Electronic Supplementary Information

A mechanistic insight into the rapid and selective removal of Congo Red by an amide functionalised Zn(II) coordination polymer

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Contents:

Table S2. Hydrogen bond geometry (Å, °) in compounds **1**, **2** and **3.**

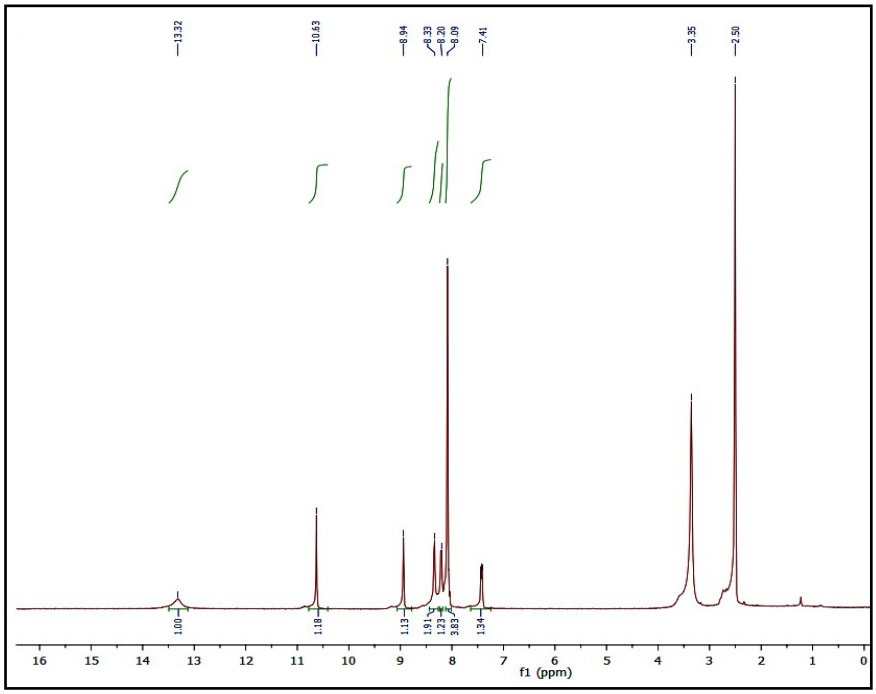


Fig. S1. ^{1}H-NMR spectrum of **HL** recorded in DMSO-d_6.

