SUPPORTING INFORMATION

Structural Analysis and Water Adsorption Properties of Chloranilate Anion–Terpyridine Metal Complexes forming Hydrogen-Bonded Frameworks

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Table S1 Selected bond distance (Å) and angle (°) for **Fe-A** and **Co-A**.

Fe-A

Atom1	Atom2	Distance (Å)
Fe01	N1	1.9869(18)
Fe01	N2	1.8871(17)
Fe01	N3	1.9839(19)
Fe01	N4	1.9819(18)
Fe01	N5	1.8859(16)
Fe01	N6	1.9808(18)

Atom1	Atom2	Atom3	Angle (°)
N2	Fe01	N4	101.79(7)
N2	Fe01	N3	80.88(7)
N2	Fe01	N1	80.81(7)
N2	Fe01	N6	96.56(8)
N3	Fe01	N1	161.62(7)
N4	Fe01	N3	90.90(7)
N4	Fe01	N1	91.16(7)
N5	Fe01	N2	177.50(8)
N5	Fe01	N4	80.69(7)
N5	Fe01	N3	98.84(7)
N5	Fe01	N1	99.53(7)
N5	Fe01	N6	80.96(7)
N6	Fe01	N4	161.64(7)
N6	Fe01	N3	91.52(8)
N6	Fe01	N1	92.26(8)

Co-A

Atom1	Atom2	Distance (Å)
Co1	N1	2.0932(19)
Co1	N2	1.9137(17)
Co1	N3	2.097(2)
Co1	N4	2.0692(19)
Co1	N5	1.8979(17)
Co1	N6	2.0663(19)

Atom1	Atom2	Atom3	Angle (°)
N1	Co1	N3	159.21(7)
N2	Co1	N4	103.02(7)
N2	Co1	N1	79.66(7)
N2	Co1	N6	96.86(7)
N2	Co1	N3	79.66(7)
N4	Co1	N1	91.78(7)
N4	Co1	N3	90.76(7)
N5	Co1	N2	176.88(7)
N5	Co1	N4	79.87(7)
N5	Co1	N1	101.53(7)
N5	Co1	N6	80.25(7)
N5	Co1	N3	99.23(7)
N6	Co1	N4	160.11(7)
N6	Co1	N1	92.23(7)
N6	Co1	N3	92.36(8)

Table S2 Selected bond distance (Å) and angle (°) for **Fe-B** and **Co-B**.

Fe-B

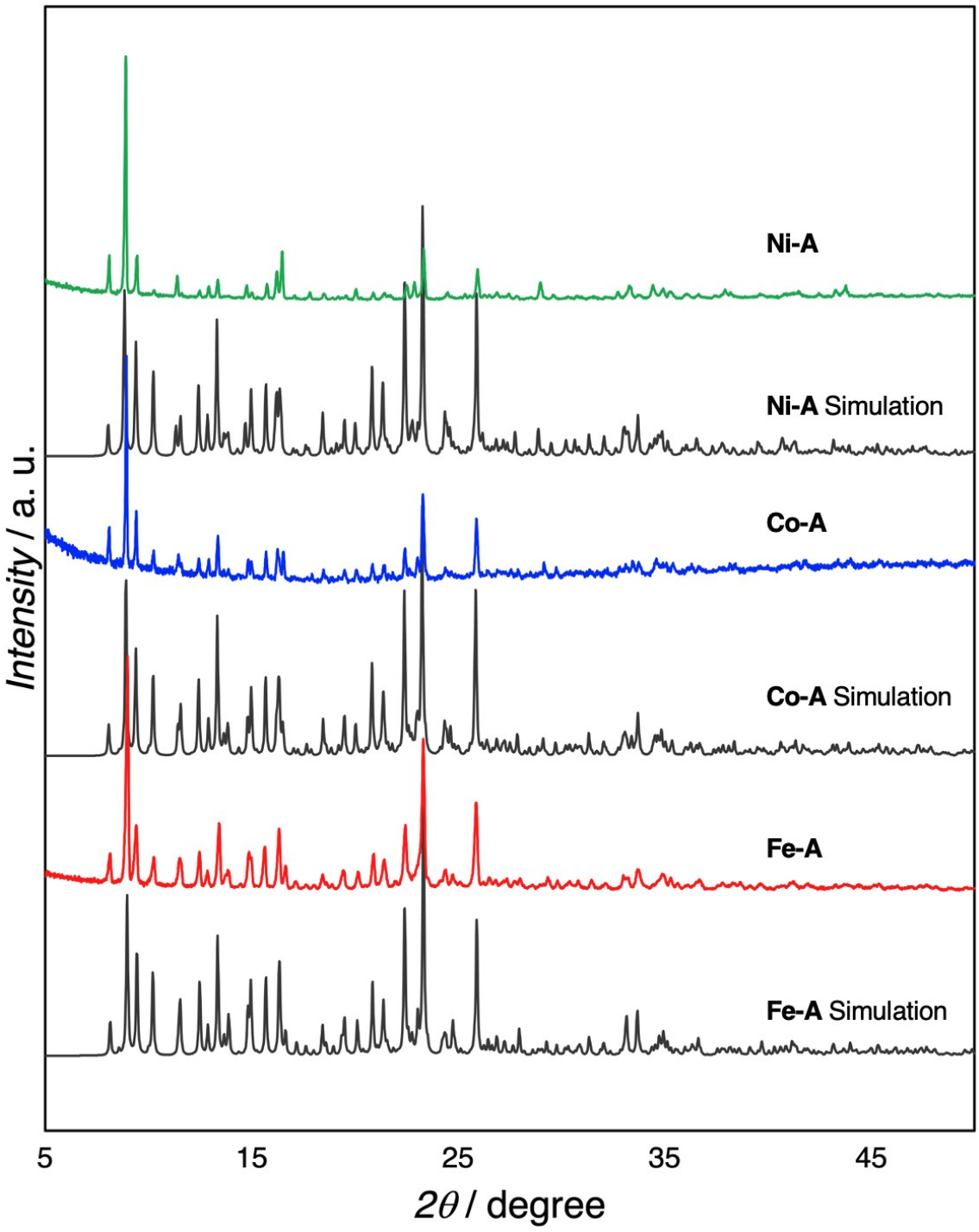
Atom1	Atom2	Distance (Å)
Fe01	N1	1.9796(16)
Fe01	N2	1.8882(14)
Fe01	N3	1.9804(15)
Fe01	N4	1.9798(16)
Fe01	N5	1.8882(14)
Fe01	N6	1.9854(16)

Atom1	Atom2	Atom3	Angle (°)
N1	Fe01	N3	161.93(6)
N1	Fe01	N6	91.94(6)
N1	Fe01	N4	91.05(6)
N2	Fe01	N3	80.90(6)
N2	Fe01	N6	98.08(6)
N2	Fe01	N1	81.07(6)
N2	Fe01	N4	99.95(6)
N3	Fe01	N6	91.65(6)
N4	Fe01	N3	90.99(6)
N4	Fe01	N6	161.97(6)
N5	Fe01	N3	99.87(6)
N5	Fe01	N2	178.85(7)
N5	Fe01	N6	81.06(7)
N5	Fe01	N1	98.19(6)
N5	Fe01	N4	80.91(7)

