Supporting information for

Structural analysis and catalytic activity of tetranuclear metal carboxylate clusters with $[KZn_3(\mu_3\text{-}OH)(OOCCPh_3)_6]$ or $[Zn_4(\mu_4\text{-}O)(OOCCPh_3)_6]$ central motif

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Crystallographic Data for Compounds 1-3.

Table S1. Crystal and data collection parameters for compounds **1-3**.

Crystal	**1**·4CH_3CN·0.2C_6H_{14}	**1**·**2**·3.58CH_3CN·0.21C_6H_{14}	**3**·5CH_3CN
Chemical formula	$C_{131.2}H_{108.8}N_5O_{13}Zn_3K$	$C_{130.42}H_{107.6}N_{4.58}O_{13}Zn_{3.08}K_{0.92}$	$C_{124}H_{96}N_2O_{13}Zn_4$
Formula Mass	2198.71	2184.33	2288.86
Crystal system	Triclinic	Triclinic	Triclinic
Space group	$P\bar{1}$	$P\bar{1}$	$P\bar{1}$
a/Å	14.302(4)	14.301(4)	13.610 (3)
b/Å	15.362(5)	15.348 (4)	15.338 (4)
c/Å	27.872 (9)	27.869 (8)	29.649 (8)
α/°	74.68 (3)	74.64 (3)	92.10 (3)
β/°	84.79 (3)	84.79 (3)	97.87 (3)
γ/°	66.28 (3)	66.31 (3)	112.25 (3)
Unit cell volume/Å^3	5406 (3)	5401 (3)	5648(3)
Temperature/K	100(2)	100(2)	100(2)
Z	2	2	2
Radiation type	MoKα	MoKα	MoKα
Absorption coefficient, μ/mm^{-1}	0.767	0.781	0.907
No. of reflections measured	60695	71595	49124
No. of independent reflections	27833	23571	24365
No. of observed reflections ($I > 2\sigma(I)$)	22907	19892	14784
R_{int}	0.0282	0.0297	0.0525
Final R_1 values ($I > 2\sigma(I)$)	0.0393	0.0404	0.0539
Final $wR(F^2)$ values ($I > 2\sigma(I)$)	0.1134	0.1046	0.1167
Final R_1 values (all data)	0.0476	0.0515	0.0998
Final $wR(F^2)$ values (all data)	0.1166	0.1112	0.1279
Goodness of fit on F^2	1.104	1.037	0.927
Δρmax/eÅ^{-3}	1.03	1.55	0.72
Δρmin/eÅ^{-3}	-0.75	-1.03	-0.82