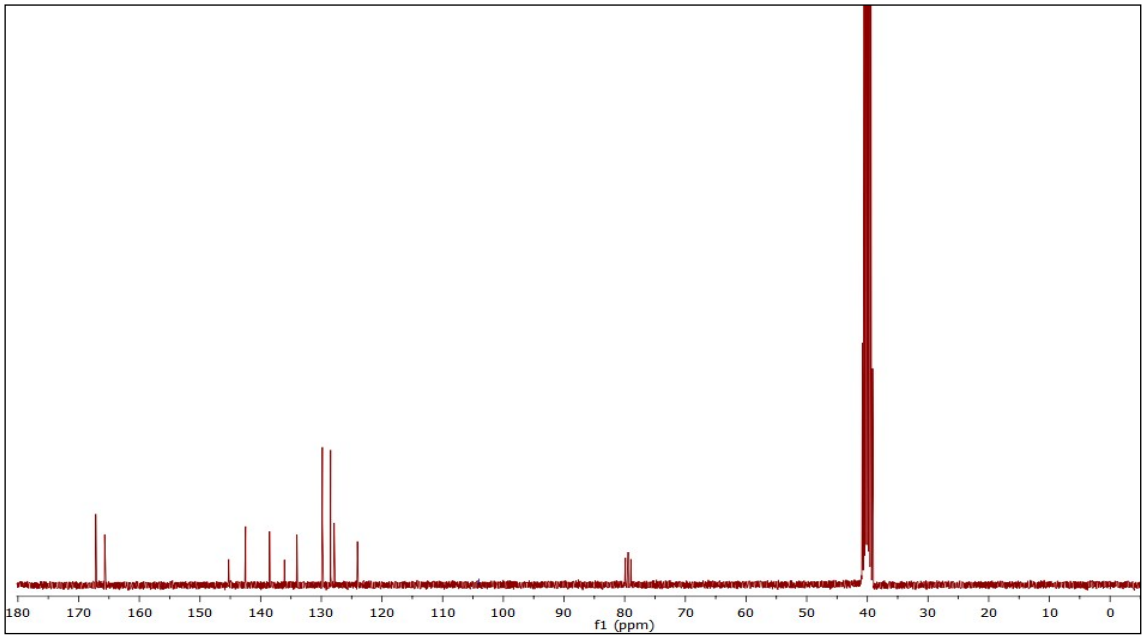


Fig. S2. ^{13}C-NMR spectrum of **HL** recorded in DMSO-d_6.

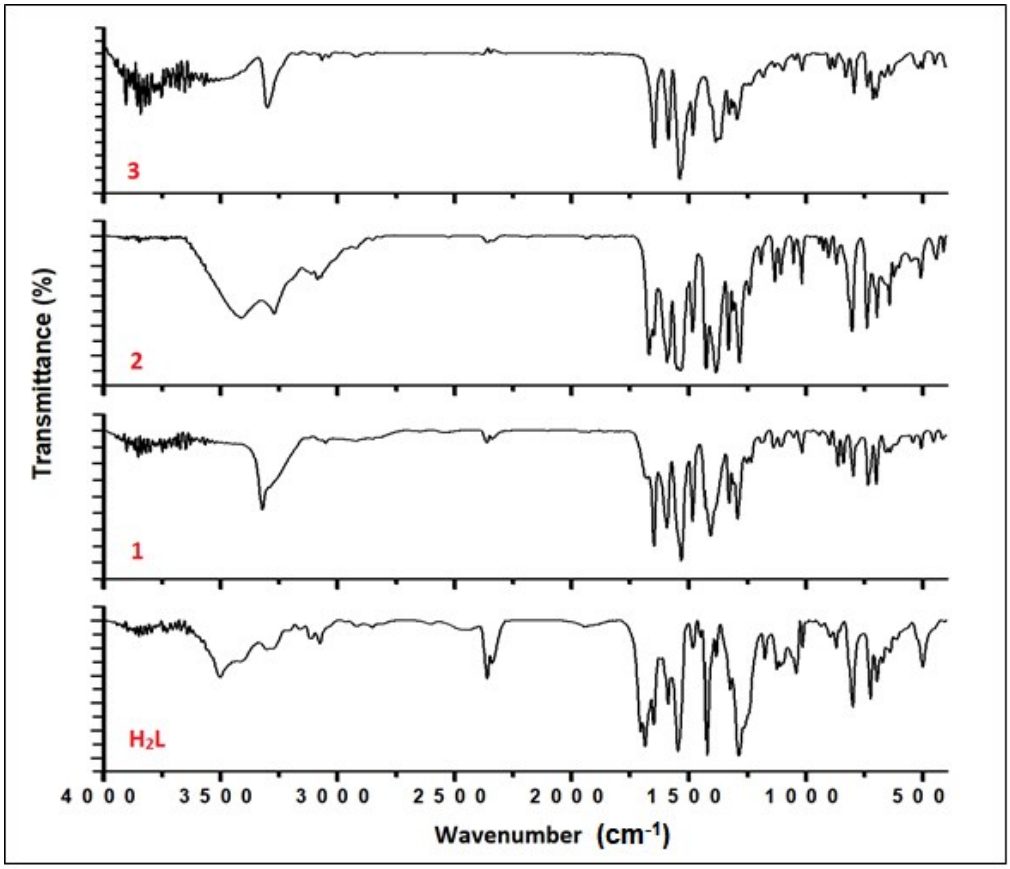


Fig. S3. IR Spectra of **HL** and CPs **1-3**.

