Electronic Supplementary Material for CrystEngComm

Electronic Supplementary Information for MS:

Solid State Crystal-to-Crystal Transformation From Monomeric Structure to One-dimensional Coordination Polymers on Anion Exchange

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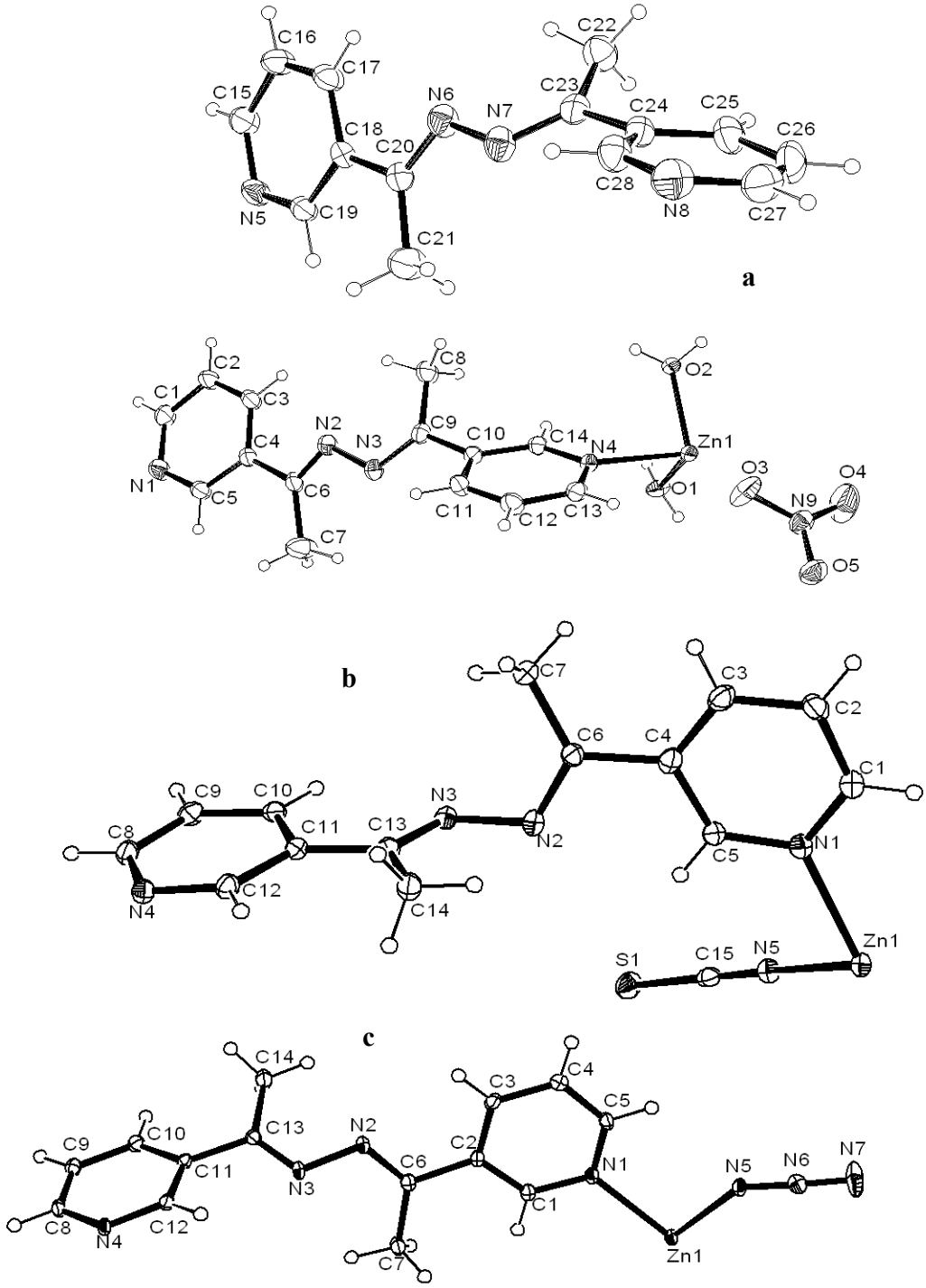

Figure S1. ORTEP diagram of the asymmetric unit **a**) compound $[Zn(bpdh)_2(H_2O)_4](NO_3)_2.2bpdh$ (**1**), **b**) compound $[Zn(\mu\text{-}bpdh)_2(NCS)_2]_n$ (**2**) and **c**) compound $[Zn(\mu\text{-}bpdh)_2(N_3)_2]_n$ (**3**). Ellipsoids 30% probability.

