Electronic Supplementary Material (ESI) for Inorganic Chemistry Frontiers.

Selective anionic dye adsorption, Topology and Luminescence study of structurally diverse cadmium(II) coordination polymers

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SI 1. Table : Selected bond lengths (Å) and bond angles (º) for complexes **1**, **2, 3** and **4**.

1			
Cd(1)-O(1)	2.363(3)	O(1)-Cd(1)-N(2)	127.59(13)
Cd(1)-N(1)	2.433(4)	O(1)-Cd(1)-O(7)	82.80(13)
Cd(2)-O(10)	2.239(3)	N(2)-Cd(1)-N(1)	145.38(13)
Cd(3)-O(5)	2.422(3)	O(10)-Cd(2)-O(18)	169.07(15)
O(5)-C(1)	1.254(5)	O(19)-Cd(3)-O(21)	91.55(16)
N(2)-C(5)	1.469(6)	C(1)-O(5)-Cd(1)	116.9(3)
O(14)-N(5)	1.236(6)	C(5)-N(2)-C(2)	110.3(4)
2			
Cd(2)-O(1)	2.246(7)	N(002)-Cd(2)-O(2)	86.3(3)
Cd(2)-N(016)	2.310(8)	O(1)-Cd(2)-O(2)	83.8(2)
Cd(1)-O(16)	2.279(6)	N(002)-Cd(2)-N(016)	174.3(3)
Cd(1)-N(013)	2.349(8)	O(16)-Cd(1)-O(15)	164.9(2)
Cd(5)-N(20)	2.424(8)	O(16)-Cd(1)-N(013)	86.9(2)
N(007)-C(1)	1.322(13)	O(37)-Cd(5)-O(008)	87.7(2)

3			
Cd(1)-N(1)	2.323(9)	N(1)-Cd(1)-O(8)	91.1(3)
Cd(1)-O(8)	2.333(7)	O(8)-Cd(1)-O(17)	91.9(3)
Cd(2)-O(1)	2.331(7)	O(9)-Cd(2)-O(1)	99.2(3)
Cd(2)-N(18)	2.444(9)	O(1)-Cd(2)-N(18)	135.8(3)
Cd(3)-O(1)	2.396(7)	N(18)-Cd(2)-N(20)	143.3(3)
O(1)-C(36)	1.275(13)	C(42)-O(5)-Cd(2)	113.1(6)
4			
Cd(1)-O(2)	2.266(2)	O(2)-Cd(1)-N(2)	89.32(10)
Cd(1)-N(2)	2.291(3)	O(2)-Cd(1)-O(1)	84.64(8)
Cd(2)-O(5)	2.382(3)	O(5)-Cd(2)-N(3)	85.59(9)
Cd(2)-N(4)	2.431(3)	O(5)-Cd(2)-O(3)	87.24(9)
O(7)-C(25)	1.272(4)	N(3)-Cd(2)-N(4)	141.46(9)
N(1)-C(1)	1.329(4)	C(29)-O(13)-Cd(2)	119.70(19)

SI 2. Table: Weak interaction for Complexes **1-4.**

D-H···A	D-H (Å)	H···A (Å)	D···A (Å)	DHA (°)	Symmetry code
1					
O17 --H17A ..O4	0.87	2.37	3.1474(3)	148	--
O17 --H17A ..O9	0.87	2.15	2.7823(2)	129	--
O17 --H17B ..O16	0.88	2.12	2.9948(2)	169	1+x,y,z
O18 --H18A ..O11	0.85	2.47	2.8439(2)	107	--
O18 --H18A ..O20	0.85	2.02	2.7943(2)	152	-1+x,y-1+z
O18 --H18B ..O8	0.85	2.54	2.9306(2)	109	-x,1-y,1-z
O19 --H19A ..O13	0.85	2.50	2.8205(2)	103	1-x,-y,1-z
O19 --H19B ..O3	0.85	2.07	2.7750(2)	140	--
O21 --H21A ..O11	0.86	2,47	3.2926(3)	161	1+x,y,1+z
O21 --H21A ..O14	0.86	2.34	2.9071(2)	124	1+x,y,1+z
O21 --H21B ..O2	0.86	2.01	2.8150(2)	156	1-x,-y,2-z
O22 –H22A ..O13	0.86	2.37	2.8680(2)	118	1+x,y,1+z
O22 --H22A ..O20	0.86	2.59	2.9169(2)	104	--
O22 --H22B ..O13	0.86	2.53	2.8680(2)	105	1+x,y,1+z
O23 --H23A ..O1	0.85	2.57	3.1426(3)	126	1+x,y,z

O23 --H23B ..O16	0.85	2.34	2.9872(2)	133	1+x,y,1+z
O7 --H7B ..O15	0.97	2.46	3.3626(30)	155	1+x,y,1+z

2

O1 --H1B …O20	0.87	1.83	2.6825(3)	165	x,1-y,-1/2+z
O15 --H15A …N01	0.88	1.93	2.7891(4)	164	x,1+y,z
O16 --H16A ...N008	0.87	1.93	2.7663(4)	162	x,1+y,z
O16 --H16B ...N034	0.87	1.83	2.6948(3)	173	--
O20 --H20A …N09	0.86	1.86	2.7023(3)	165	--
O20 --H20B …O1	0.86	1.86	2.6825(3)	159	x,1-y,1/2+z
O31 --H31A ..O26	0.86	2.25	3.0573(4)	145	-1/2+x,1/2-y,-1/2+z
O31 --H31B ..O45	0.85	2.57	3.3009(4)	145	-1/2+x,1/2-y,-1/2+z
O31 --H31B ..O45	0.85	2.20	2.8694(4)	135	-1/2+x,1/2-y,-1/2+z
O31 --H31B ..O46	0.85	1.83	2.6539(3)	162	-1/2+x,1/2-y,-1/2+z
O32 --H32A ..O6	0.85	2.18	2.6852(3)	162	--
O32 --H32B ..O19	0.85	2.43	2.7672(4)	104	1/2+x,-1/2+y,z
O33 --H33A ..O37	0.85	2.08	2.9262(4)	171	1/2+x,-1/2+y,z
O35 --H35B ..O41	0.85	2.32	2.8830(4)	124	--
O47 --H47A ..O7	0.85	2.23	3.0258(4)	156	--