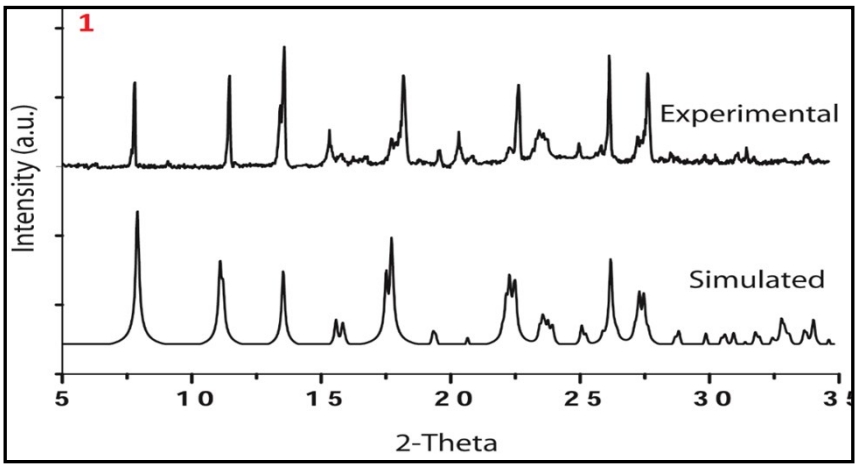


Figure S4: Simulated and Experimental PXRD of **1**.

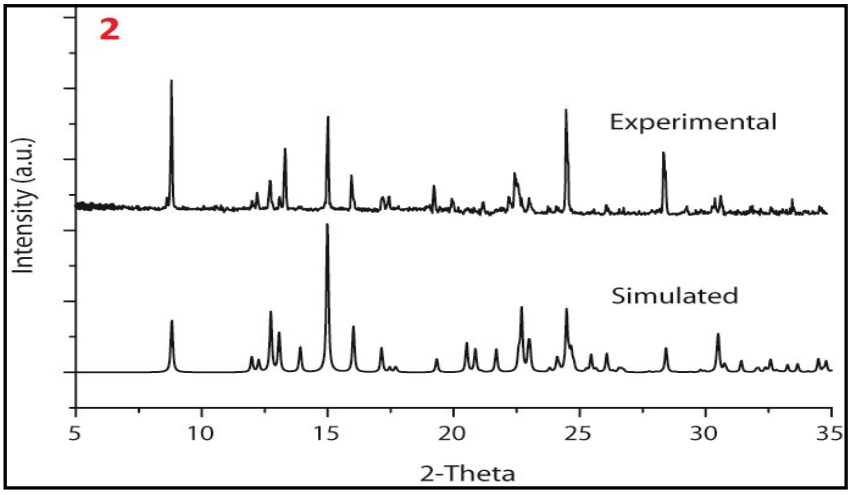


Fig. S5: Simulated and Experimental PXRD of **2**.