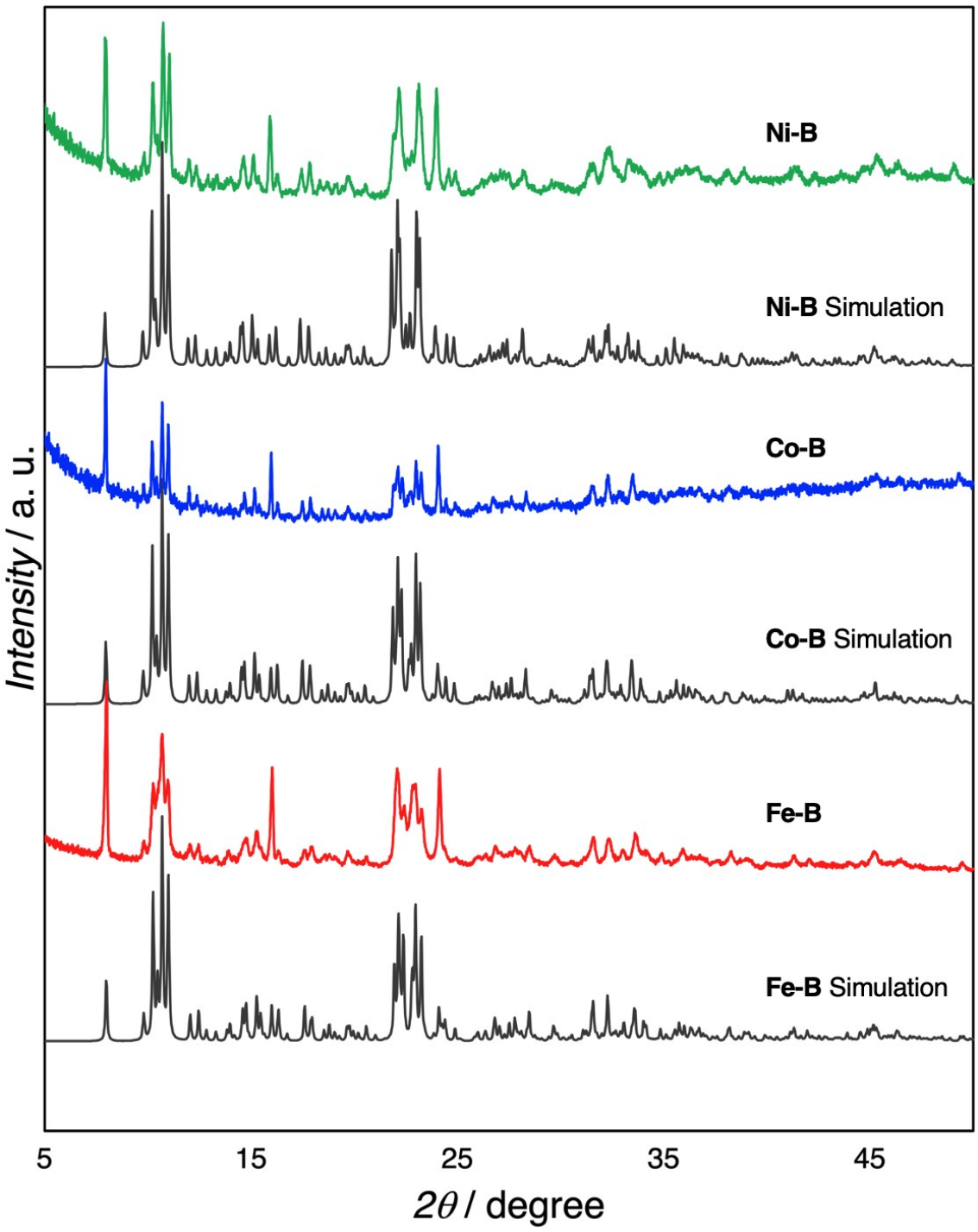
Co-B

Atom1	Atom2	Distance (Å)
Co1	N6	2.0702(14)
Co1	N3	2.0757(14)
Co1	N1	2.0784(14)
Co1	N4	2.0706(14)
Co1	N2	1.9028(13)
Co1	N5	1.8985(13)

Atom1	Atom2	Atom3	Angle (°)
N2	Co1	N6	100.97(5)
N2	Co1	N3	79.94(6)
N2	Co1	N1	80.18(6)
N2	Co1	N4	98.66(5)
N3	Co1	N1	160.09(5)
N4	Co1	N3	91.79(5)
N4	Co1	N1	92.07(5)
N5	Co1	N6	80.16(6)
N5	Co1	N3	101.50(5)
N5	Co1	N1	98.40(5)
N5	Co1	N4	80.23(6)
N5	Co1	N2	178.18(6)
N6	Co1	N3	91.48(5)
N6	Co1	N1	91.41(5)
N6	Co1	N4	160.38(5)



FigS1. PXRD patterns of **Fe-A**, **Co-A** and **Ni-A**.



FigS2. PXRD patterns of **Fe-B**, **Co-B** and **Ni-B**.

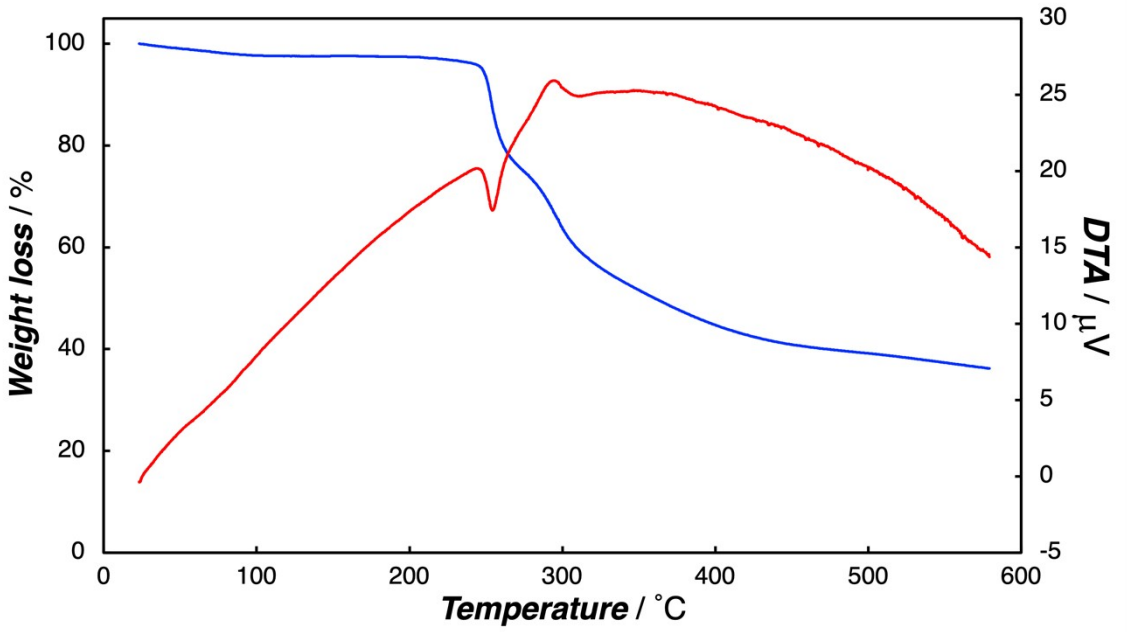


Fig.S3 TGA (bule) and DTA (red) curves of **Fe-A**.

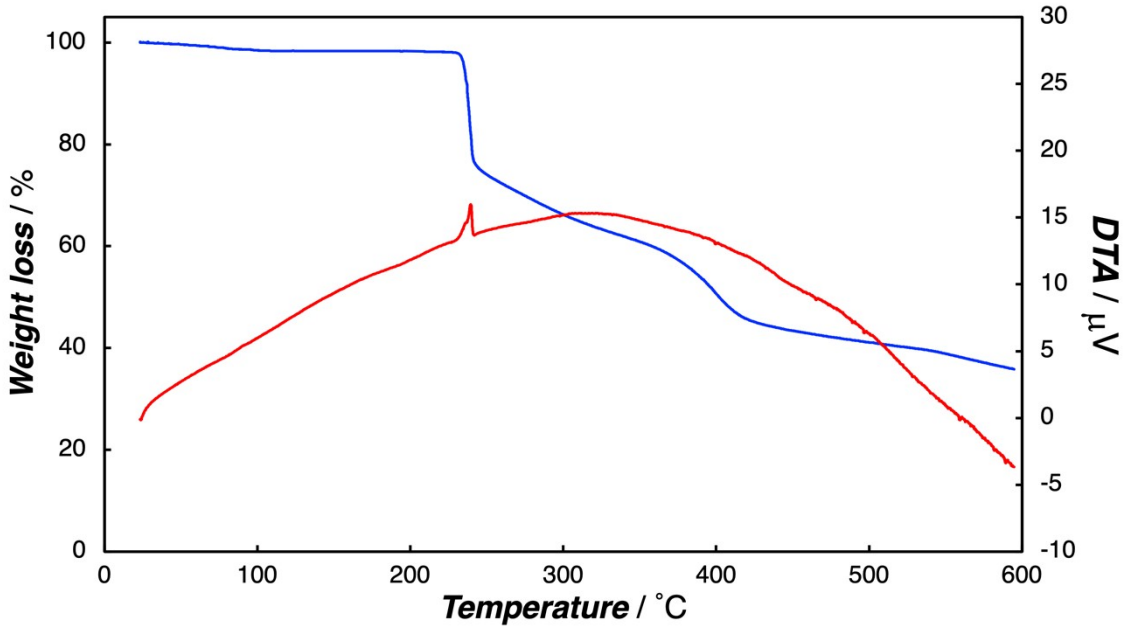


Fig.S4 TGA (bule) and DTA (red) curves of **Co-A**.

