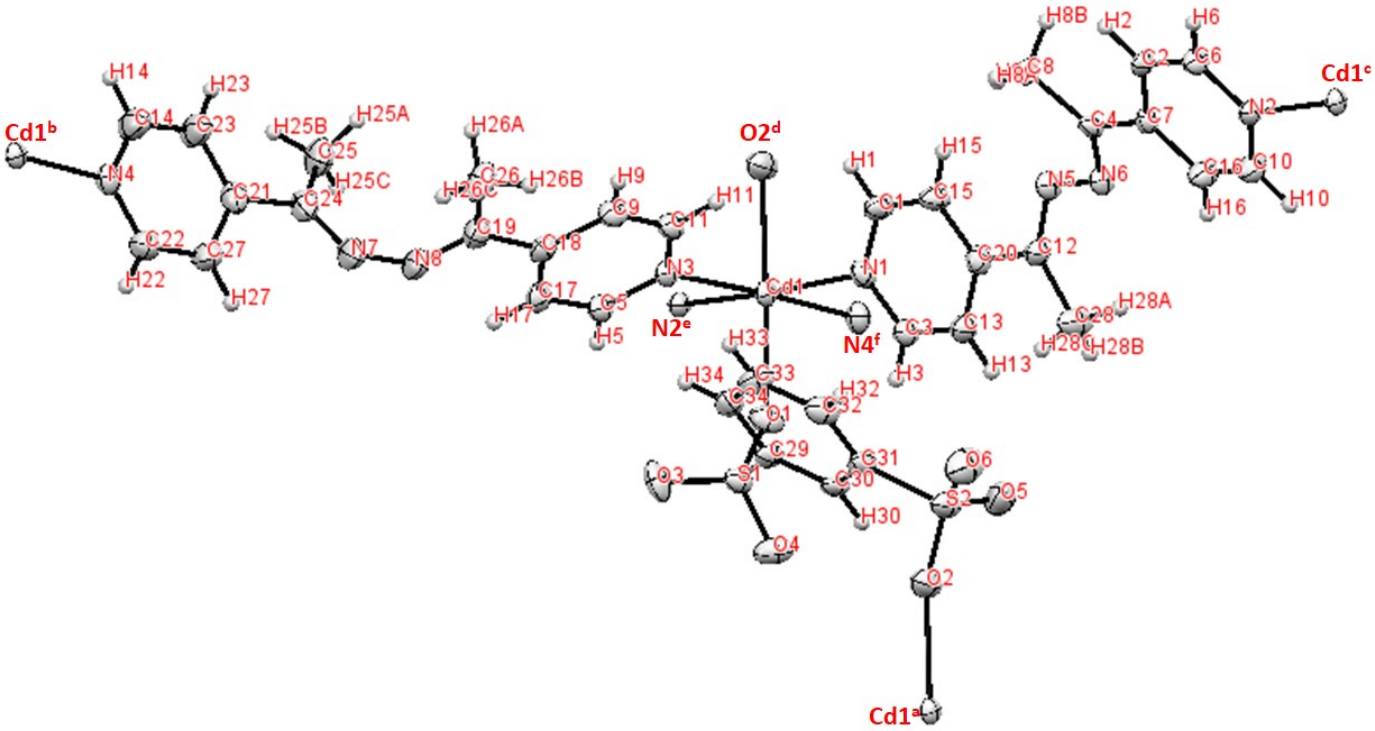


Fig. S14 ORTEP drawing of **CP2** showing thermal ellipsoids at the 50% probability level, Symmetry Codes: a: 1+x, y, z; b: x, y, 1+z; c: 1+x, 1+y, z; d: x-1, y, z; e: x-1, y-1, z; f: x, y, z-1

