

Supplementary Materials: A Family of Nitrogen Enriched Metal Organic Frameworks with CCS Potential

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Table S1. Selected crystallographic parameters for MOF coordination polymers.

Compound	Co-pytz	Ni-pytz	Zn-pytz(hydro)
Formula	C ₃₇ H ₂₆ Cl ₂ Co ₂ N ₂₂ O ₁₂	C _{18.5} H ₁₃ ClN ₁₁ NiO ₆	C ₂₆ H ₃₀ N ₈ O ₁₀ Zn
Formula weight	1159.56	579.56	679.95
Crystal system	Monoclinic	Monoclinic	Triclinic
Space Group	P2 ₁ /c	P2 ₁ /c	P-1
λ Å	1.5418	1.5418	0.71073
a Å	15.0829 (4)	15.0373 (8)	7.5735 (5)
b Å	15.3730 (5)	15.2694 (10)	9.2742 (6)
c Å	24.4188 (8)	24.337 (2)	11.7874 (8)
α°	90	90	91.365 (5)
β°	97.922(3)	97.945 (6)	107.279 (6)
γ°	90	90	222.294 (6)
Volume Å ³	5607.9 (3)	5534.4 (7)	728.50 (8)
Temp. K	123 (2)	123 (2)	123 (2)
Z	4	8	1
Refls. Collected	21735	21737	6924
Refls. Independent	10571	10460	3536
Rint	0.0564	0.0545	0.0317
Goodness of Fit	0.949	0.886	1.013
R[I > 2σ(I)], F	0.0707	0.2548	0.0723
Rw, F ²	0.1999	0.1628	0.0547

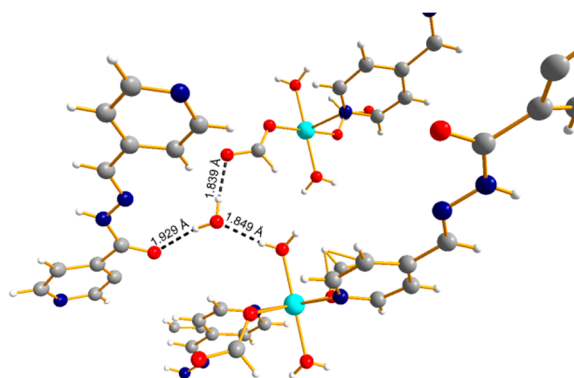


Figure S2. Unit structure of [Zn(pytz(hydrolyzed))₂(OH₂)₂(OCOCH₃)₂]₂·H₂O, highlighting hydrogen bonding between guest water molecules and coordinated species.