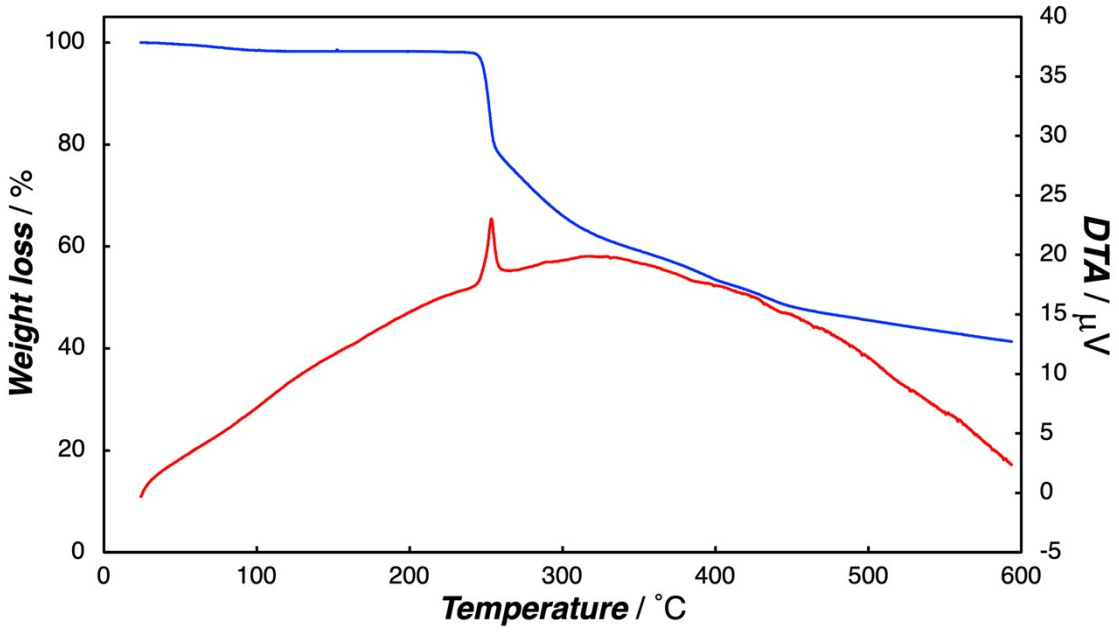


Fig.S5 TGA (bule) and DTA (red) curves of **Ni-A**.

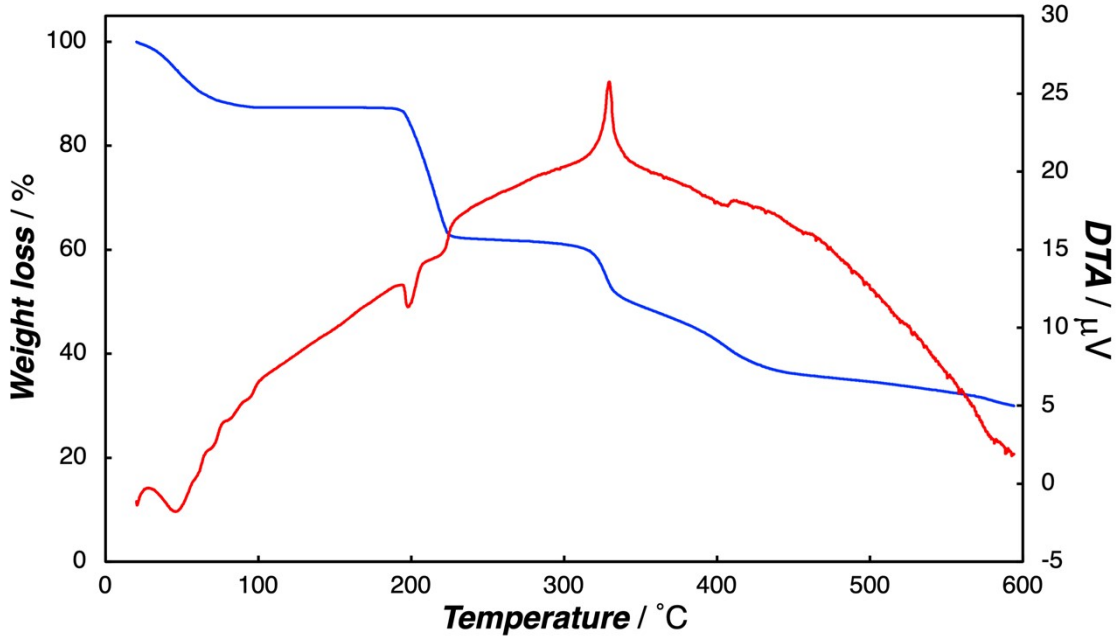


Fig.S6 TGA (bule) and DTA (red) curves of **Fe-B**.

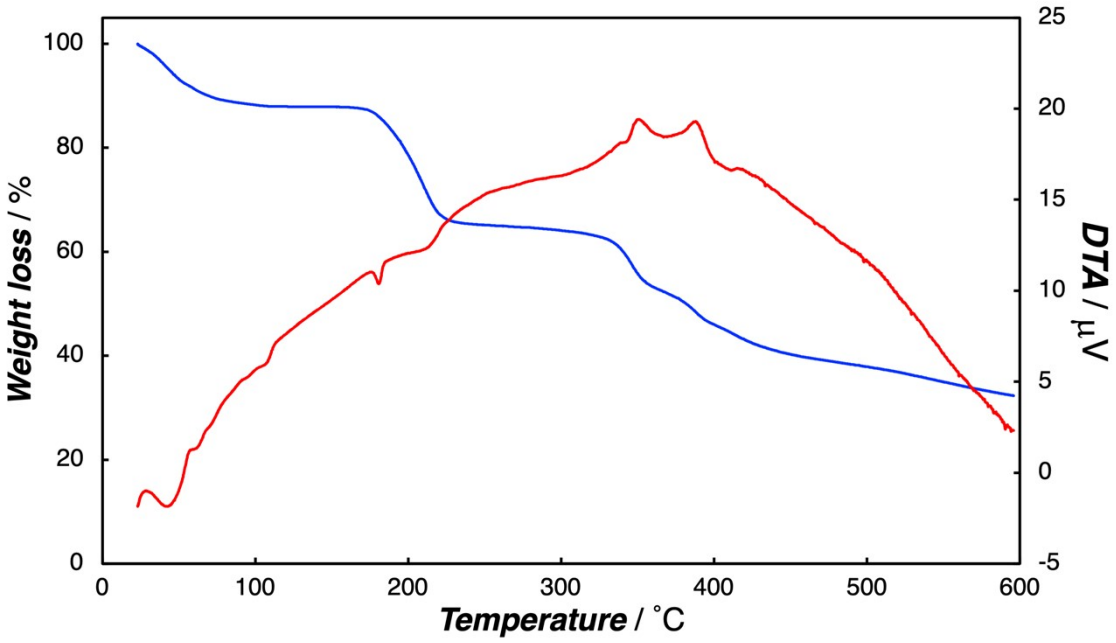


Fig.S7 TGA (bule) and DTA (red) curves of **Co-B**.

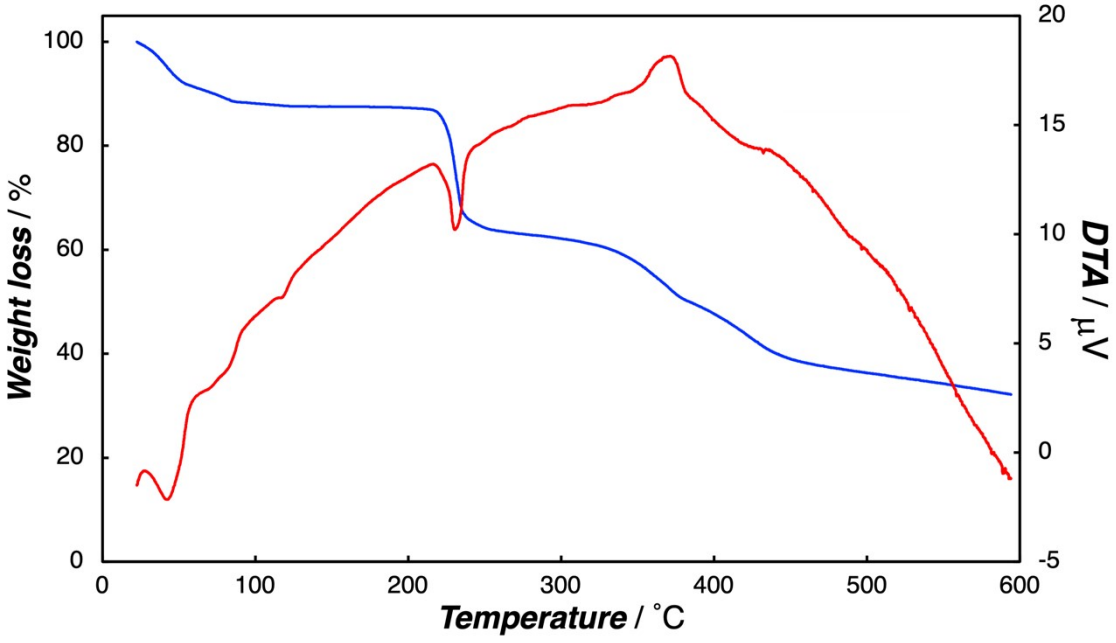


Fig.S8 TGA (bule) and DTA (red) curves of **Ni-B**.