O47	--H47B	..O48	0.85	2.13	2.9270(4)	157	--
O48	--H48A	..O19	0.85	2.20	2.8191(4)	130	1/2+x,-1/2+y,z
O48	--H48B	..O55	0.85	2.01	2.8434(4)	168	1/2+x,1/2-y,-1/2+z
C2	--H2	..O28	0.93	2.36	3.2705(4)	167	x,1+y,z
C6	--H6	..O31	0.93	2.37	3.2946(4)	176	--
C9	--H9	..O46	0.93	2.48	3.2684(4)	142	--
C11	--H11	..O008	0.93	2.50	3.1949(4)	132	--
C02G	--H02C	..O33	0.97	2.47	3.3753(4)	156	-1/2+x,1/2+y,z
C031	--H03B	..O33	0.97	2.51	3.4405(4)	160	-1/2+x,1/2+y,z
C035	--H03C	..O31	0.97	2.51	3.3066(4)	139	1/2+x,1/2-y,1/2+z
C23	--H23B	..O2	0.97	2.55	3.0971(4)	116	--
C037	--H03F	..O16	0.97	2.49	3.4360(4)	166	1/2+x,-1/2+y,z
C27	--H27	..O00W	0.93	2.49	3.2231(4)	136	-1/2+x,3/2-y,-1/2+z
C33	--H33	..O26	0.93	2.48	3.1569(4)	129	-1/2+x,3/2-y,-1/2+z
C36	--H36	..O009	0.93	2.41	3.1081(4)	132	--
C39	--H39	..O32	0.93	2.42	3.2802(4)	155	x,1-y,1/2+z
C41	--H41	..O45	0.93	2.53	3.2415(4)	134	-1/2+x,1/2+y,z
C52	--H52	..O27	0.93	2.59	3.3543(4)	139	

C56	--H56	..O27	0.93	2.53	3.3377(4)	145	
C59	--H59	..O49	0.93	2.52	3.3840(4)	154	
C64	--H64B	..O47	0.97	2.49	3.4450(4)	168	x,1-y,1/2+z

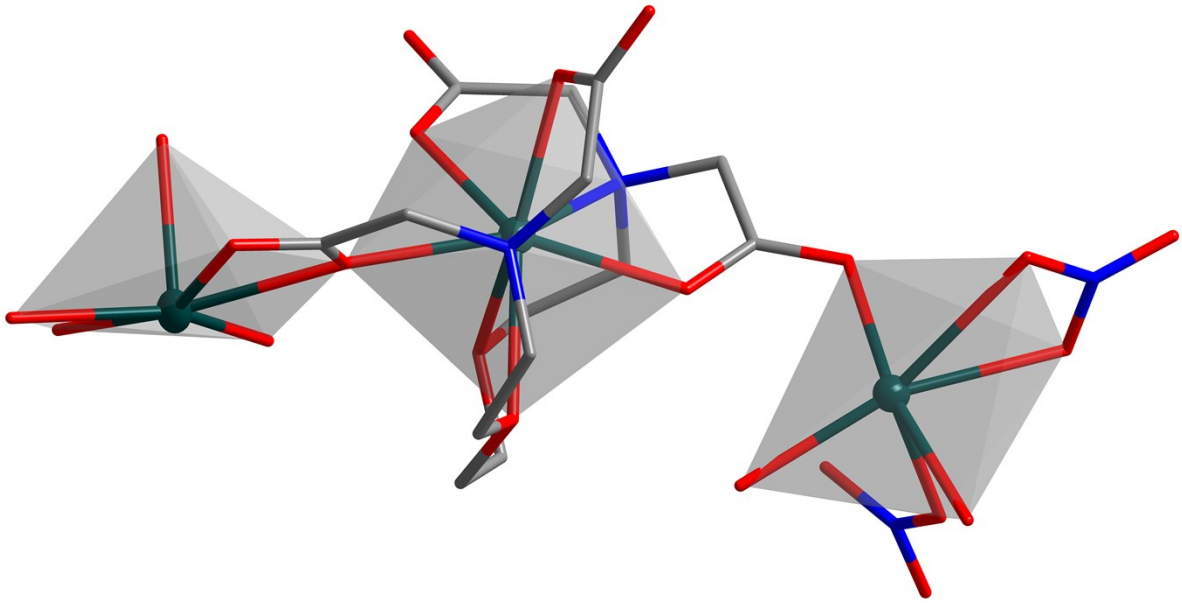
3

O12	--H12B	..O11	0.87	1.89	2.6742(13)	149	
O16	--H16A	..O24	0.85	2.01	2.7599(14)	146	
O16	--H16B	..O6	0.85	1.93	2.7299(14)	155	1-x,1-y,-z
5 O27	--H27C	..O24	0.85	1.94	2.7844(14)	171	1-x,1-y,-z
5 O27	--H27D	..O16	0.85	2.42	2.9283(15)	119	
7 O31	--H31A	..O24	0.85	2.22	2.6828(13)	115	
7 O31	--H31B	..O28	0.85	1.96	2.7989(14)	167	
8 O41	--H41D	..O28	0.85	2.47	2.7665(14)	101	-1+x,y,z
1 C27	--H27A	..O11	0.97	2.58	3.1577(16)	118	1+x,y,z
10 Intra 1 C30	--H30A	..O2	0.97	2.57	3.0541(15)	111	
11 Intra 1 C46	--H46A	..O9	0.97	2.49	3.0063(15)	113	
12 Intra 1 C50	--H50	..O9	0.93	2.42	3.2926(16)	157	1-x,1-y,-z

