Electronic Supplementary Material (ESI) for RSC Advances.

Electronic Supplementary Information

Engineered Fe_3 triangle for rapid and selective removal of aromatic cationic pollutants: Complexity is not a necessity

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Table 1 ESI Selected bond angles and bond distance parameter

Bond Distances (Å)	
Fe1–O1	2.0508(15)
Fe1–O1	2.0508(15)
Fe1–O4	1.9796(15)
Fe1–O4	1.9796(15)
Fe1–O004	1.895(2)
Fe1–O11	2.059(2)
Fe2–O2	1.9997(15)
Fe2–O004	1.8990(10)
Fe2–O5	2.0345(15)
Fe2–O7	1.9849(15)
Fe2–O8	2.0352(15)
Fe2–O10	2.0784(16)
Bond Angle (degree)	
O1–Fe1–O1	167.35(9)
O4–Fe1–O1	90.24(6)
O4–Fe1–O1	90.24(6)
O4–Fe1–O1	88.69(6)
O4–Fe1–O1	88.69(6)
O4–Fe1–O4	170.32(9)
O004–Fe1–O1	96.33(4)
O004–Fe1–O1	96.33(4)
O004–Fe1–O4	94.84(5)
O004–Fe1–O4	94.84(5)
O11–Fe1–O1	83.67(4)
O11–Fe1–O1	83.67(4)
O11–Fe1–O4	85.16(5)
O11–Fe1–O4	85.16(5)
O11–Fe1–O004	180.0
O004–Fe2–O2	96.61(6)
O5–Fe2–O2	88.97(6)
O5–Fe2–O004	95.91(6)
O7–Fe2–O2	168.60(6)
O7–Fe2–O004	94.79(6)
O7–Fe2–O5	89.75(7)
O8–Fe2–O2	87.76(6)
O8–Fe2–O004	94.54(6)
O8–Fe2–O5	169.34(6)
O8–Fe2–O7	91.45(6)
O10–Fe2–O2	85.73(6)

O10–Fe2–O004	177.42(7)
O10–Fe2–O5	85.21(6)
O10–Fe2–O7	82.88(6)
O10–Fe2–O8	84.44(6)
C1–O1–Fe1	129.11(14)
C1–O2–Fe2	135.27(14)
C9–O4–Fe1	136.65(15)
Fe2–O004–Fe1	119.86(5)
Fe2–O004–Fe1	119.86(5)
Fe2–O004–Fe2	120.29(11)
C9–O5–Fe2	128.45(14)