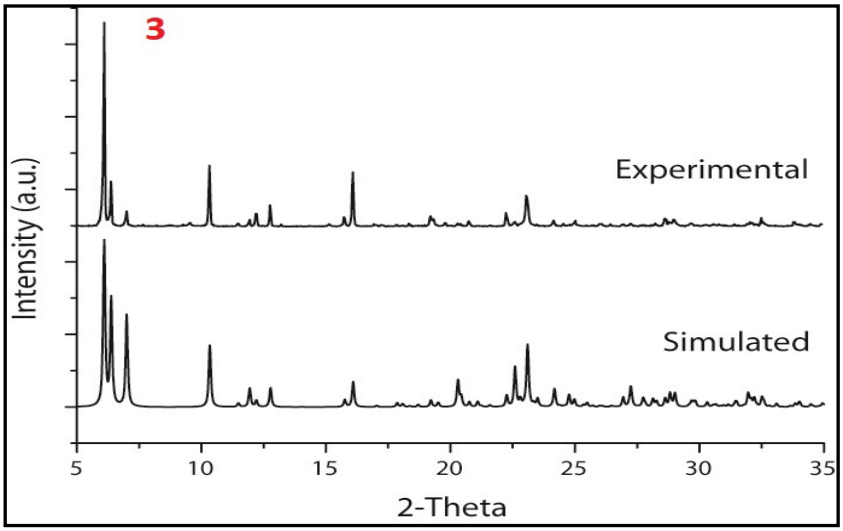
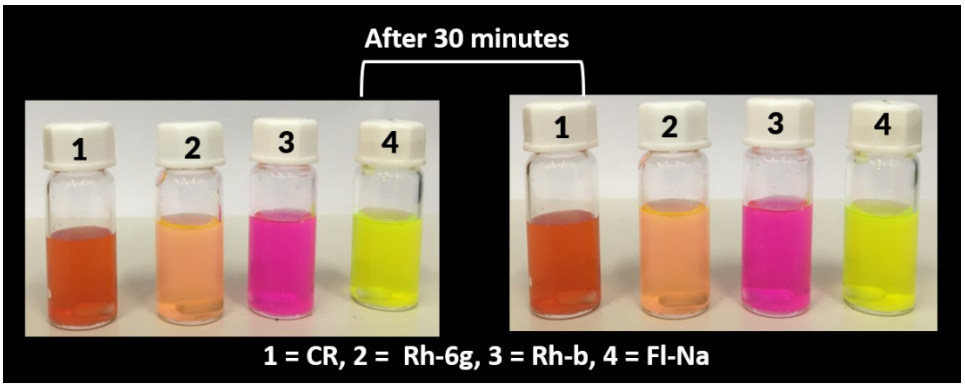
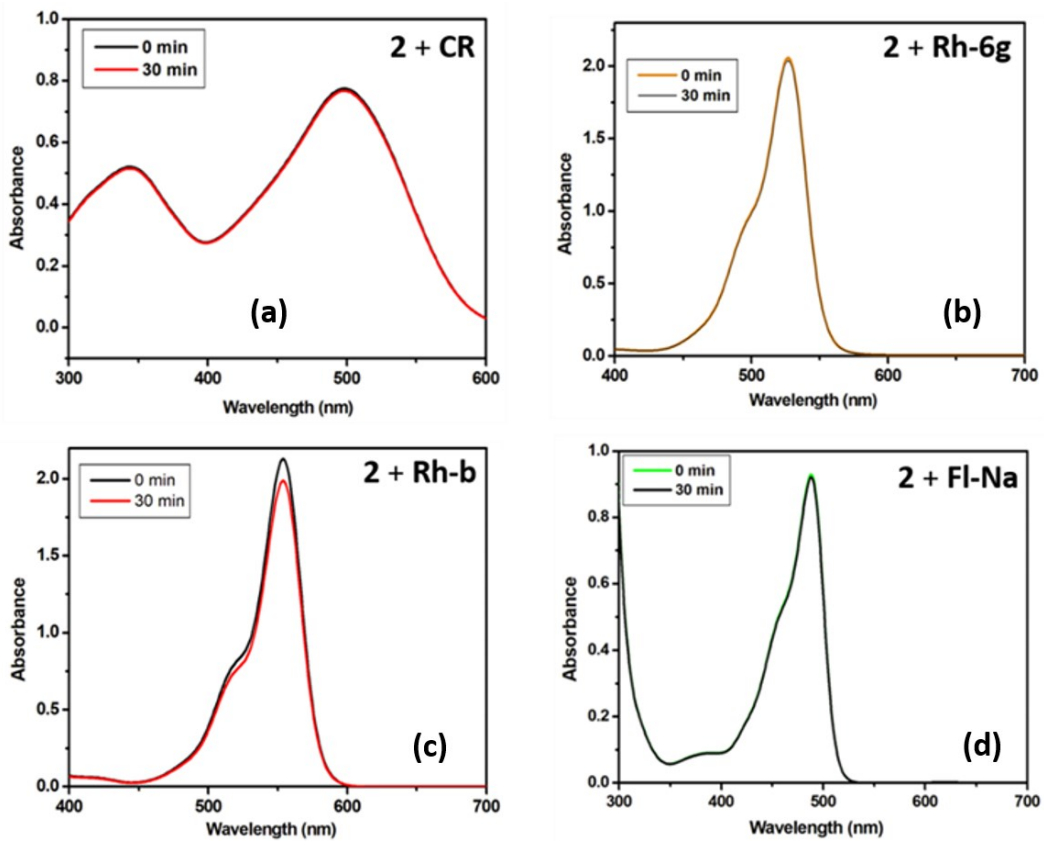


Fig. S6. Simulated and Experimental PXRD of **3**.