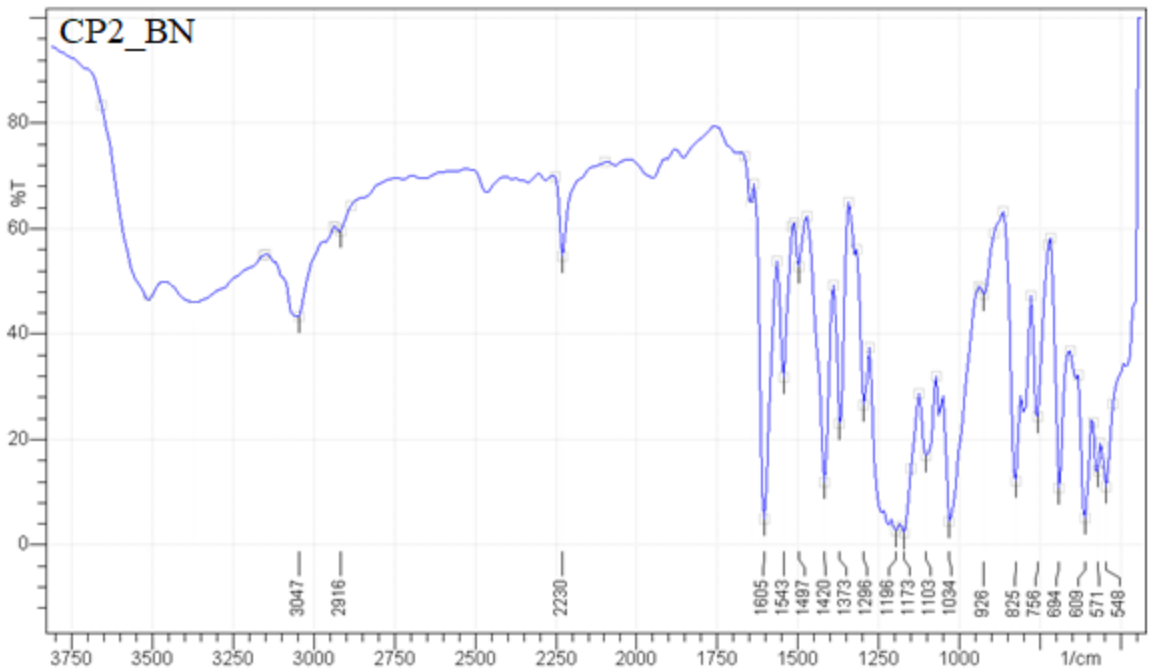
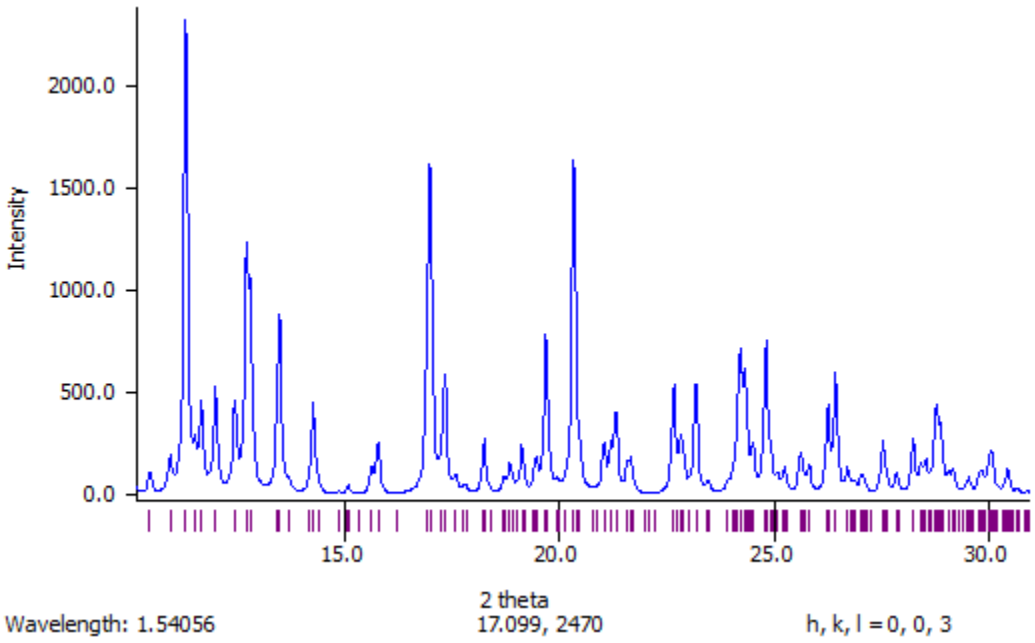