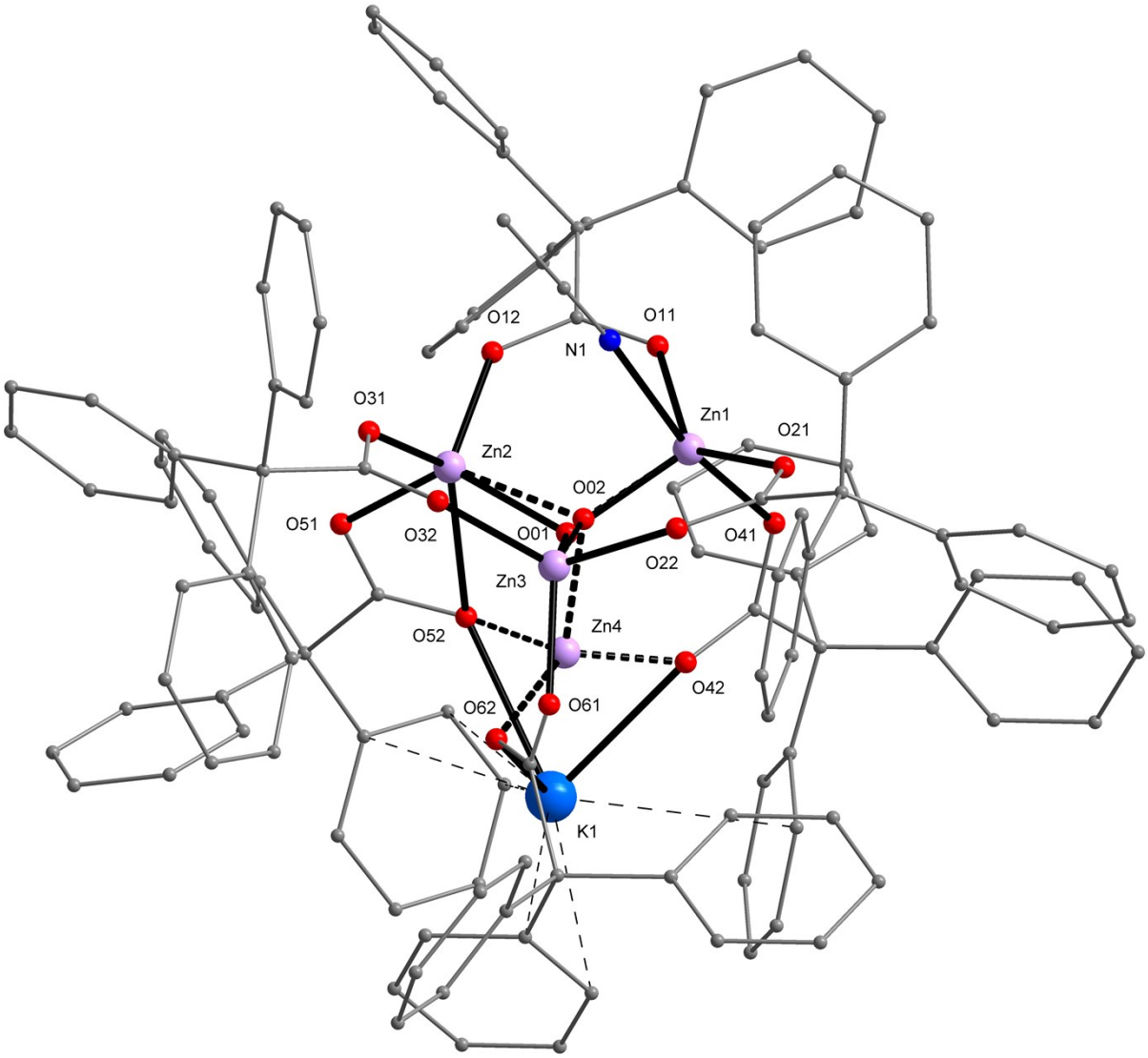

Figure S1. Molecular structures of $[KZn_3(\mu_3\text{-}OH)(Ph_3CCOO)_6(MeCN)]_{0.92}\cdot[Zn_4(\mu_4\text{-}O)(Ph_3CCOO)_6(MeCN)_2]_{0.08}\cdot 3.58MeCN\cdot 0.21C_6H_{14}$, (**1**·**2**·3.58MeCN·0.21C_6H_{14}). Hydrogen atoms and solvent molecules are omitted for clarity.