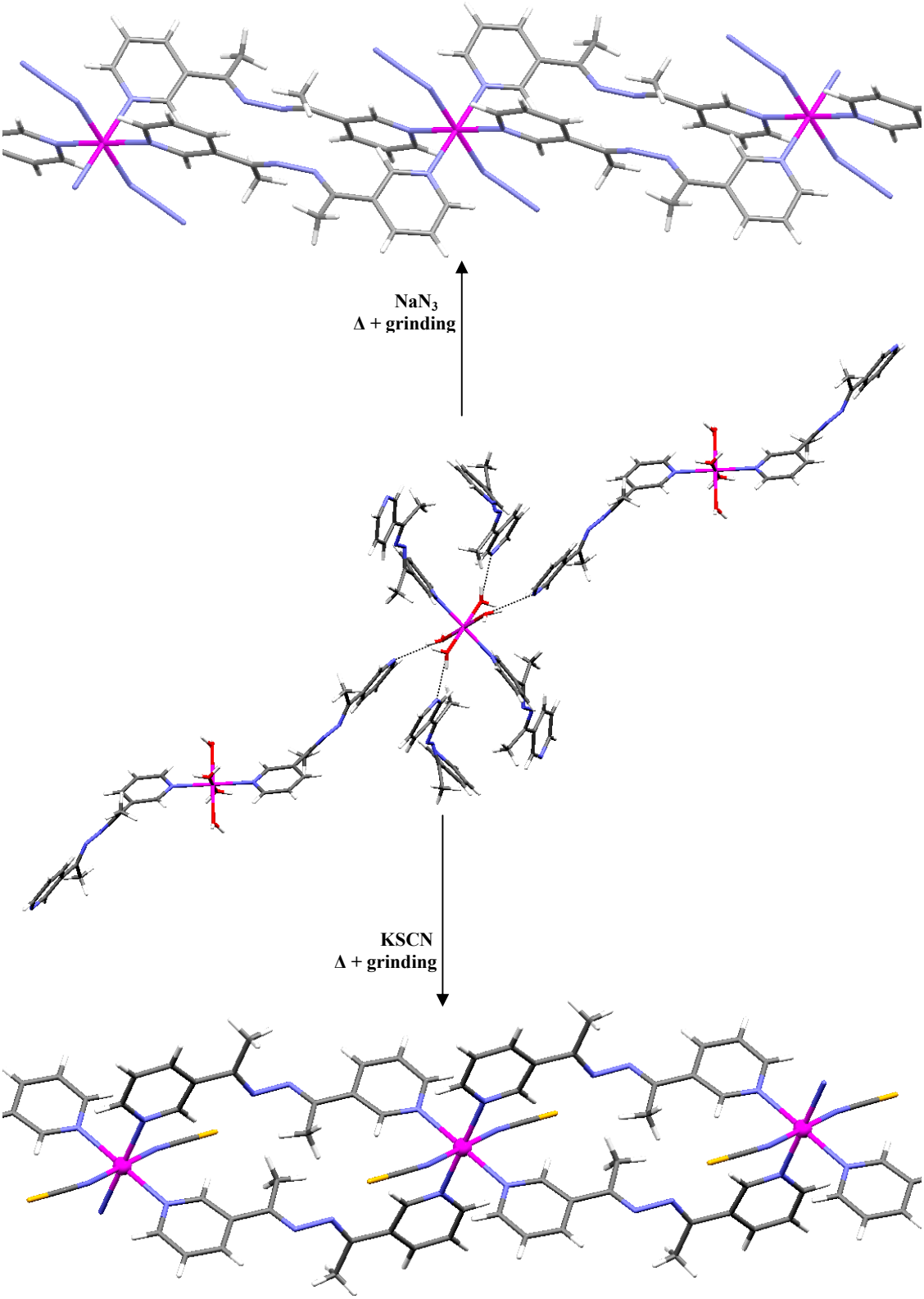

Figure S2. Schematic representation of the solid-state conversion of monomeric structure to 1D coordination polymers structures by anion exchange.