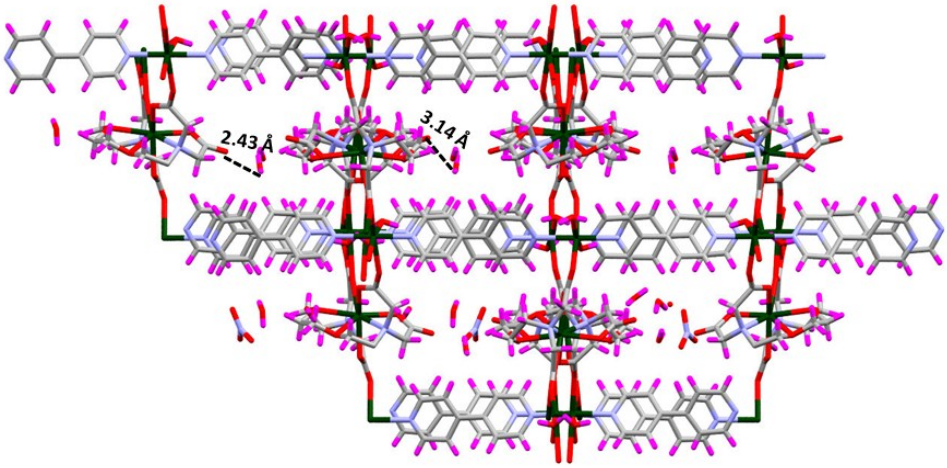
4

Intra	1 O1	--H1A	..O3	0.86	2.07	2.8102(2)	143	
Intra	1 O1	--H1B	..O13	0.81	1.88	2.6905(2)	172	x,1-y,-1/2+z
	2 O4	--H4A	..O12	0.85	2.39	3.2316(2)	173	1/2-x,1/2-y,1-z
	2 O4	--H4B	..O5	0.74	2.12	2.8402(2)	165	
	3 O35	--H35A	..O12	0.85	1.90	2.7471(2)	171	1/2-x,1/2-y,1-z
	3 O35	--H35B	..O6	0.85	2.03	2.8192(2)	153	
	4 O37	--H37B	..O6	0.85	2.30	2.8418(2)	122	
	4 O37	--H37B	..O38	0.85	2.48	3.1052(2)	336	
	1 C00N	--H00B	..O4	0.97	2.55	3.4498(2)	154	
Intra	1 C5	--H5	..O13	0.93	2.47	3.3581(2)	160	x,1-y,-1/2+z
	1 C7	--H7	..O37	0.93	2.53	3.3864(2)	153	
	1 C9	--H9	..O37	0.93	2.51	3.3737(2)	154	-x,y,1/2-z
	1 C10	--H10	..O38	0.93	2.54	3.2278(2)	131	-x,1-y,-z
Intra	1 C12	--H12	..O2	0.93	2.50	3.1447(2)	127	
	1 C17	--H17B	..O1	0.97	2.52	3.4863(2)	175	1-x,y,1/2-z
	1 C18	--H18B	..O12	0.97	2.57	3.5061(2)	163	1-x,1-y,1-z
	1 C26	--H26B	..O2	0.97	2.30	3.1428(2)	145	1/2-x,1/2+y,1/2-z

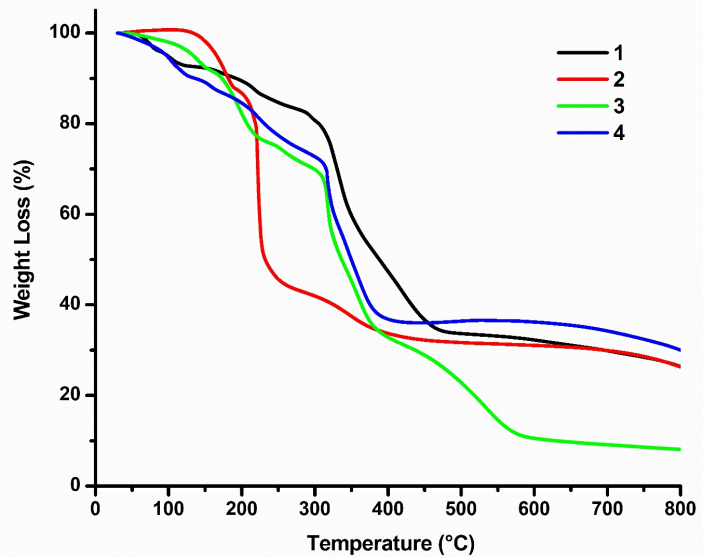
SI3 Different types of geometry of complex **1.**