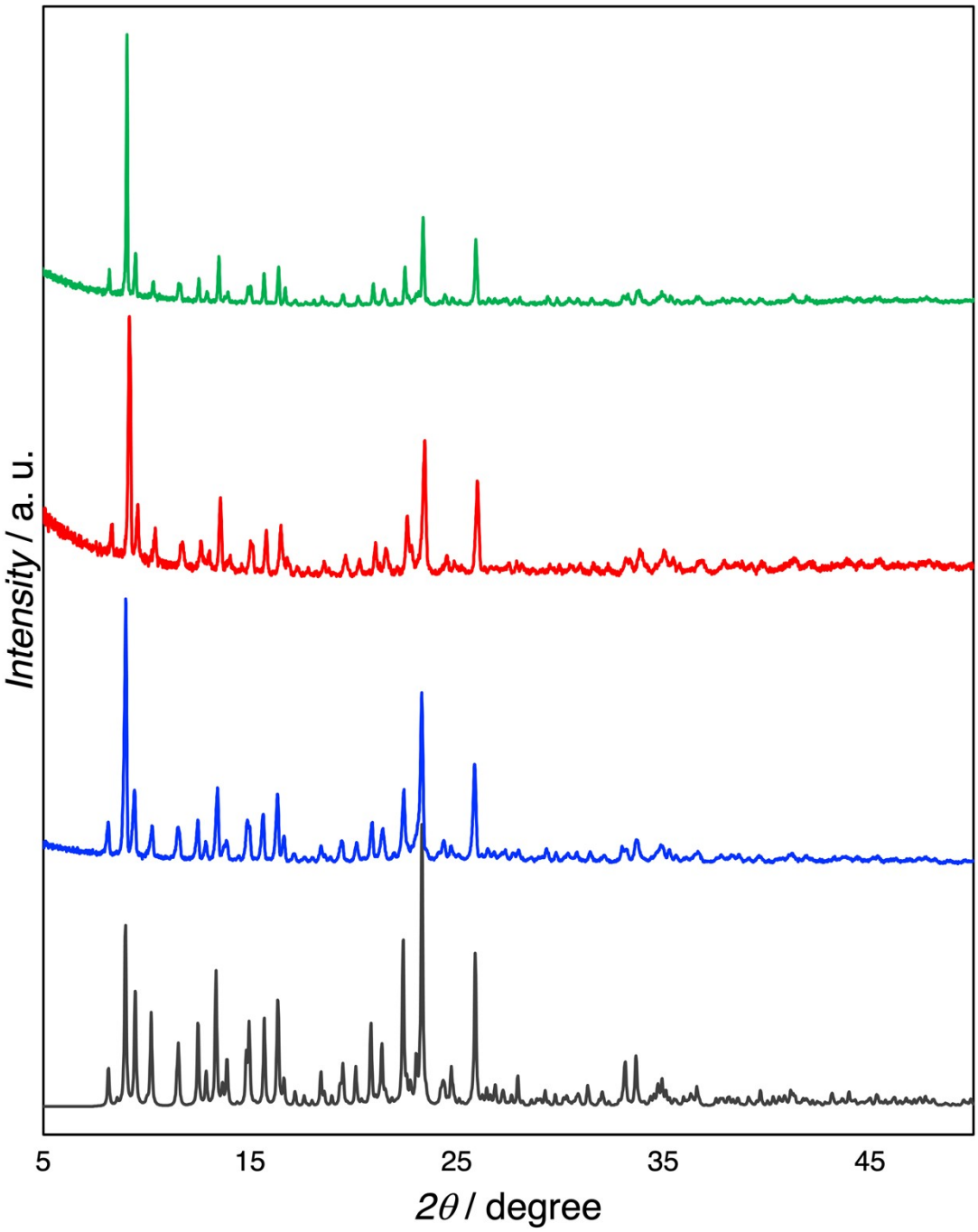


Fig.S9 PXRD patterns of **Fe-A**. Black) simulation from the single crystal, bule) as-synthesis, red) dehydration, green) rehydration.

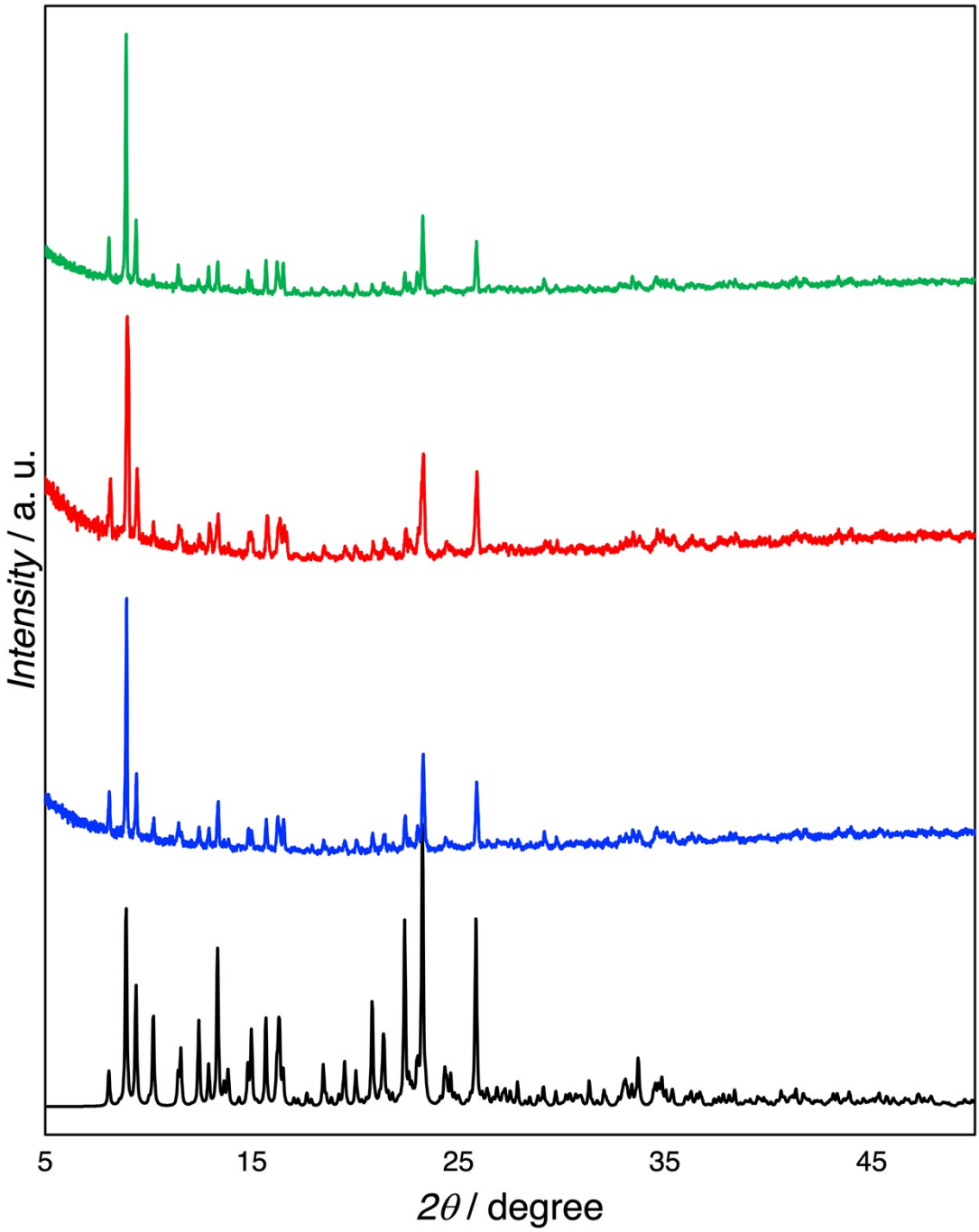


Fig.S10 PXRD patterns of **Co-A**. Black) simulation from the single crystal, bule) as-synthesis, red) dehydration, green) rehydration.