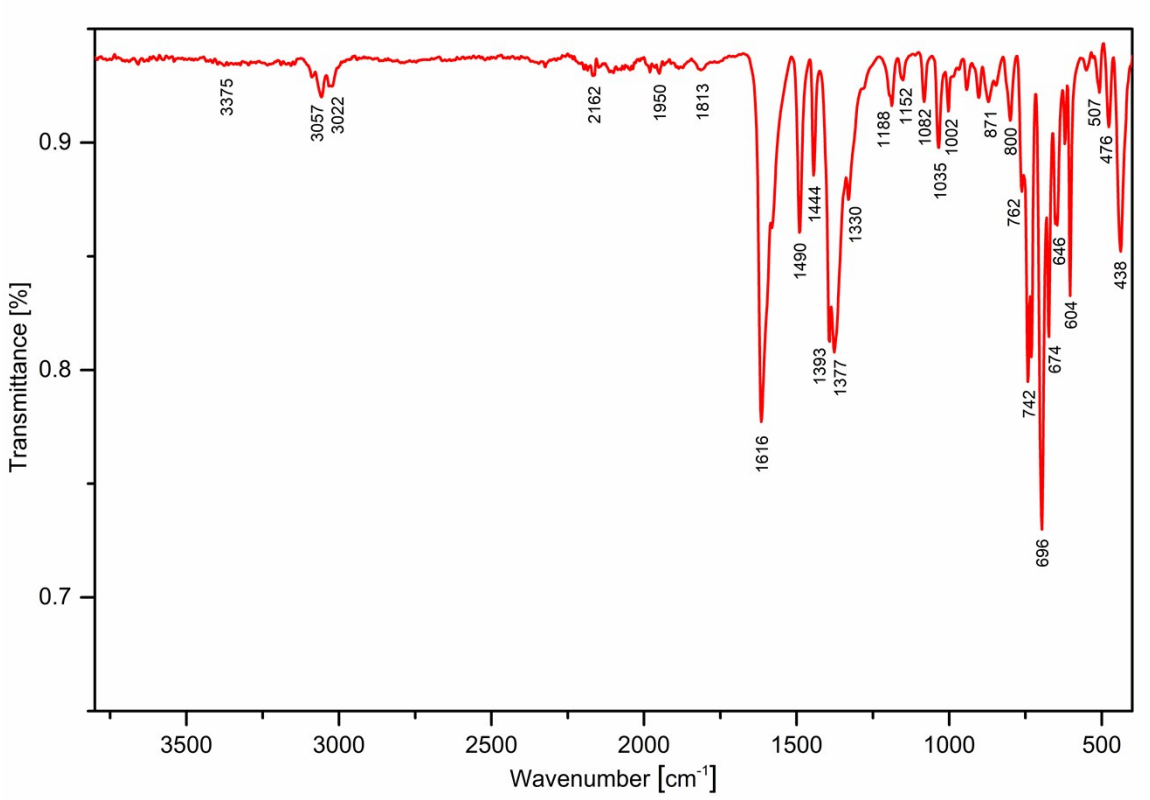

Figure S2. FTIR-ATR spectra of **1**.

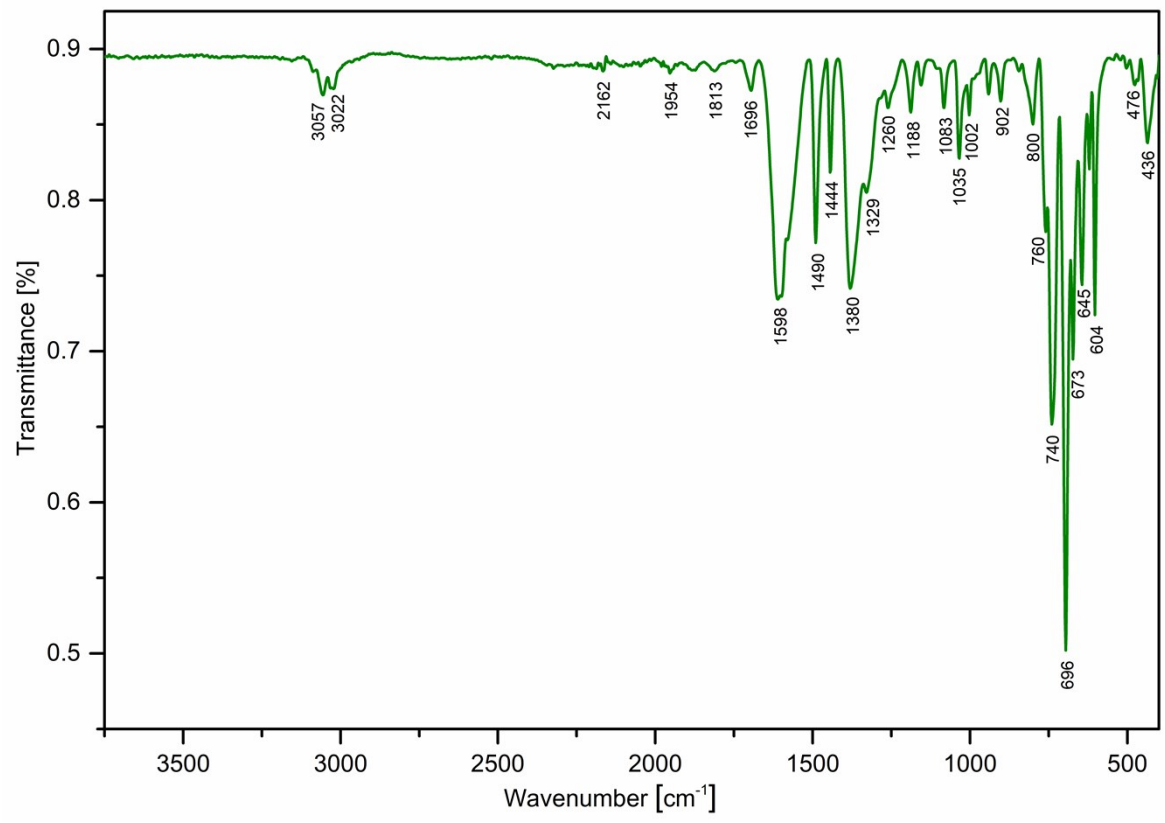

Figure S3. FTIR-ATR spectra of **1**·**2**.