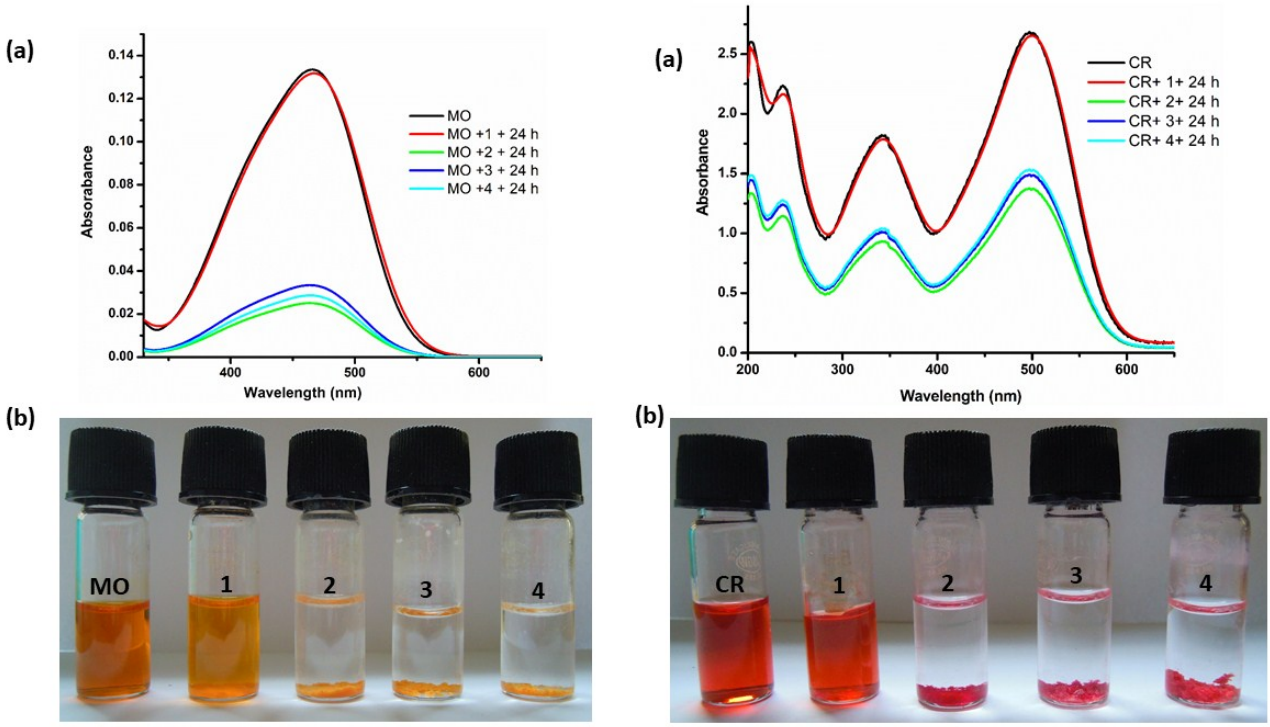
SI 4 Hydrogen bonding in complex **2.**



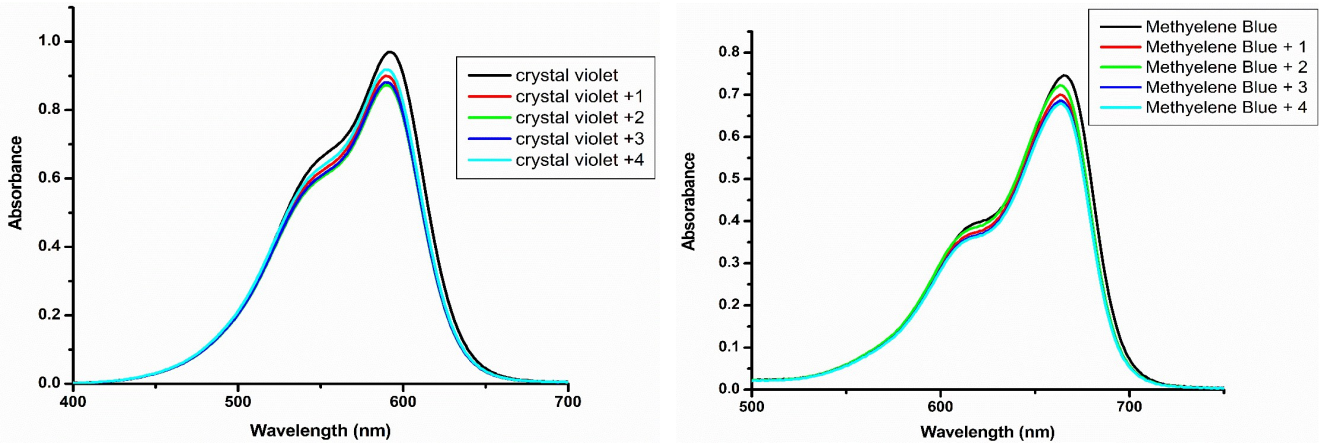
SI 5. The Thermogravimetric curves for complexes **1-4**.



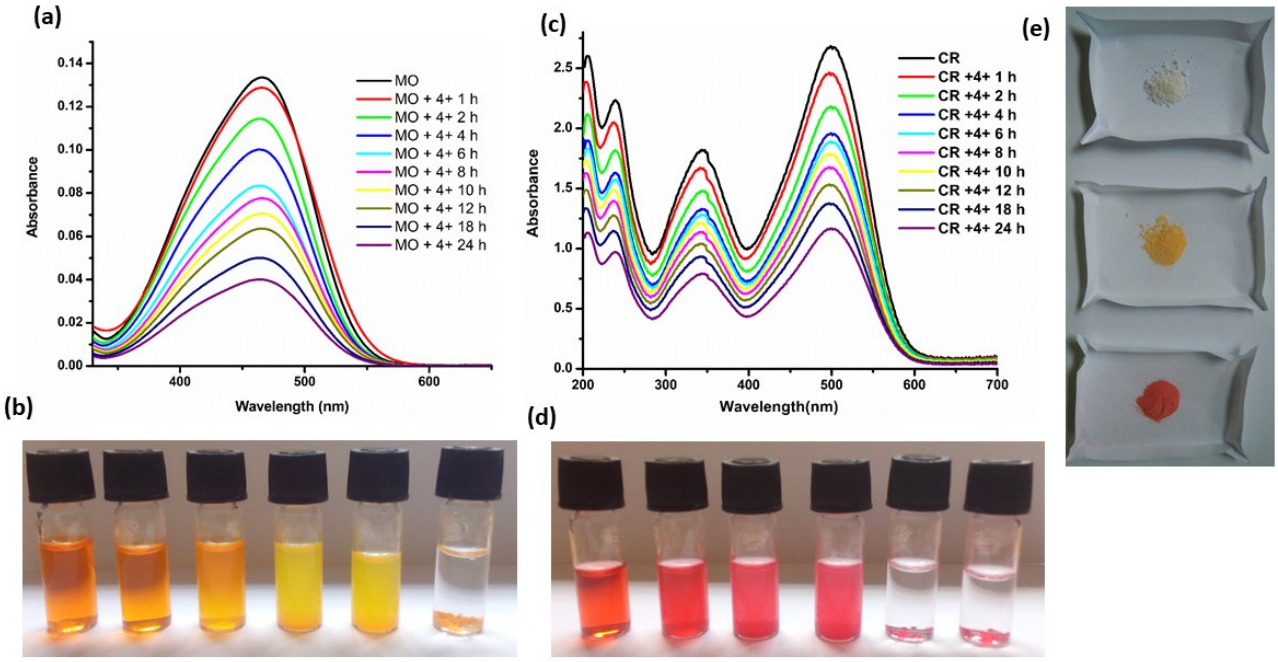
SI 6a. UV-vis spectra and colorimetric adsorption of anionic dyes of methyl orange by complexes **2, 3** and **4** after 24 h.