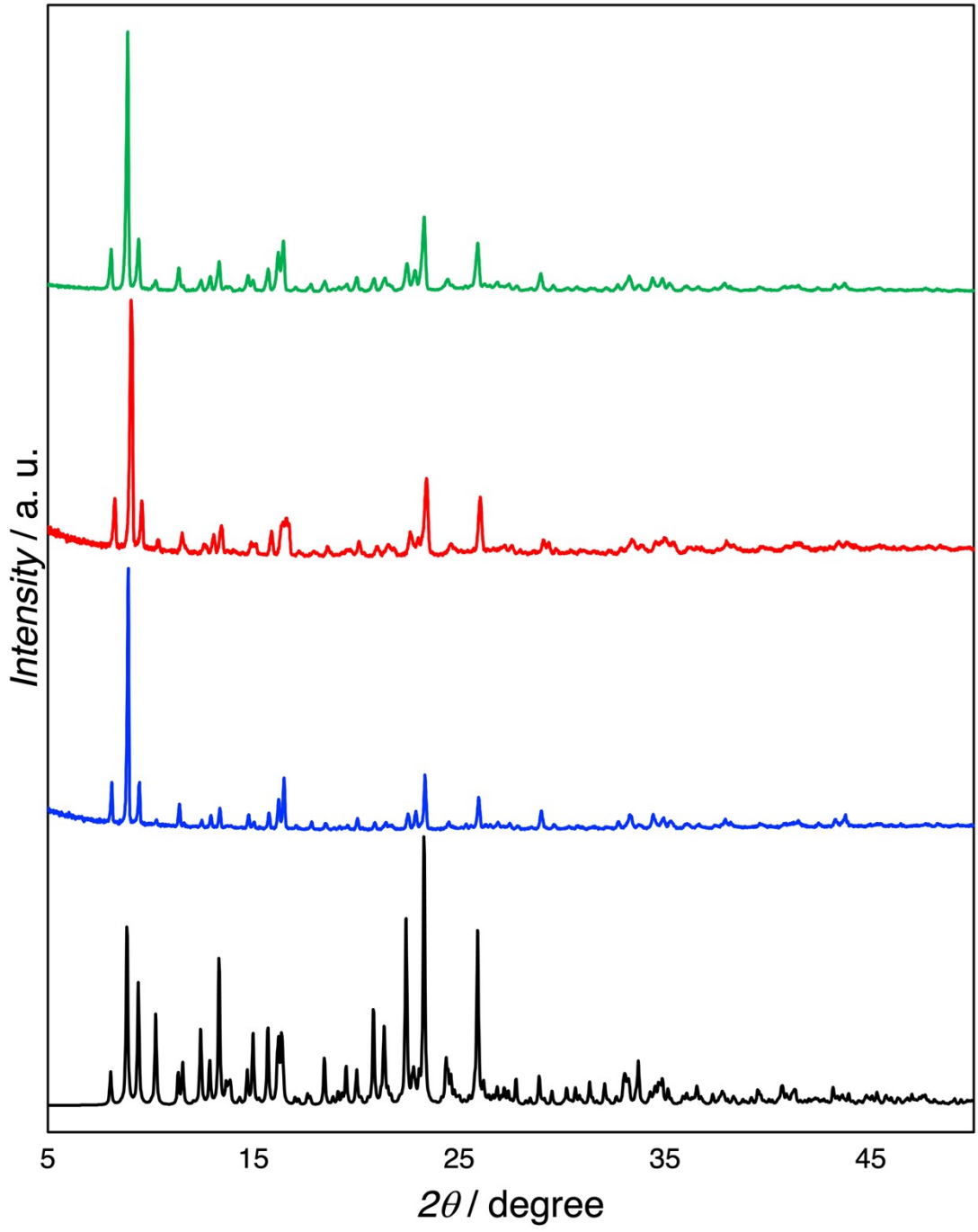


Fig.S11 PXRD patterns of **Ni-A**. Black) simulation from the single crystal, bule) as-synthesis, red) dehydration, green) rehydration.

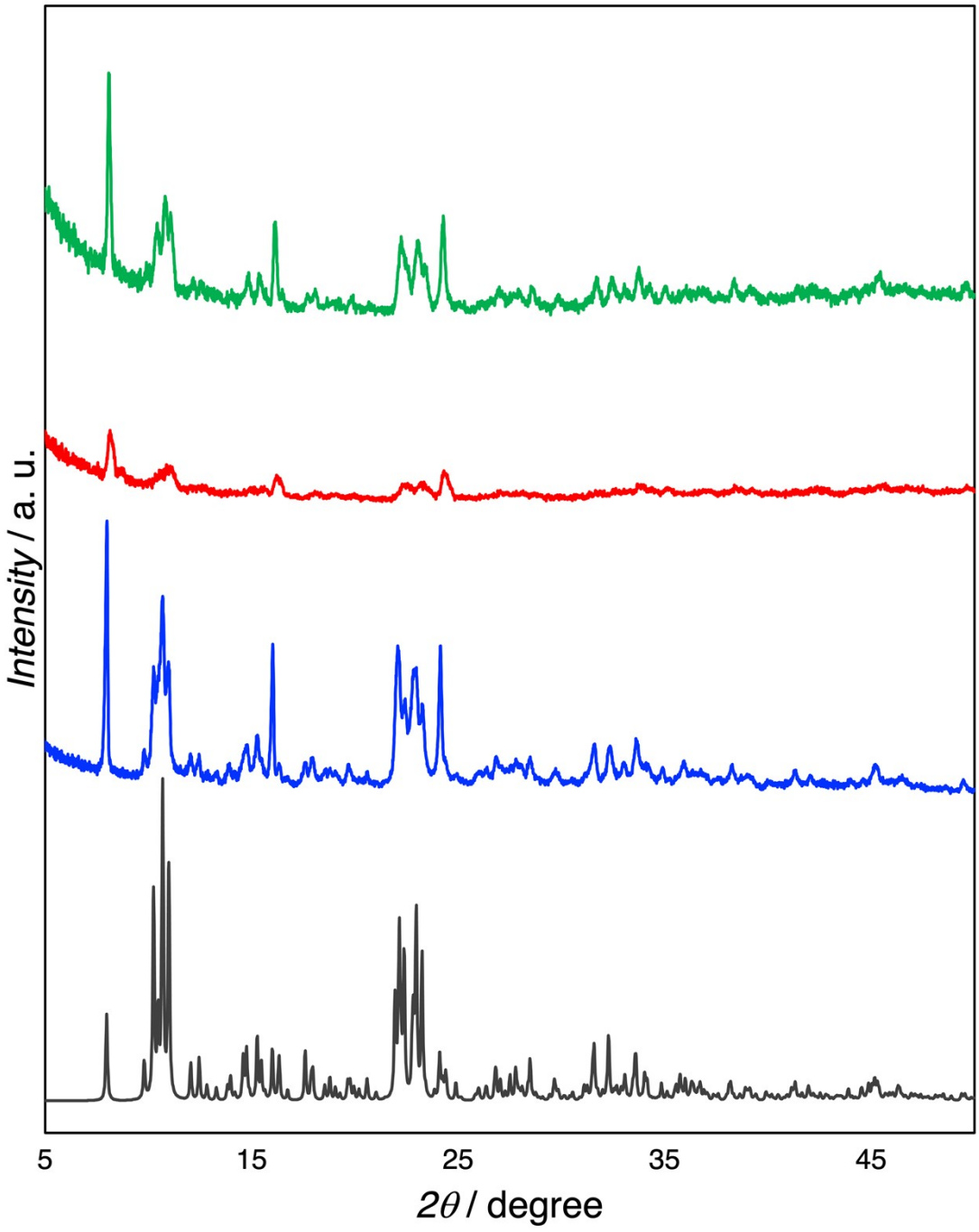


Fig.S12 PXRD patterns of **Fe-B**. Black) simulation from the single crystal, bule) as-synthesis, red) dehydration, green) rehydration.

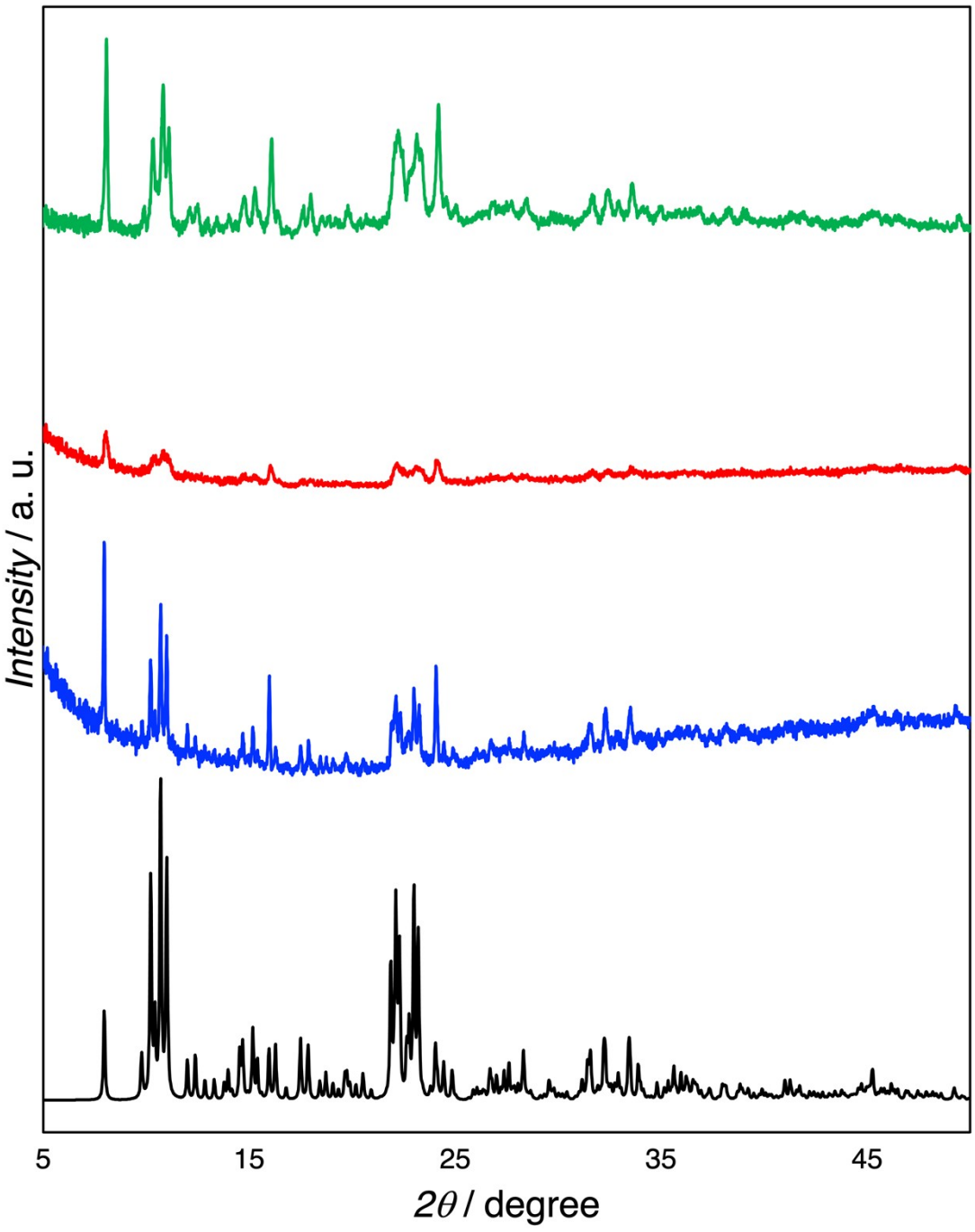


Fig.S13 PXRD patterns of **Co-B**. Black) simulation from the single crystal, bule) as-synthesis, red) dehydration, green) rehydration.