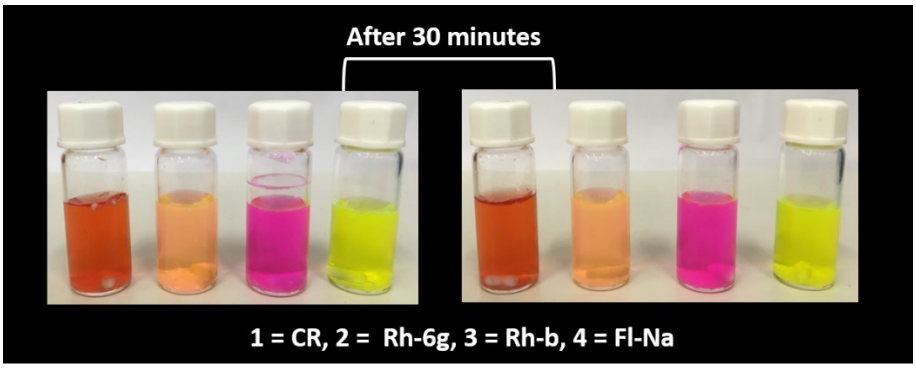


(**A**)

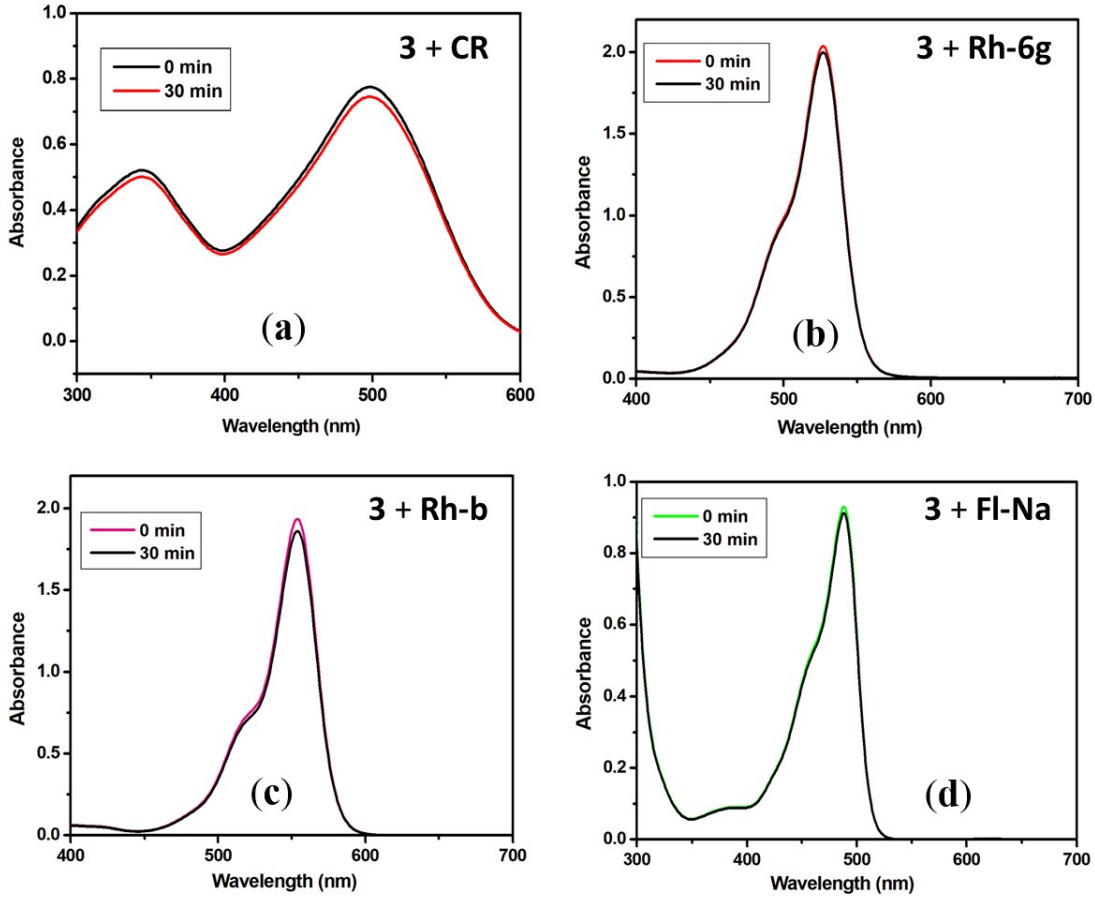


(**B**)

Fig. S7. (**A**) Naked eye visualization on the removal of dyes by **2** at room temperature. (**B**) UV-vis spectra of dye solutions upon adsorption on **2** at room temperature: (a) Congo red, (b) rhodamine 6g, (c) rhodamine B, and (d) fluorescein natrium.



(**A**)



(**B**)