Fig. S15 IR spectra of **CP2_BN**



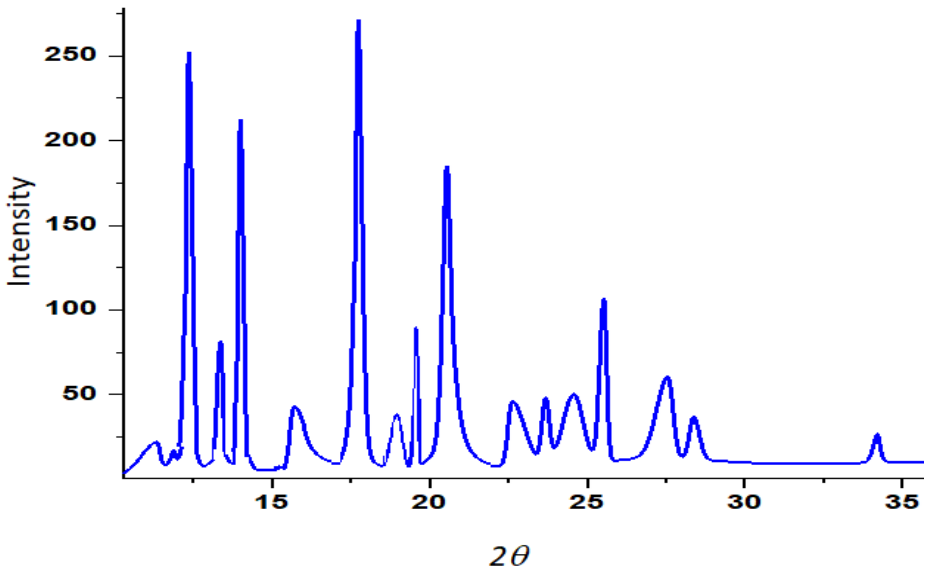


Fig. S16 Calculated and experimental PXRD of **CP2_BN**

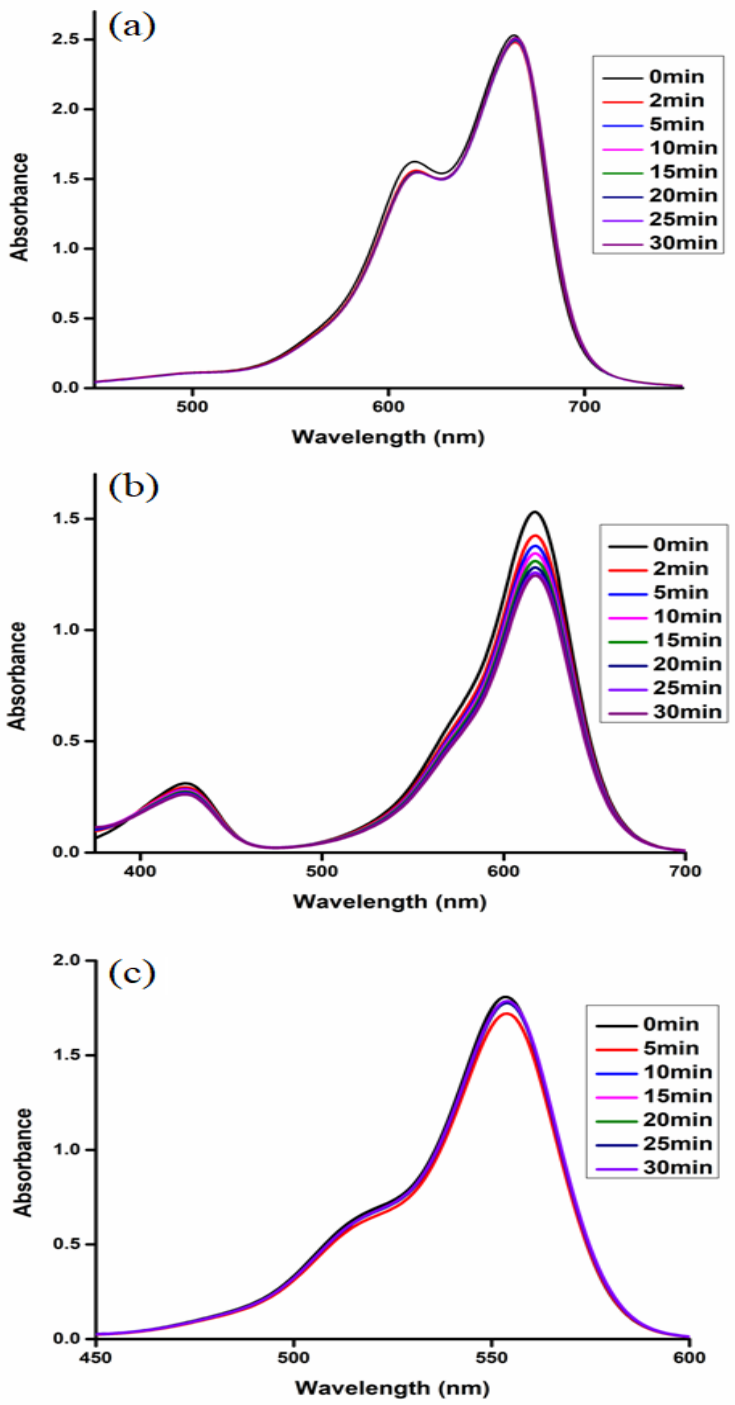


Fig. S17 UV-Visible spectra of dye degradation by **CP2** from aqueous solutions of (a) 5×10^{-4}M MB, (b)10^{-5}M MG, and (c) 2×10^{-5}M RB

Table S1 Crystallographic data and refinement parameters of **CP2_BN**

Compound	**CP2_BN**

Empirical formula	$C_{36.8}$ H_{34} Cd $N_{8.4}$ O_6 S_2
Formula Wt.	866.45
Temperature/K	298.15
Crystal system	Triclinic
Space group	P-1
a/Å	9.8814(3)
b/Å	14.1900(4)
c/Å	15.7164(5)
α/°	94.950(3)
β/°	91.893(3)
γ/°	100.060(3)
V/Å^3	2159.13(11)