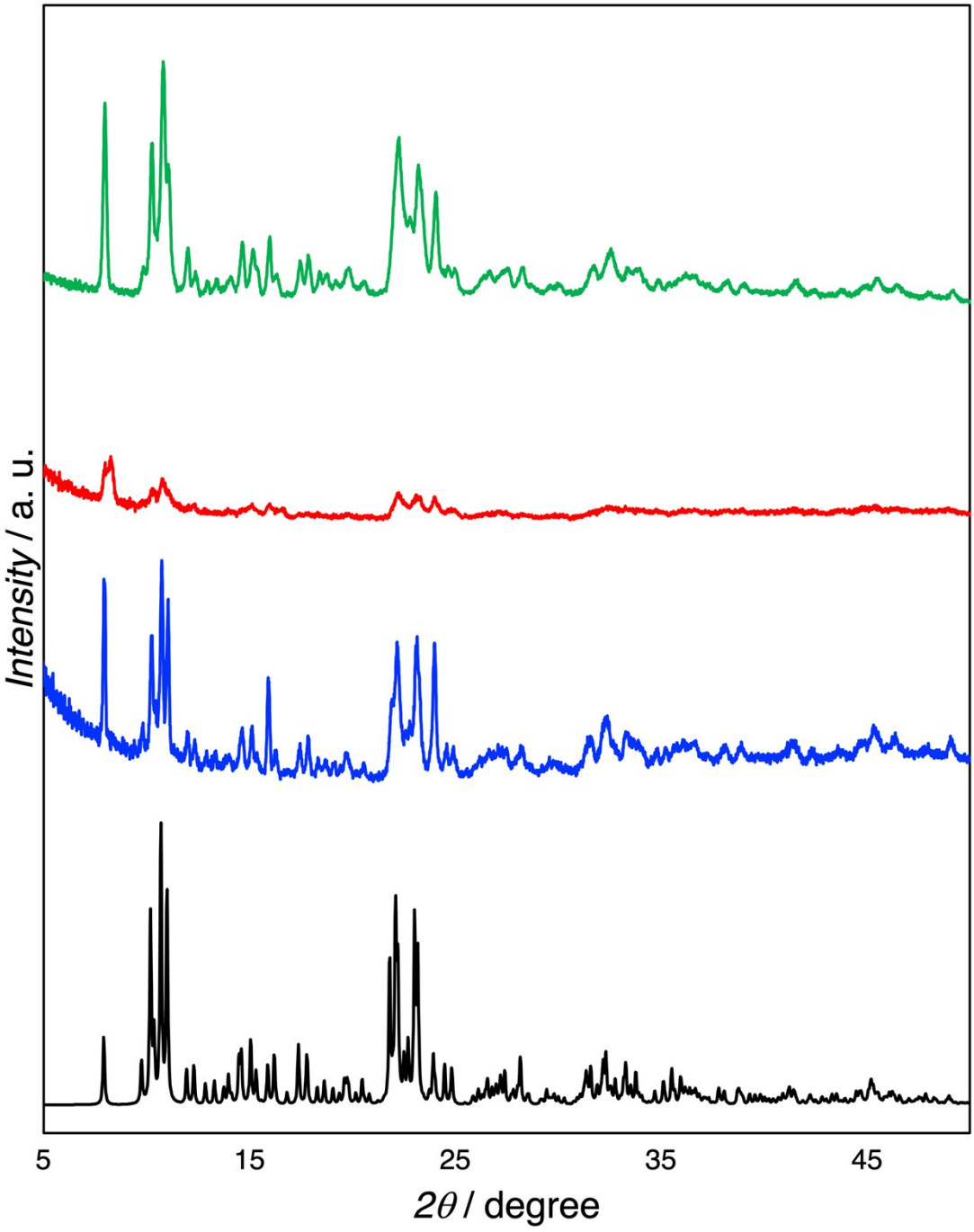


Fig.S14 PXRD patterns of **Ni-B**. Black) simulation from the single crystal, bule) as-synthesis, red) dehydration, green) rehydration.

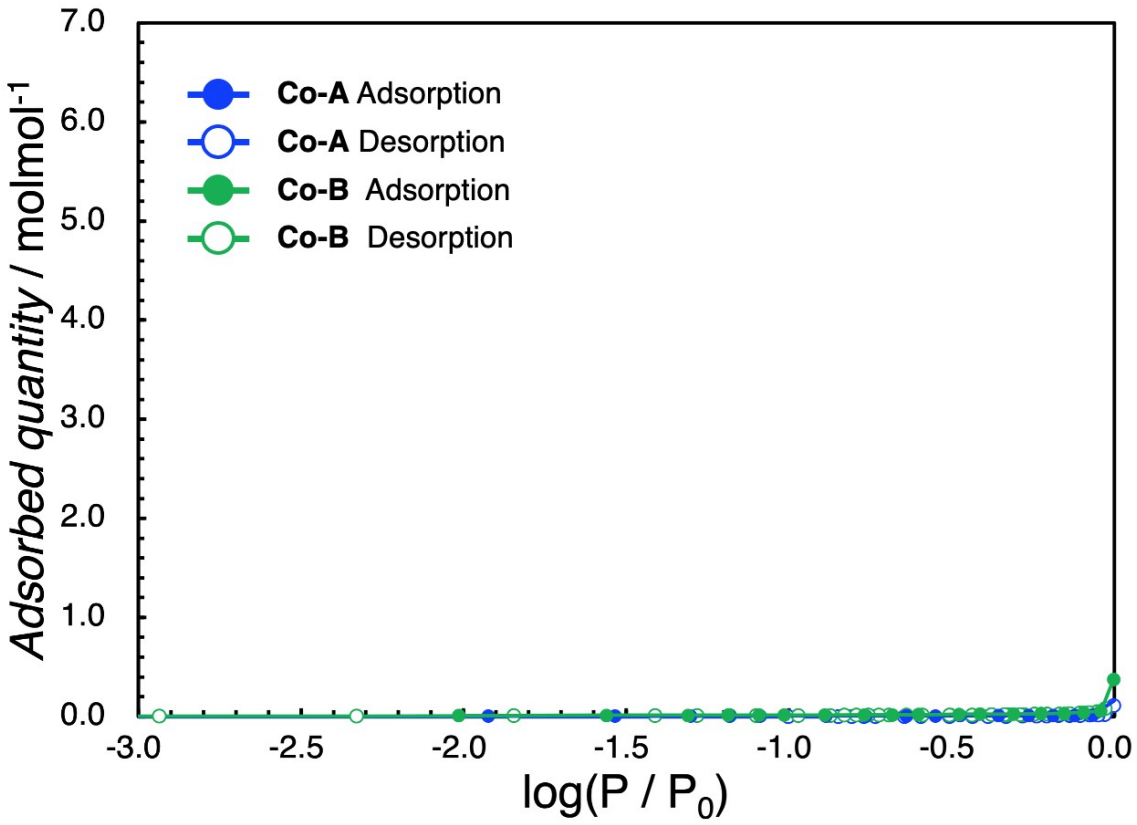


Fig. S15 N_2 adsorption isotherms at 77 K for **Co–A** (blue) and **Co–B** (green). Filled circles indicate adsorption and open circles indicate desorption.