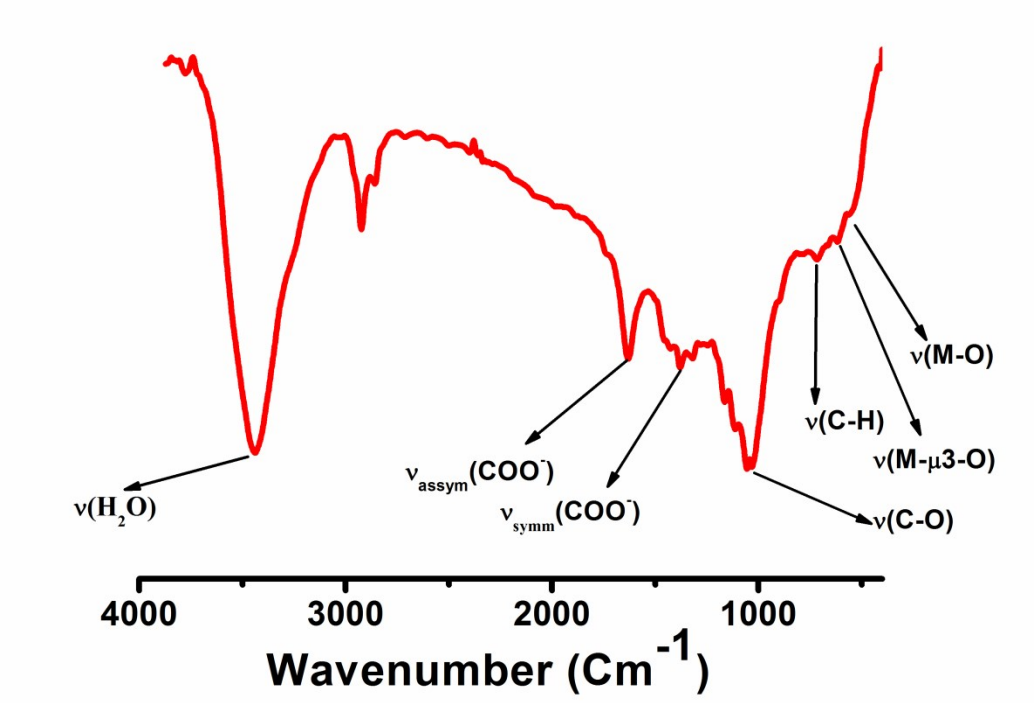

Fig. S1 ESI FTIR spectra of {Fe_3} cluster.

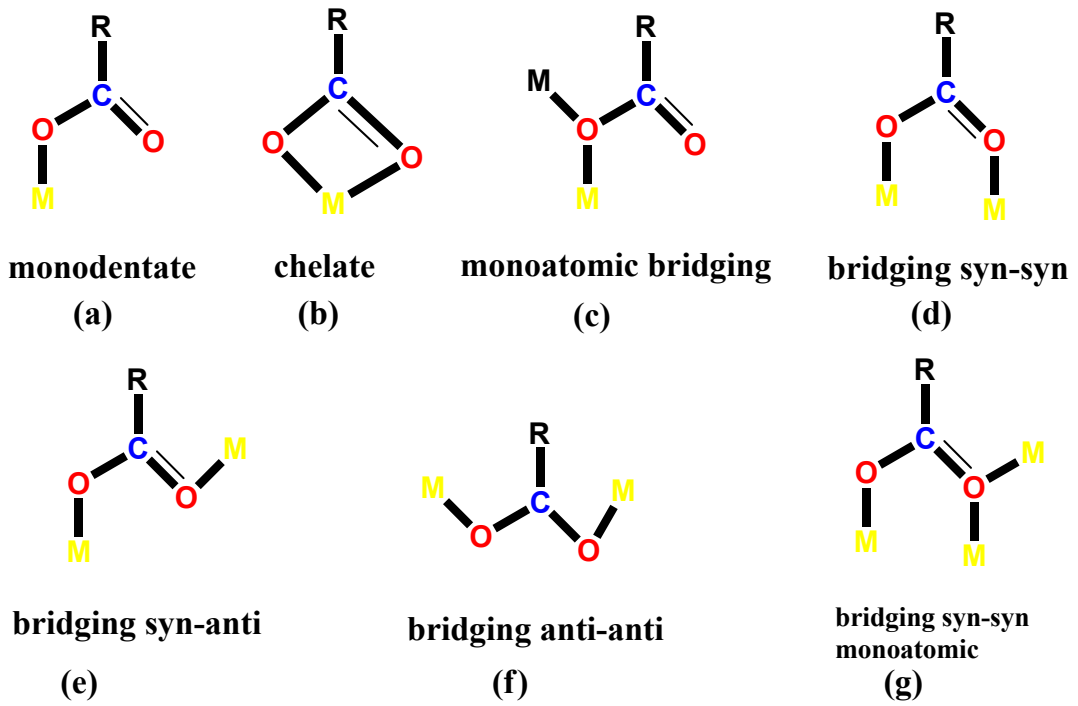

Fig. 2 ESI Different coordination modes of carboxylate group present in the benzoate ligand.