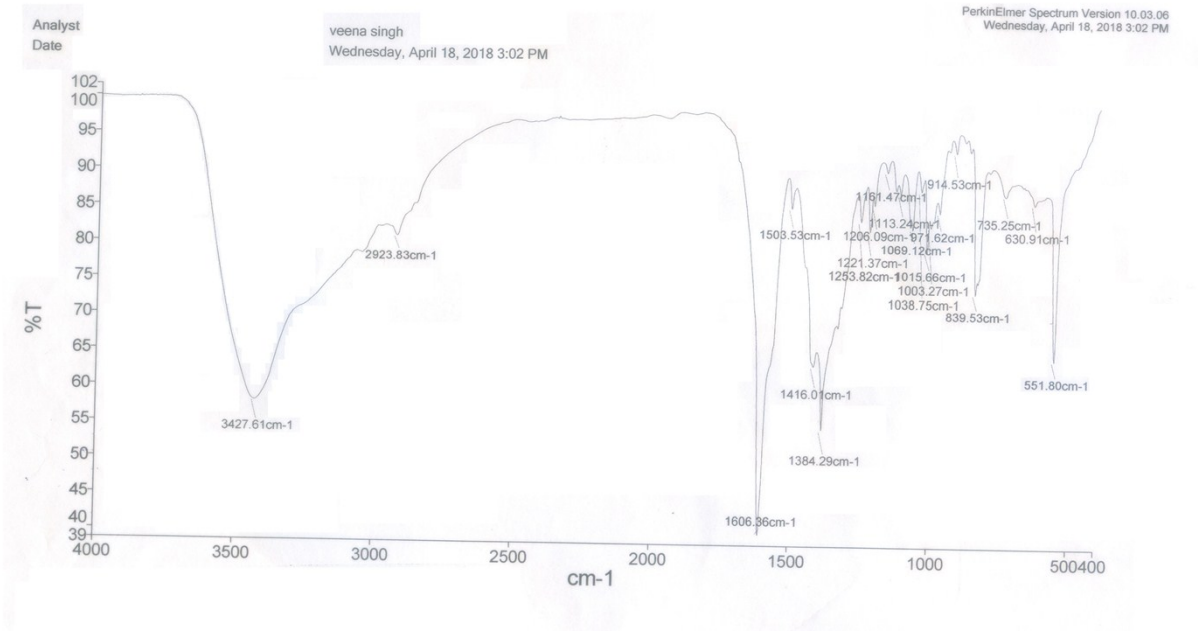
SI 6b. UV-vis spectra of aqueous cationic dyes with co-ordination polymers **1-4** after 24 h.



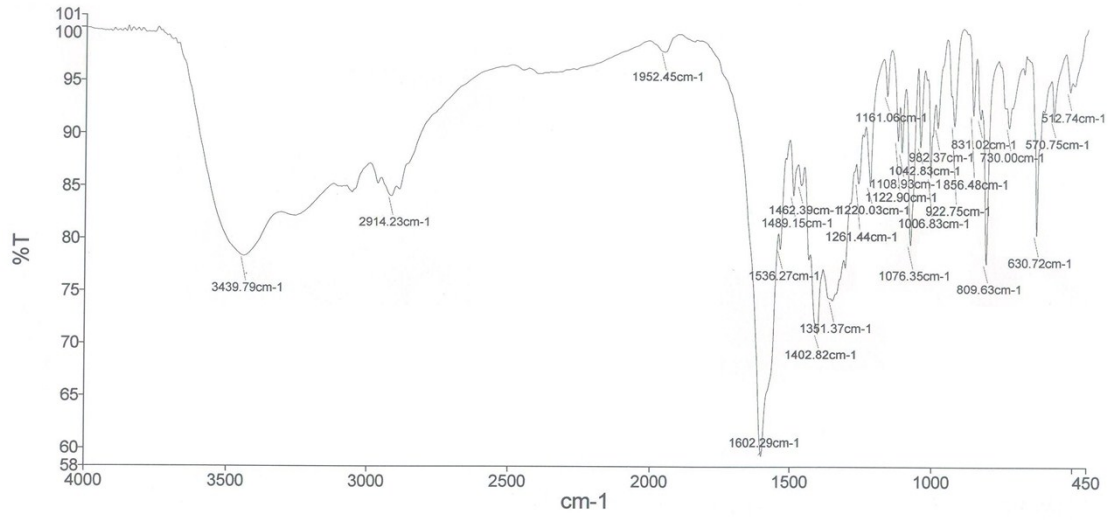
SI 7. (a) UV-vis spectra of aqueous solution of MO dye with complex **4** (b) The photograph shows the colour of dye solution changes with time in presence of **4** (c) UV-vis spectra of aqueous solution of CR dye with complex **4** (d) The photograph shows the colour of dye solution changes with time in presence of complex **4** (e) The colour of crystalline complex **4** before and after MO and CR dye adsorption.