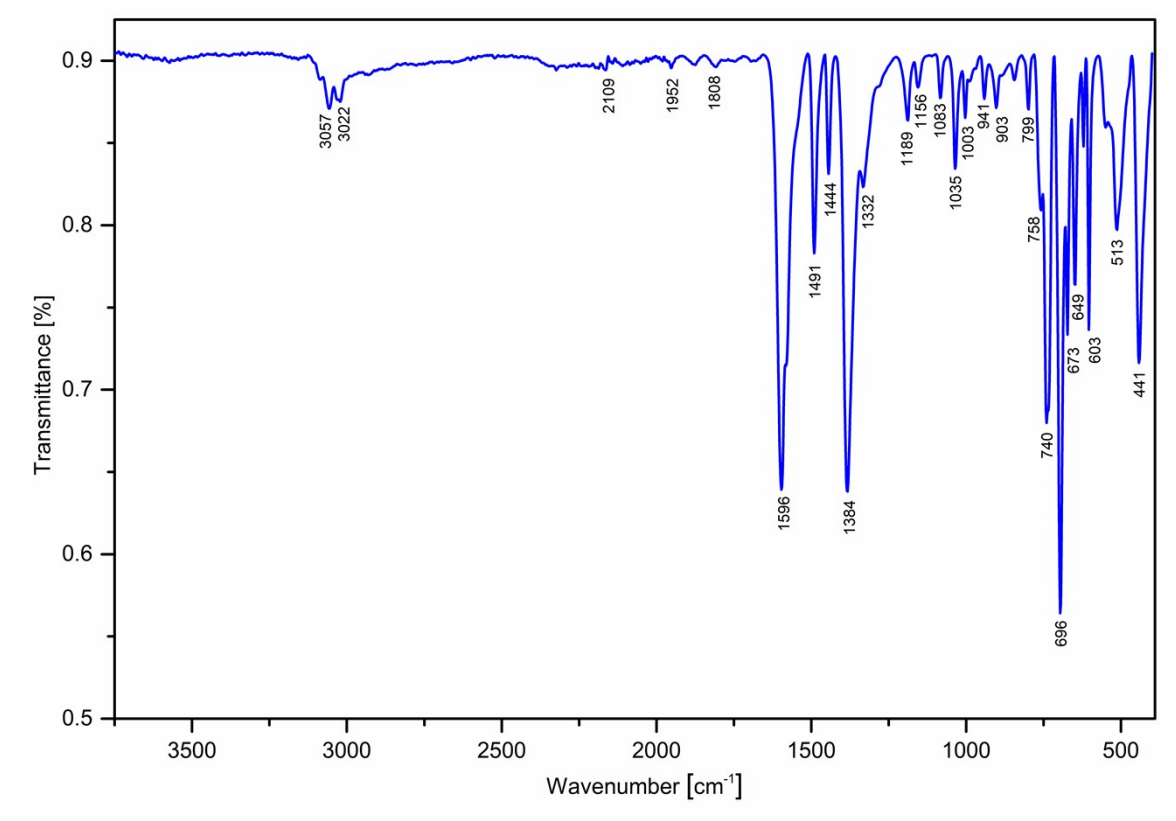

Figure S4. FTIR-ATR spectra of **3**.