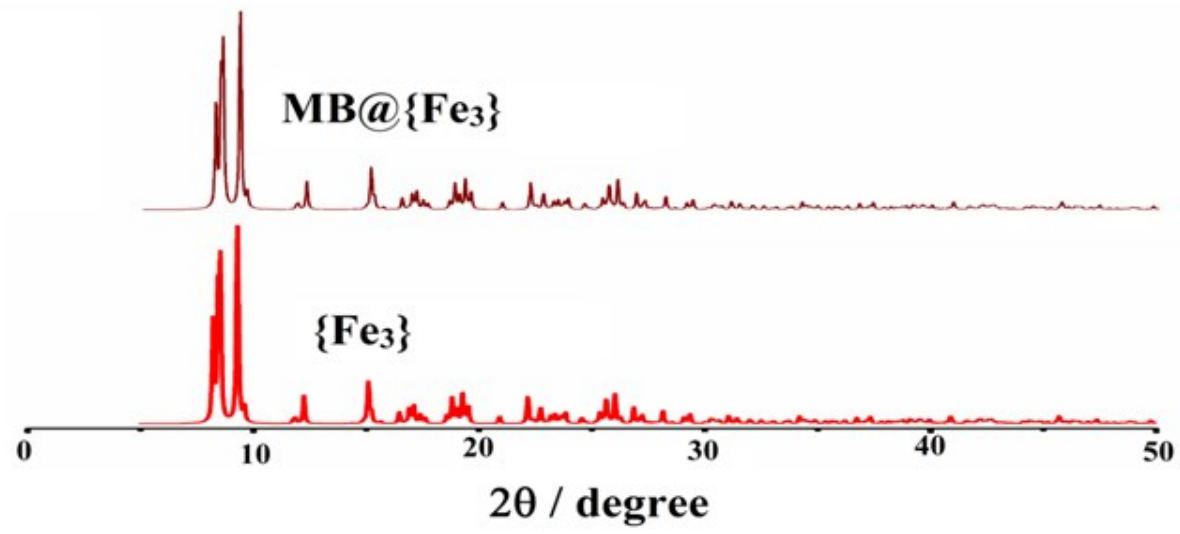

Fig. 3 ESI PXRD pattern of adsorbent $\{Fe_3\}$ cluster before and adsorption of MB dye.

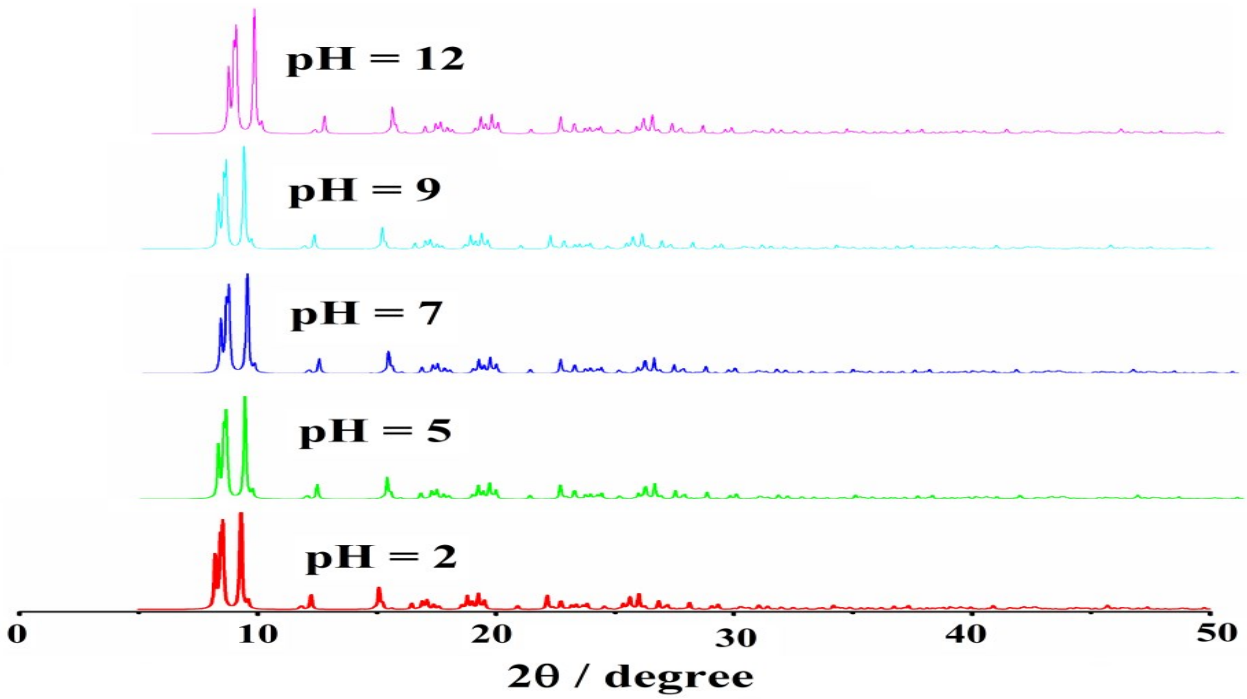

Fig. S4 ESI PXRD pattern of adsorbent {Fe_3} at different pH.