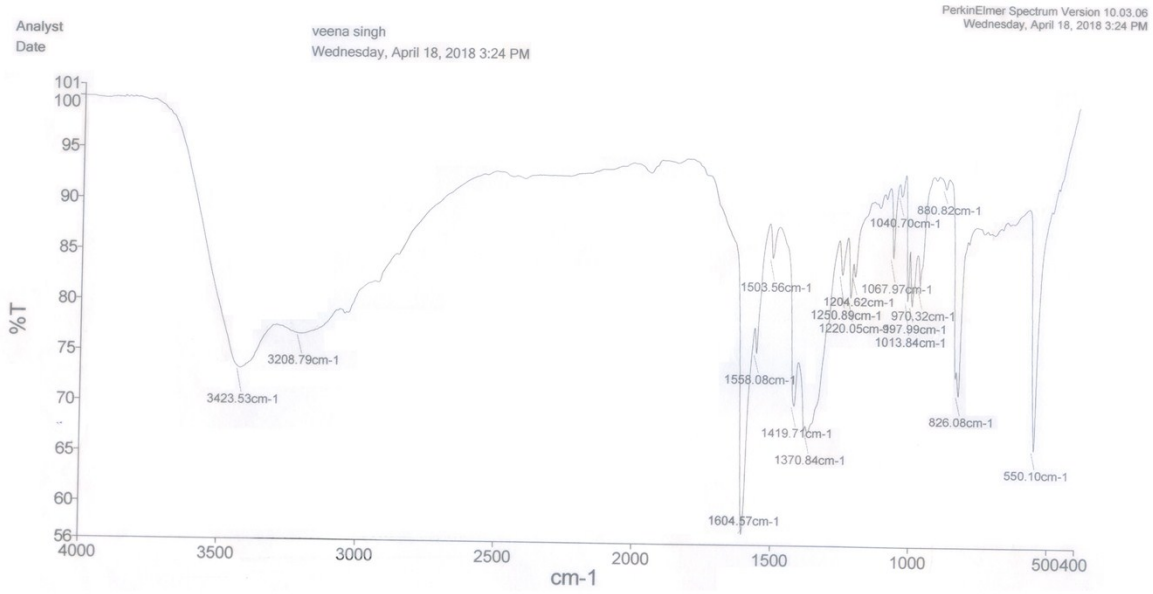
SI 8



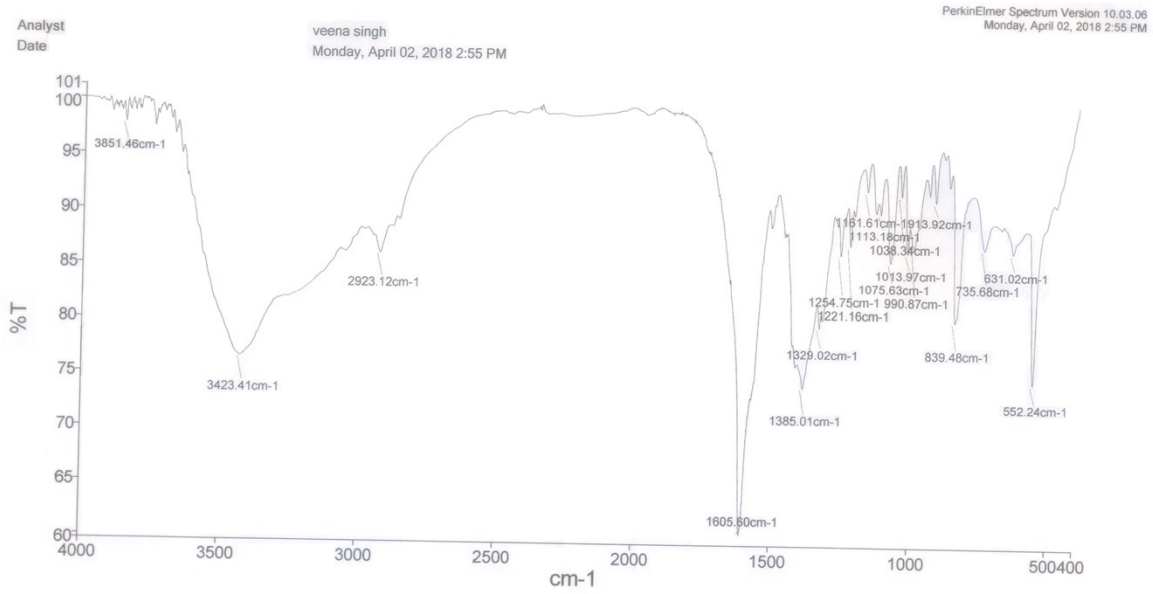
IR Spectrum of complex 2



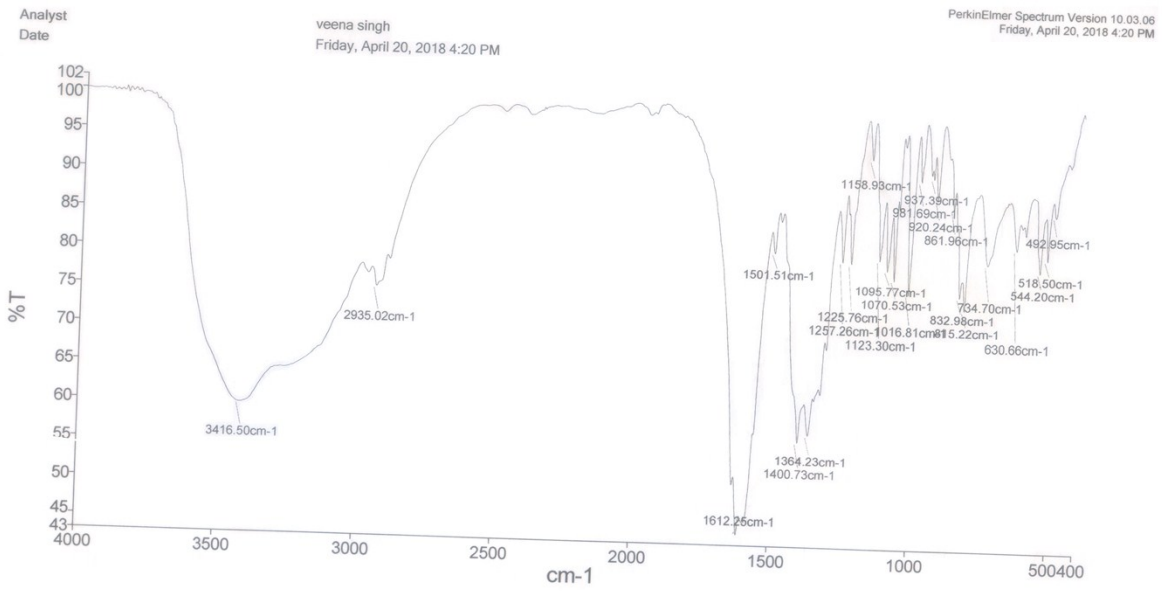
IR Spectrum of complex 2 after MO adsorption



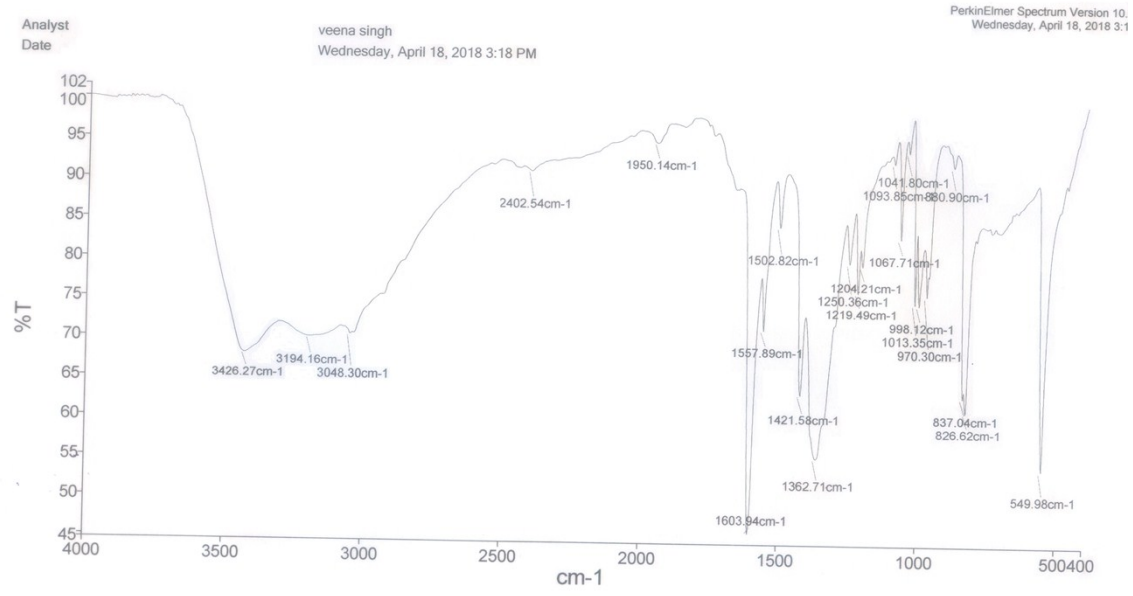
IR Spectrum of complex 2 after CR adsorption