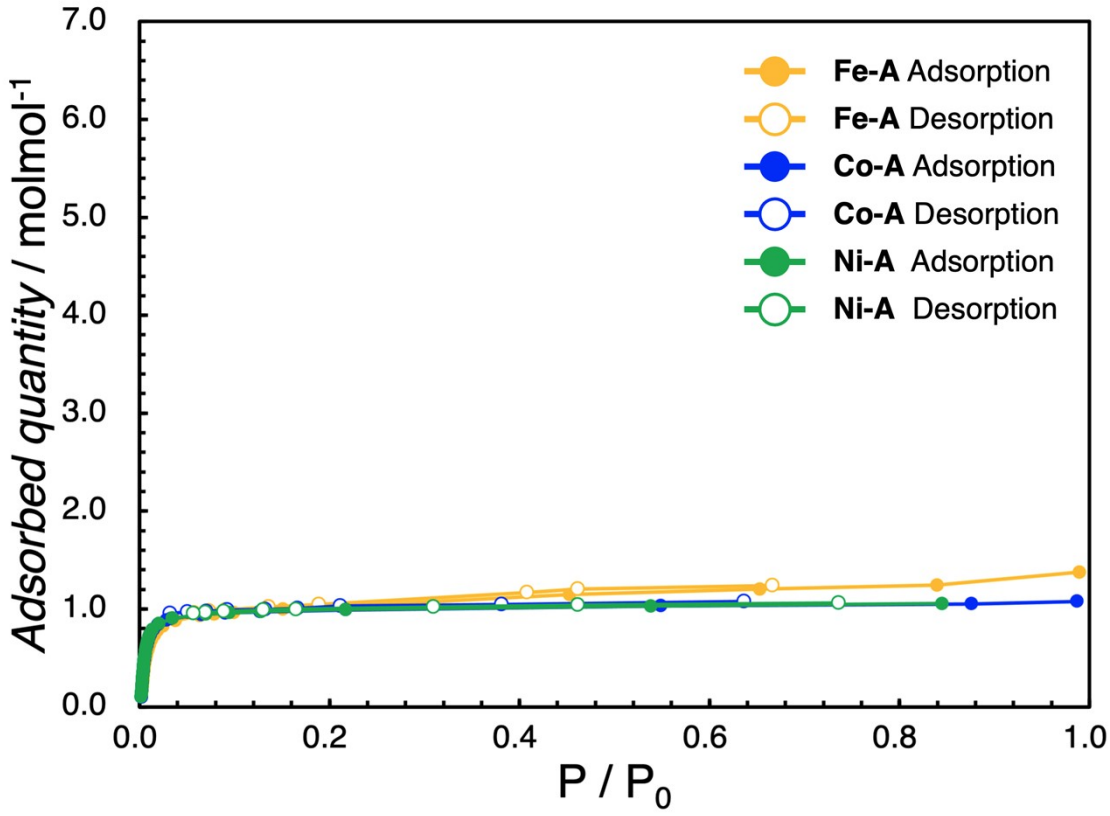


Fig. S16 Water adsorption isotherms at 298 K for **Fe–A** (yellow), **Co–A** (blue), and **Ni–A** (green). Filled circles indicate adsorption and open circles indicate desorption.

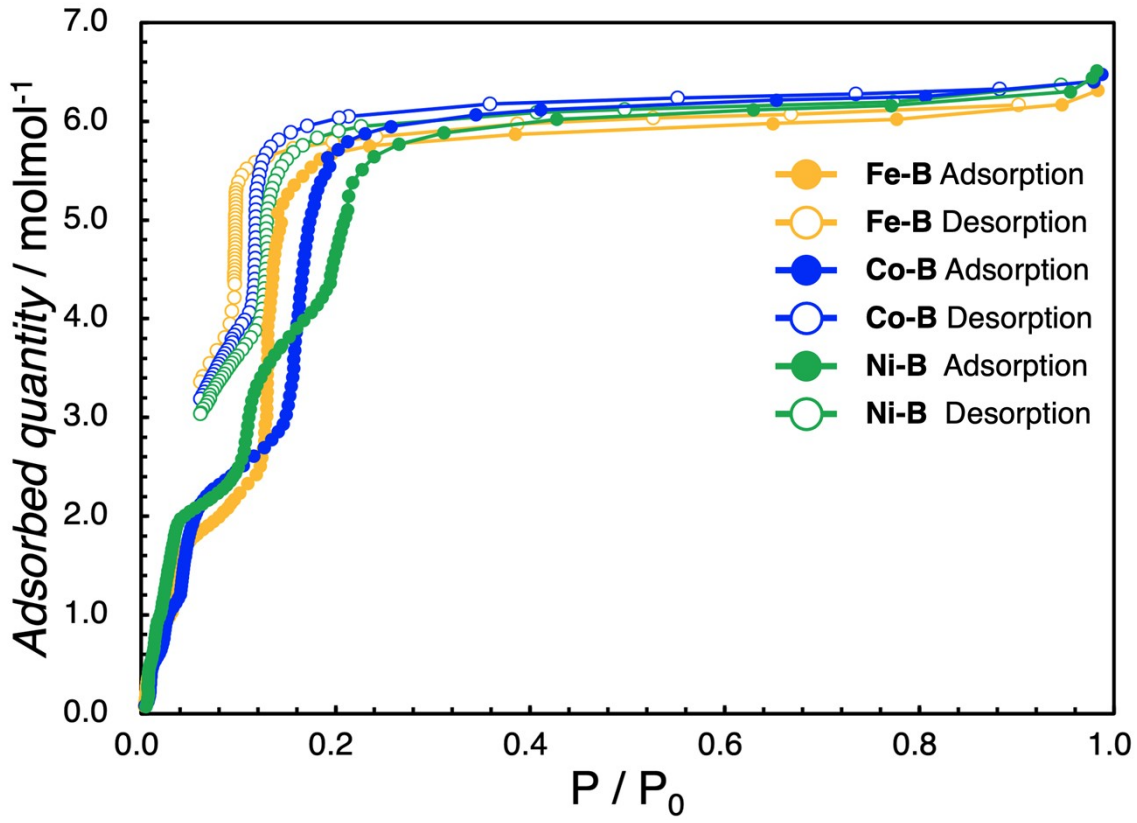


Fig. S17 Water adsorption isotherms at 298 K for **Fe–B** (yellow), **Co–B** (blue), and **Ni–B** (green). Filled circles indicate adsorption and open circles indicate desorption.

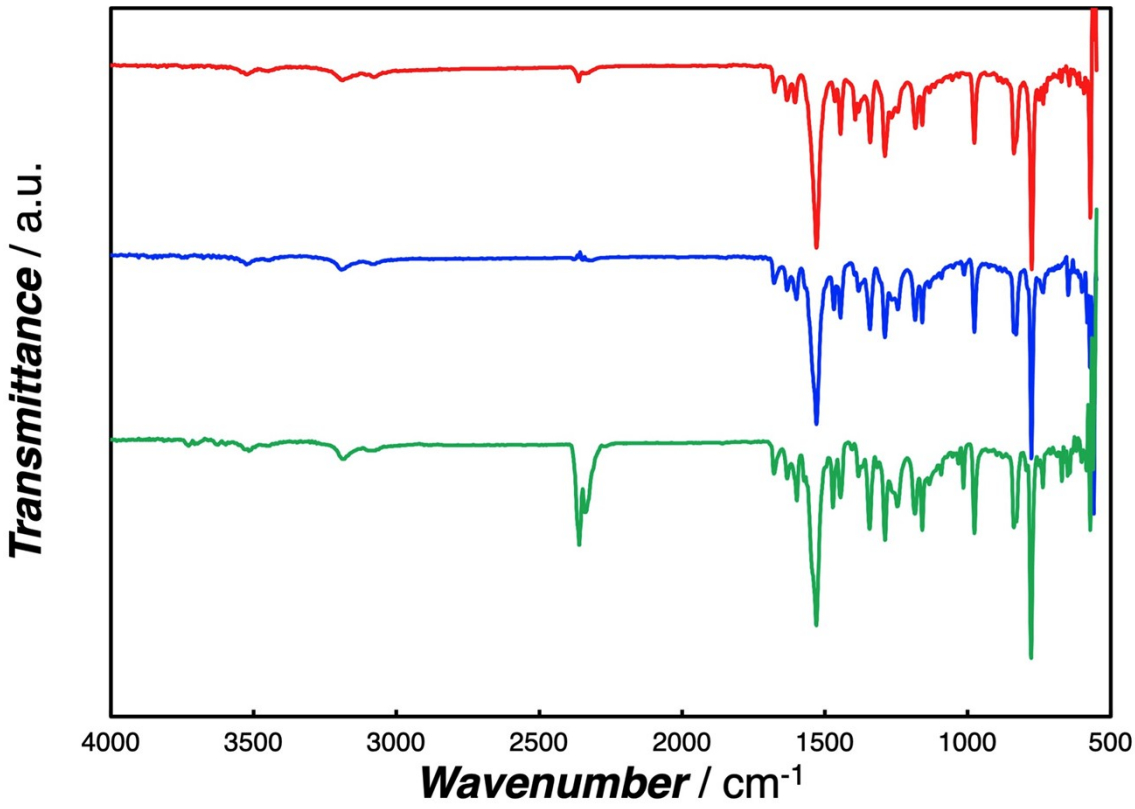


Fig. S18 FT-IR Spectra for **Fe–A** (red), **Co–A** (blue), and **Ni–A** (green).