Fig. S8. (**A**) Naked eye visualization on the removal of dyes by **3** at room temperature. (**B**) UV-vis spectra of dye solutions upon adsorption on **3** at room temperature: (a) Congo red, (b) rhodamine 6g, (c) rhodamine B, and (d) fluorescein natrium.

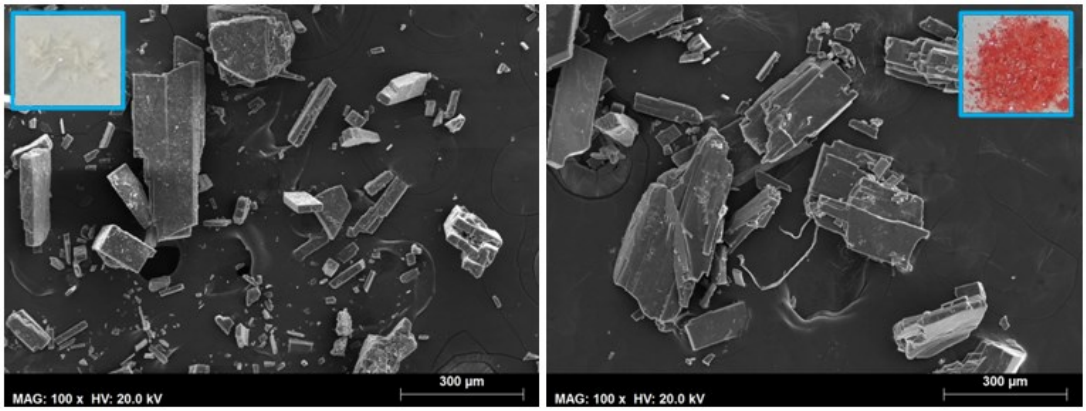


Fig. S9. SEM image of **1** recorded before and after the adsorption of CR.

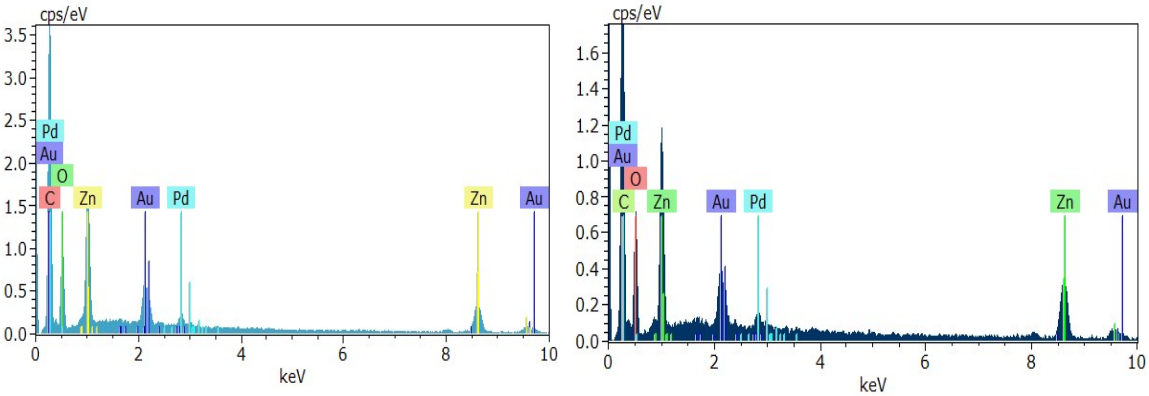


Fig. S10. EDX of **1** recorded before (left) and after (right) the adsorption of CR.