IR Spectrum of Complex 3

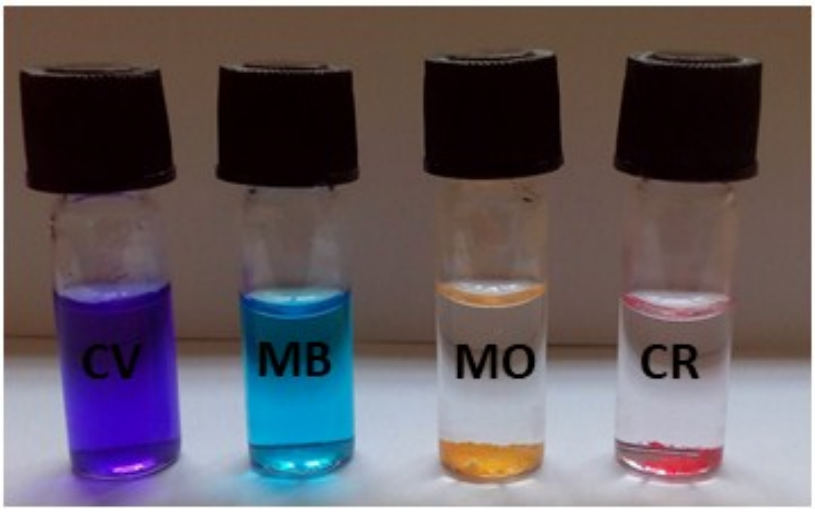


IR Spectrum of complex 3 after MO adsorption



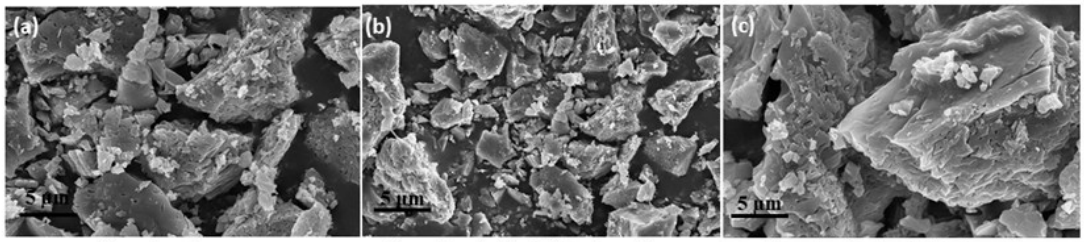
IR Spectrum of complex 3 after CR adsorption

SI 9. Selective adsorption of cationic and anionic dyes of complex **2.**



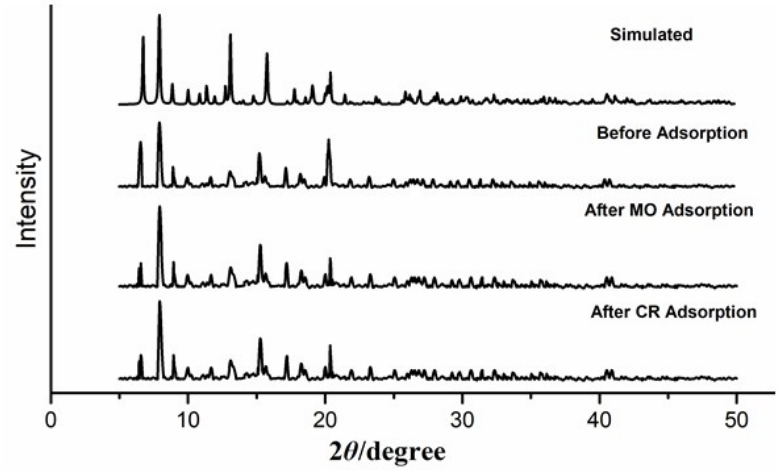
SI 10. (a) FE-SEM micrograph of complex **4** before and after adsorption of MO as well as CR dyes (b) PXRD pattern of simulated and complex **4**, before and after dye adsorption.

(a)

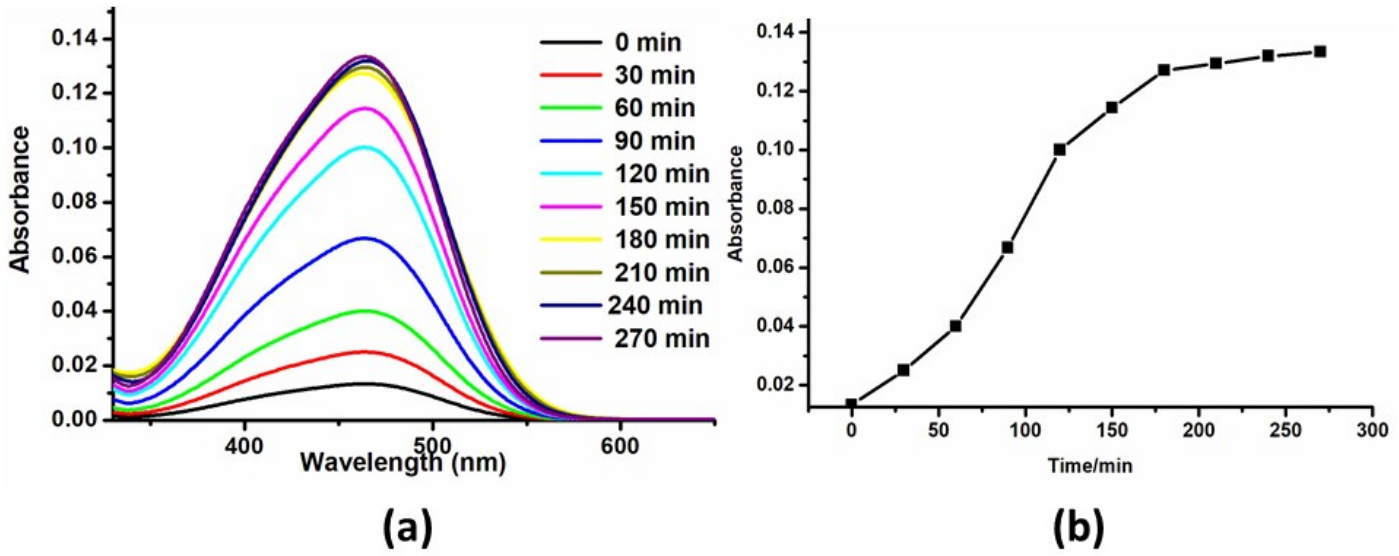


Complex 4 | Complex 4 after MO adsorption | Complex 4 after CR adsorption

(b)