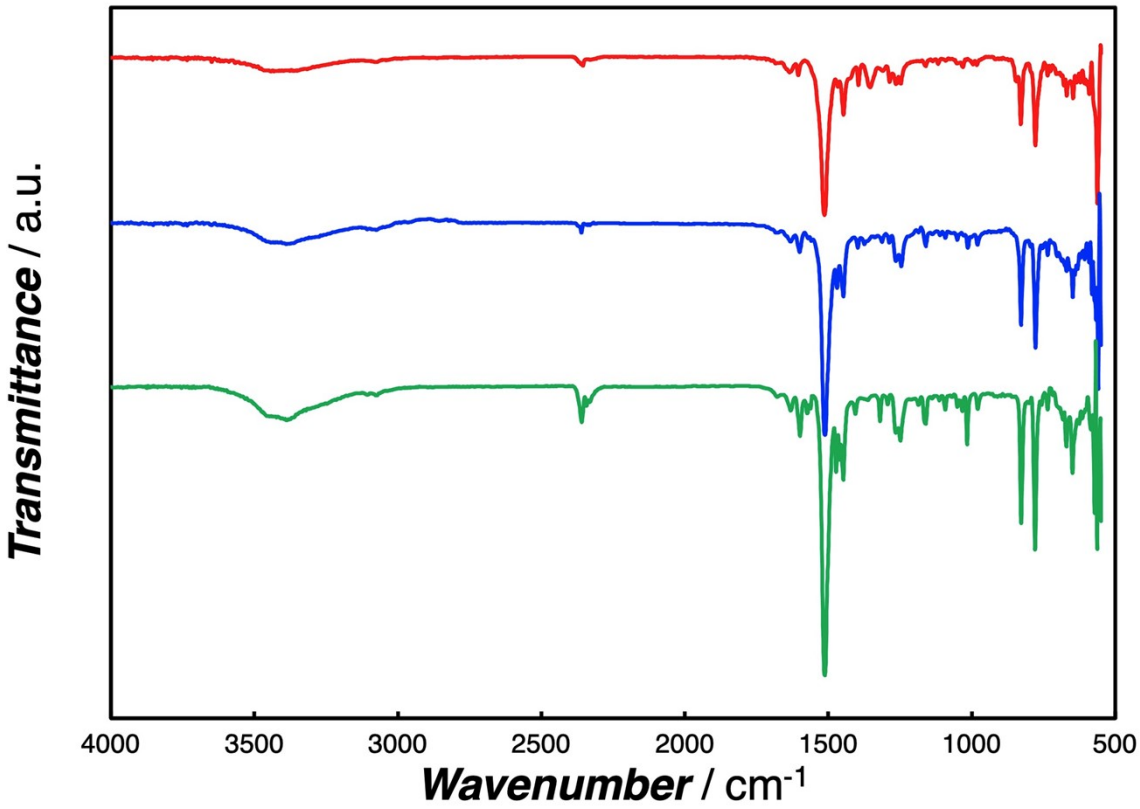


Fig. S19 FT-IR Spectra for **Fe–B** (red), **Co–B** (blue), and **Ni–B** (green).

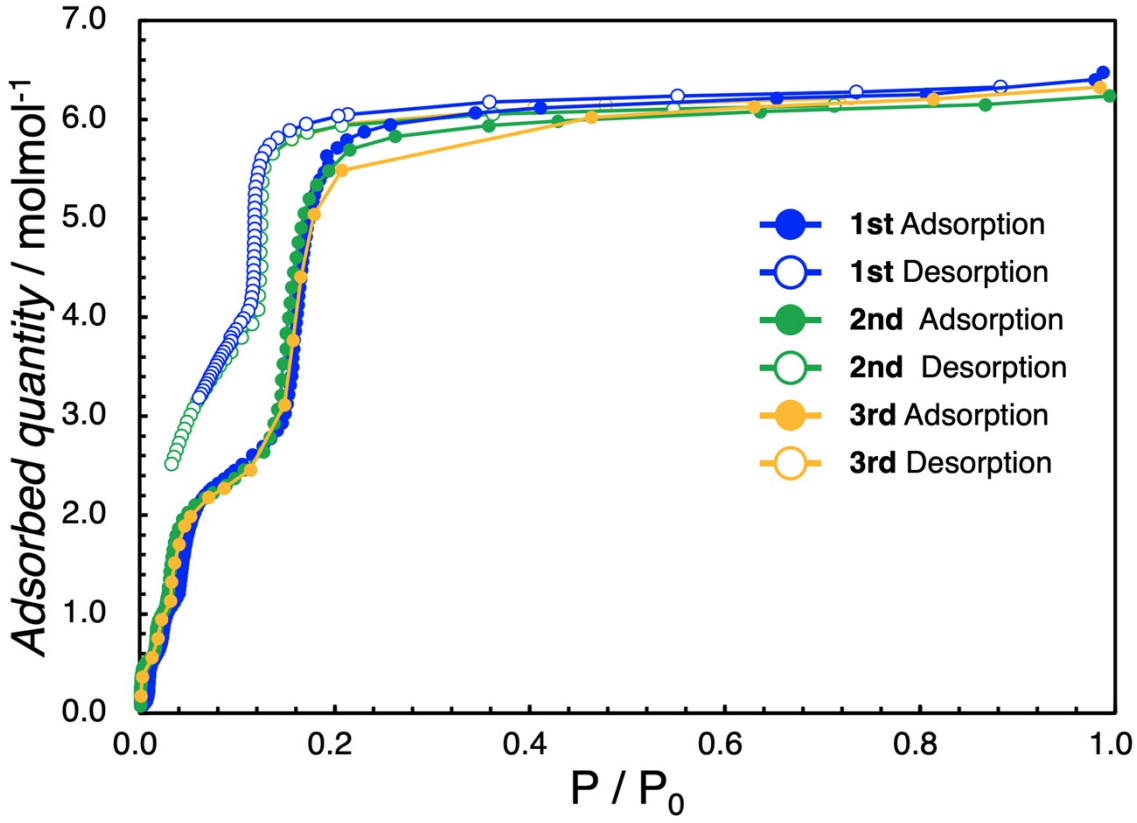


Fig. S20 Cyclic water adsorption isotherms at 298 K for **Co–B**. Filled circles indicate adsorption and open circles indicate desorption.

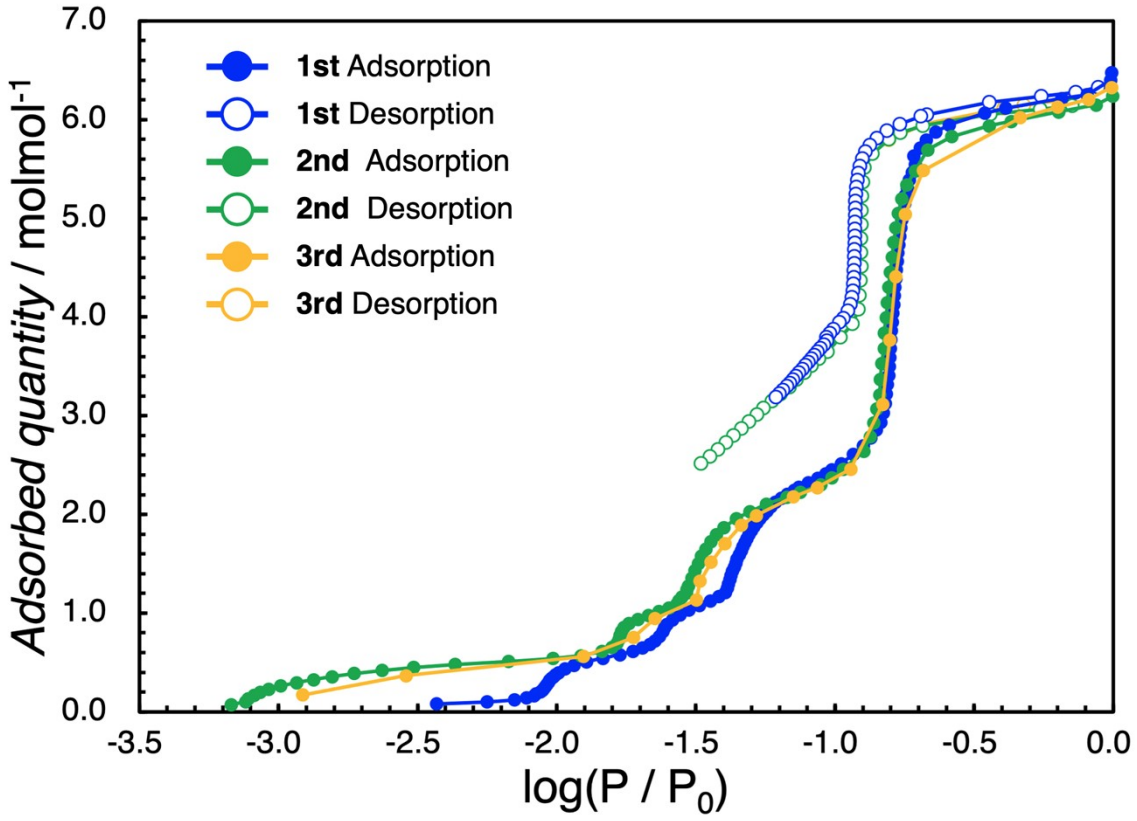


Fig. S21 Cyclic water adsorption isotherms represented in logarithmic form at 298 K for **Co–B**. Filled circles indicate adsorption and open circles indicate desorption.