SUPPLEMENTARY MATERIAL

Distortions of a Flexible Metal Organic Framework From Substituted Pendant Ligands

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Table S1: Synthesis conditions for Co(BDC)(ligand) materials

	Conditions			Molar equivalents of reagents			
Material	Temp /°C	Time/ days	Co^{2+} $Conc^{n}$ /M	Co^{2+}	BDC	PNO	Solvent (10 mL)
MIL-53(PNO-Br)	120	7	0.07	1	3	3	DMF
MIL-53(PNO-MeO)	120	2	0.07	1	2	2	DMF
MIL-53(PNO-iso)	100	6	0.03	1	3	3	DMF
MIL-53(PNO-phenyl)	120	7	0.07	1	3	3	DMF

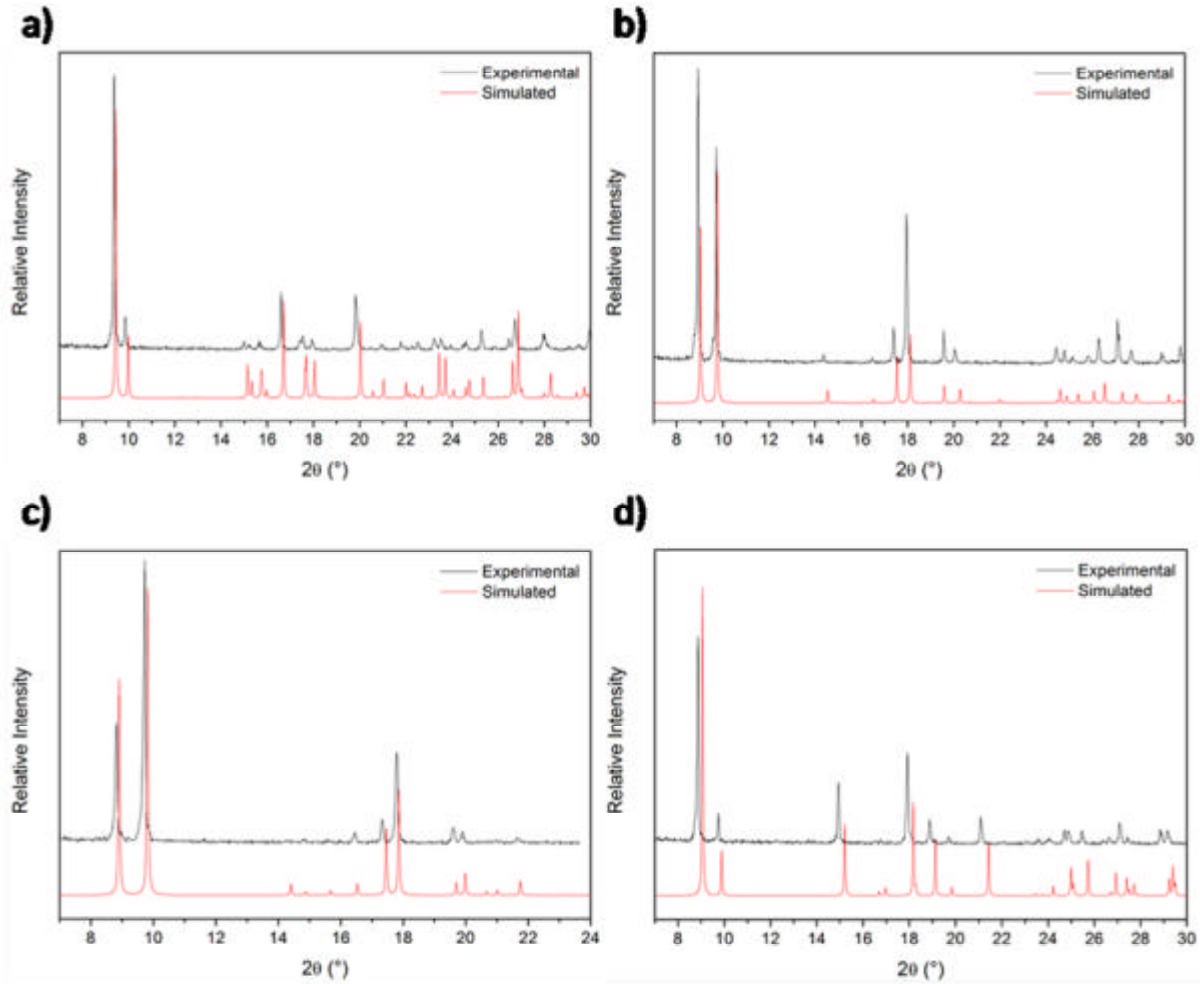

Figure S1: Powder XRD patterns of the four new materials compared with the simulated patterns from the single crystal structures. (a) Co(BDC)(3-Br-PNO), (b) Co(BDC)(4-MeO-PNO), (c) Co(BDC)(isoquinoline-N-oxide), (d) Co(BDC)(4-phenyl-PNO). Note that the powder patterns were recorded at room temperature, while the single crystal structures for (b), (c) and (d) were determined at 100(2) K.