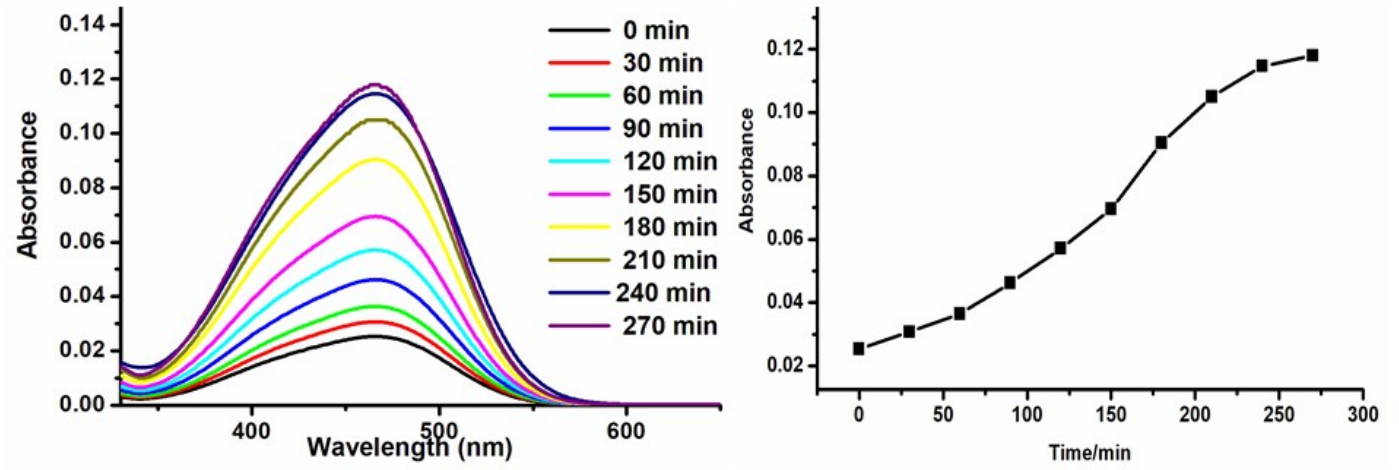


SI 11 (a) The MO release of **2** in aqueous of solution of NaCl. b) The relation between adsorption time and the concentration of the aqueous dye solution.



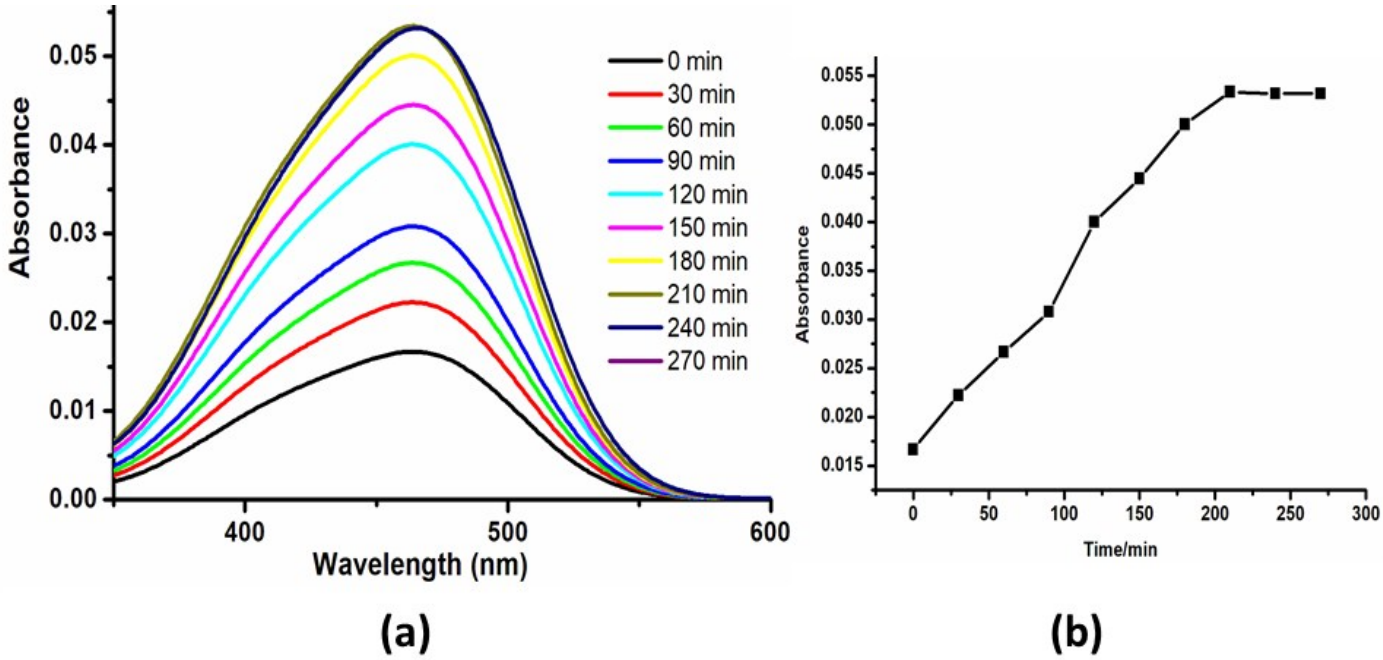
(a) (b)

SI 12 (a) The MO release of **3** in aqueous of solution of NaCl. b) The relation between adsorption time and the concentration of the aqueous dye solution.



(a) (b)

SI 13 (a) The MO release of **4** in aqueous of solution of NaCl. b) The relation between adsorption time and the concentration of the aqueous dye solution.



(a) (b)