Z	2
ρ_{calc}g/cm^3	1.334
μ/mm^{-1}	0.649
F(000)	894
Crystal size/mm^3	0.3 × 0.2 × 0.2
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	9.786 to 49.998
Index ranges	$-10 \leq h \leq 11$,
	$-16 \leq k \leq 16$,
	$-18 \leq l \leq 18$
Reflections collected	28332
Independent reflections	7608 [R_{int} = 0.0227, R_{sigma} = 0.0194]
Data / restraints / parameters	7539/0/464
Goodness-of-fit on F^2	1.065
Final R indexes [I>=2σ (I)]	R_1 = 0.0551, wR_2 = 0.1377
Final R indexes [all data]	R_1 = 0.0591, wR_2 = 0.1399

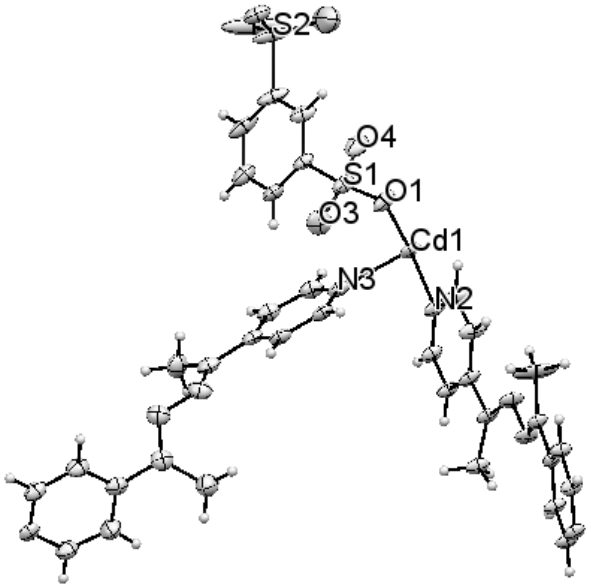


Fig S18 ORTEP of asymmetric unit of **CP2_BN** showing thermal ellipsoids at the 50% probability level