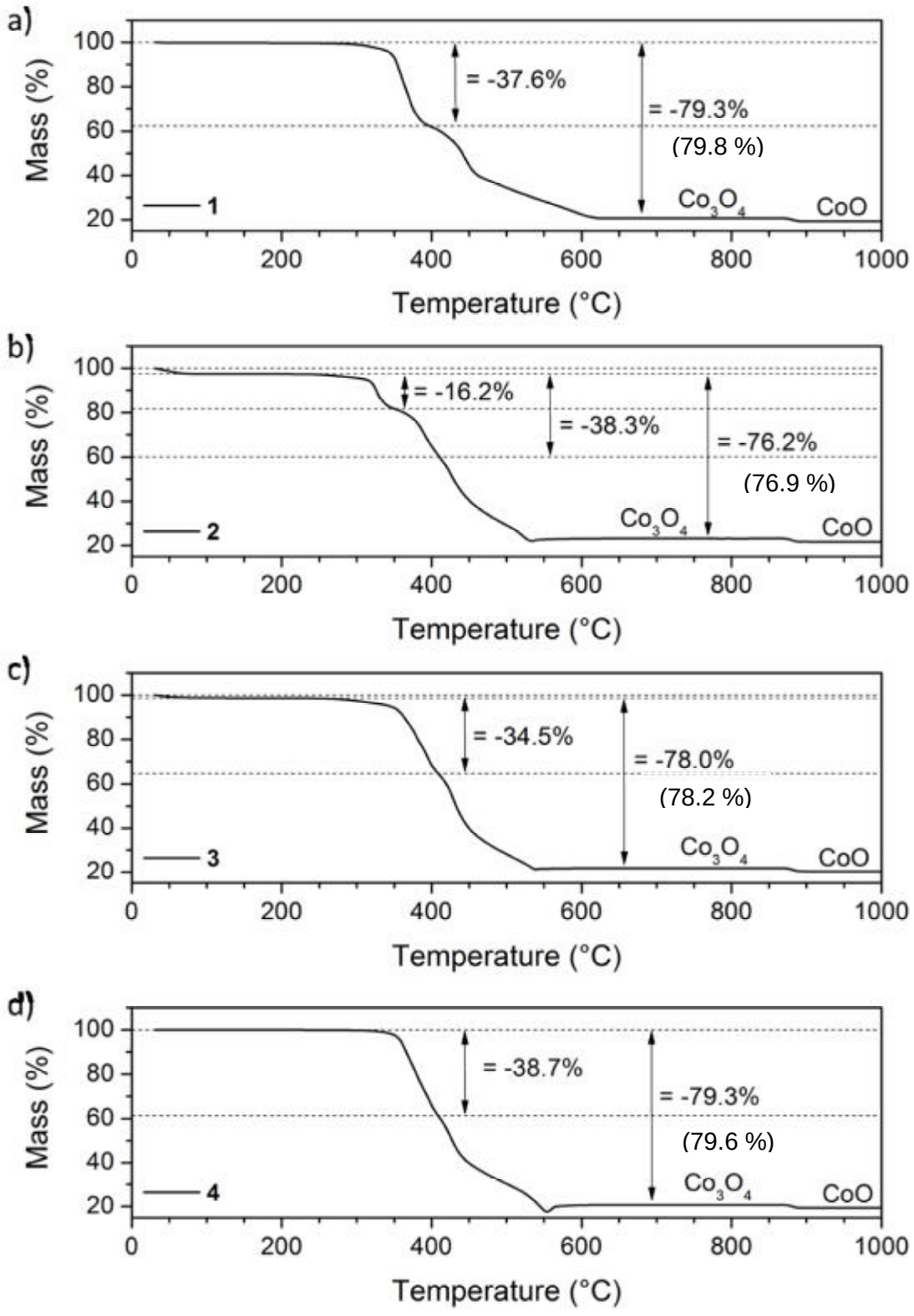

Figure S2: Thermogravimetric analysis of the four new materials, with expected mass loss for combustion of the organic given in parentheses. (a) Co(BDC)(3-Br-PNO), (b) Co(BDC)(4-MeO-PNO), (c) Co(BDC)(isoquinoline-N-oxide), (d) Co(BDC)(4-phenyl-PNO). The first loss indicated would correspond to the loss of the pyridine-N-oxide, but no crystalline product was isolated at this point.