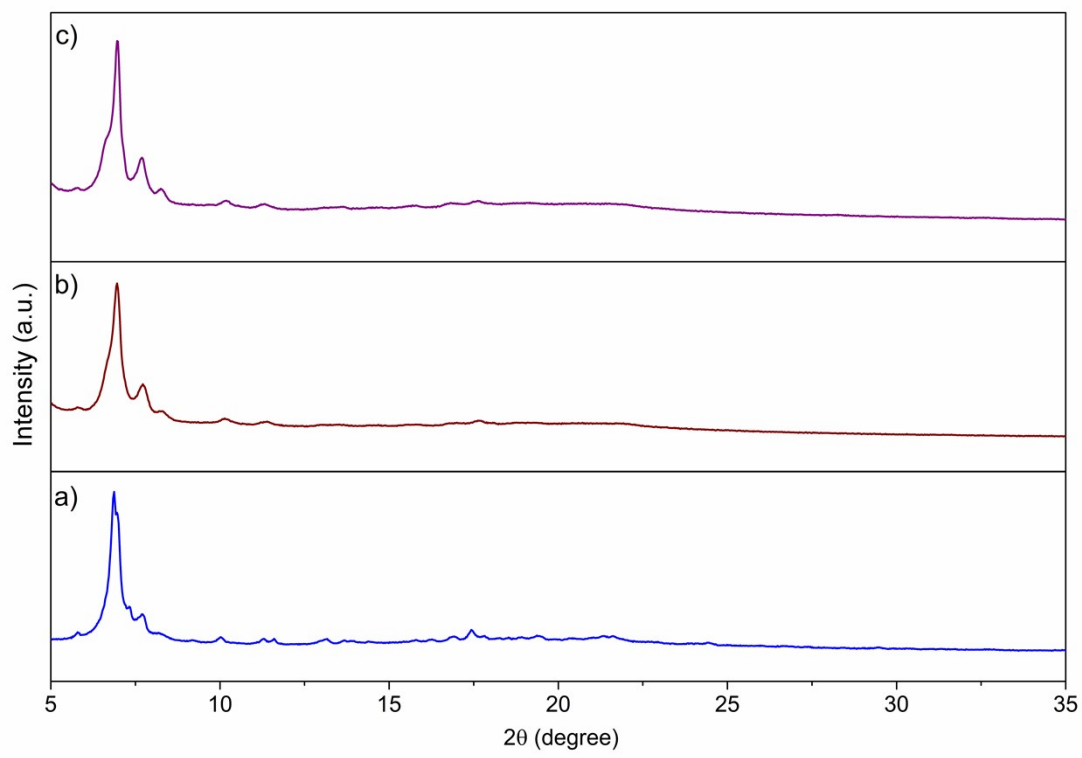

Figure S5. Comparison of PXRD patterns of **3** measured at 25 ºC for the ground crystals (a), crystals without grounding and crystalline precipitate isolated from the reaction (c).

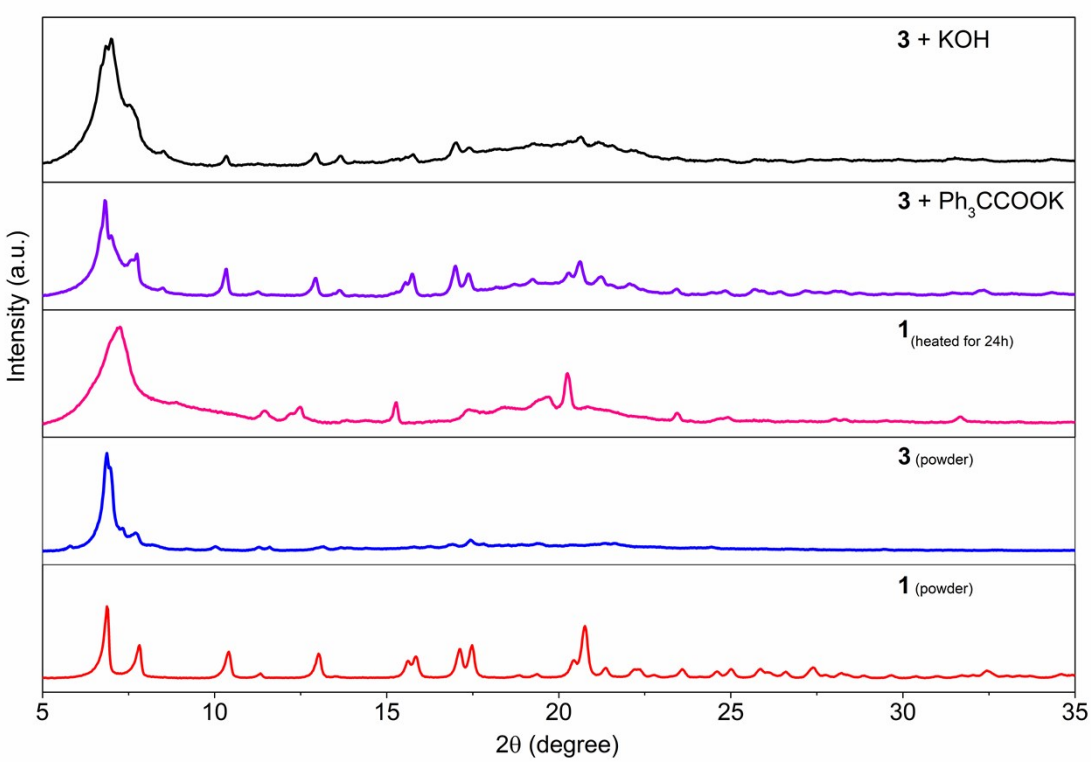

Figure S6. Comparison of PXRD patterns of **1** and **3** together with patterns of crystalline materials obtained by the heating of **1** for 24h in CH_3CN solution (pink), and reaction of **3** with Ph_3CCOOK (violet) or KOH (black).