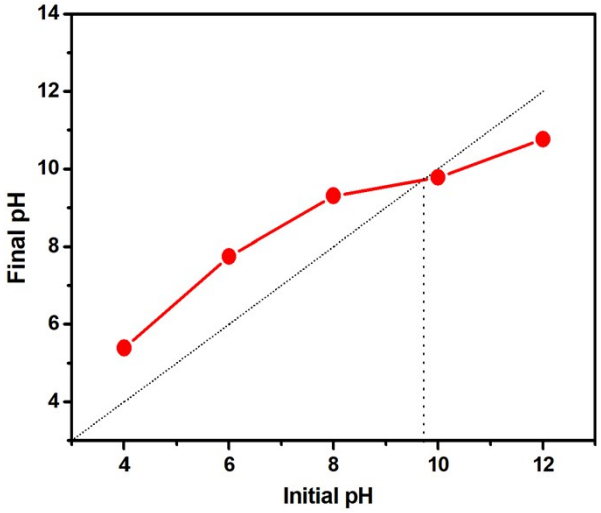


Fig. S11. Point of zero charge measurement of 1. Plot of final versus initial pH (red line).

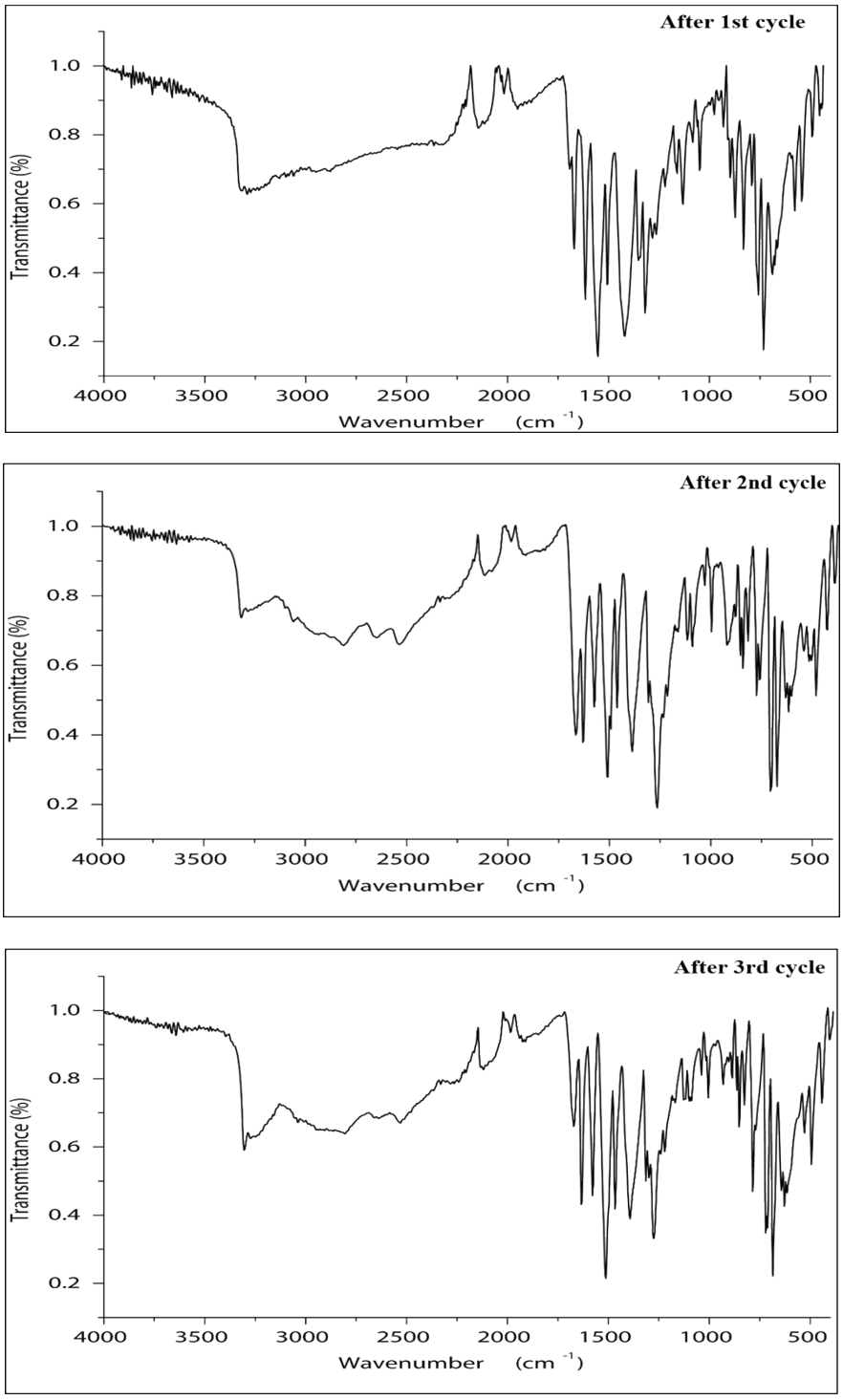


Fig. S12. IR spectra of **1** after various cycles.

Table S1. Selected bond distances (Å) and angles (°) for compounds 1-3	
1	Zn1-O2 2.006(3), Zn1-O3 2.034(2), Zn1-O4 2.431(3), Zn1-O5 2.029(3), Zn1-N2 2.064(3). <O2-Zn1-O5 101.31(13); <O2-Zn1-O3 103.12(11); <O5-Zn1-O3 99.79(11); <O2-Zn1-N2 143.16(12); <O5-Zn1-N2 92.75(11); <O3-Zn1-N2 107.81(11); <O2-Zn1-O4 92.55(11); <O5-Zn1-O4 156.53(10); <O3-Zn1-O4 58.25(9); <N2-Zn1-O4 87.15(9).
2	Cd1-O1 2.2900(12); Cd1-N2 2.3139(13); Cd1-O4 2.3425(13). <O1-Cd1-O1' 180.0; <O4-Cd1-O4' 180.00(7); <N2-Cd1-N'2 180.00(8); <O1-Cd1-N2 89.55(5); <O1'-Cd1-N2 90.45(5); <O1-Cd1-O4 93.16(5); <O1'-Cd1-O4 86.84(5); <N2-Cd1-O4 89.76(5); <N2'-Cd1-O4 90.24(5).
3	Pb1-O1 2.3821(19); Pb1-O4 2.3817(17); Pb1-N4 2.534(2). <O4-Pb1-O1 106.94(7); <O4-Pb1-N4 76.58(6); <O1-Pb1-N4 80.35(6).

Table S2. Hydrogen bond geometry (Å, °) in compounds 1-3					
Compound	D-H···A	D···H (Å)	H···A (Å)	D···A (Å)	<D−H···A(°)
1	N1-H1N···O4	0.88	2.10	2.978(4)	172
	O5-H5A···O1	0.81	1.91	2.709(4)	173
	O5-H5B···O7	0.89	1.76	2.646(5)	172
	C10-H10···O4	0.93	2.64	3.341(4)	133
	C12-H12···O1	0.93	2.36	3.068(4)	132
	C13-H13···O6	0.93	2.26	2.850(4)	121
	C22-H22B···O5	0.96	2.72	3.382(9)	126
2	O4-H4A···O2	0.93	1.79	2.6919(19)	164
	O4-H4B···O3	0.81	1.95	2.7546(19)	171
	N1-H1N···O2	0.82	2.34	3.086(2)	152
3	N1-H1N···O3	0.86	2.12	2.951(3)	162
	N2-H2N···O6	0.88	2.09	2.943(3)	163
	C10-H10···O3	0.93	2.42	2.876(3)	110
	C28-H28···O4	0.93	2.36	2.999(3)	125