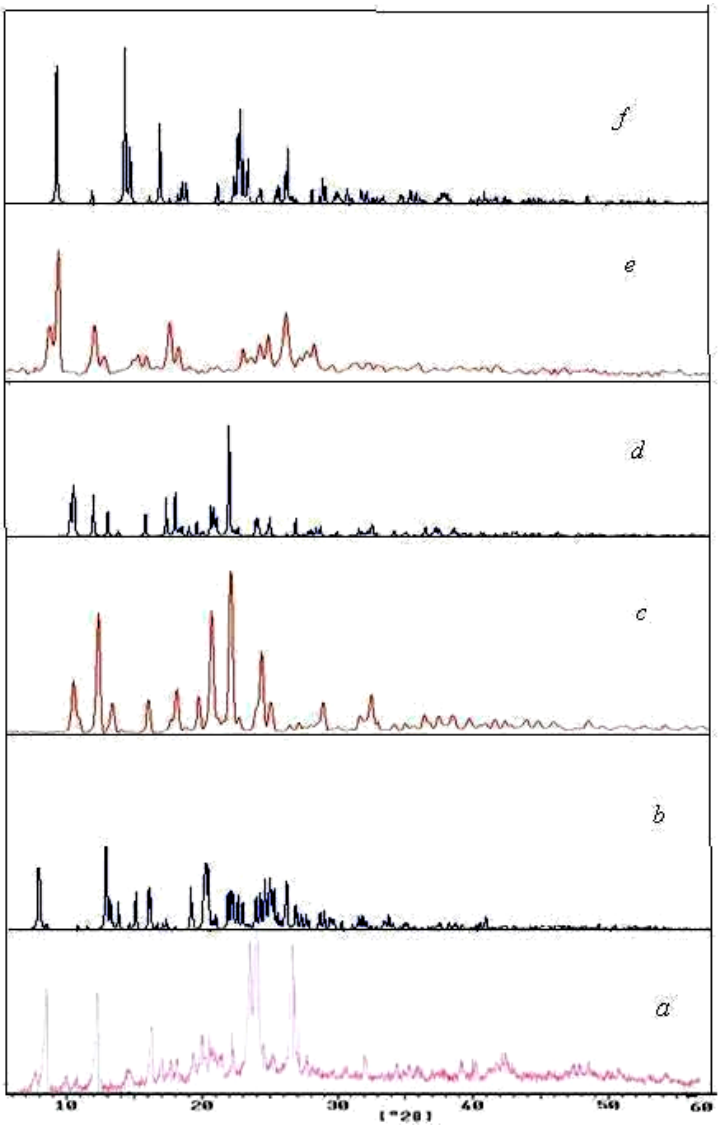

Figure S3. The XRD patterns of (**a**) bulk materials as synthesized of compound **1**; (**b**) simulated from single crystal X-ray data of compound **1**, (**c**) bulk materials obtained by anion exchange of compound **1** by potassium thiocyanate; (**d**) simulated from single crystal X-ray data of compound **2** (e) bulk materials obtained by anion exchange of compound **1** by sodium azide; (**d**) simulated from single crystal X-ray data of compound **3**.

Table S1 Crystal data and structure refinement for compound **1-3**.

Identification code	1	2	3
Empirical formula	$C_{56}H_{64}N_{18}O_{10}Zn$	$C_{30}H_{28}N_{10}S_2Zn$	$C_{14}H_{14}N_7Zn_{0.50}$
Formula weight	1214.62	658.15	313.01
Temperature	298 K	296 K	150 K
Wavelength	0.71073 Å	0.71073 Å	0.71073 Å
Crystal system	Monoclinic	Monoclinic	Monoclinic
Space group	$P2_1/c$	$P2_1/n$	$P2_1/c$
Unit cell dimensions	a = 8.7682(12) Å	a = 9.5576(5) Å	a = 12.618(4) Å
	b = 22.742(3) Å	b =16.9548(10) Å	b = 13.076(4) Å
	c = 14.533(2) Å	c = 9.6533(5) Å	c = 8.739(3) Å
	β = 91.819(2)°	β = 98.630(3)°	β =106.414(4)°
Volume	2896.5(7) Å^3	1546.6(5) Å^3	1383.2(6) Å^3
Z	2	2	4
Density (calculated)	1.393 Mg/m^3	1.413 Mg/m^3	1.503 Mg/m^3
Absorption coefficient	0.499 mm^{-1}	0.968 mm^{-1}	0.936 mm^{-1}
F(000)	1272	680	648
Crystal size	0.31×0.30×0.27 mm^3	0.21 ×0.18×018 mm^3	0.18×0.12×0.10 mm^3
Theta range for data collection	1.66 to 25.01°	2.40 to 27.58 °	3.54 to2 6.69°
Index ranges	-10≤ h ≤ 10	-12≤ h ≤ 12	-15≤ h ≤ 15
	-27≤ k ≤ 23	-22≤ k ≤ 21	-16≤ k ≤ 15
	17≤ k ≤ 16	-12 ≤ l ≤ 12	-10≤ l ≤ 11
Reflections collected	15072	39569	10473
Independent reflections	5104	3576	2701
Completeness to theta	99.8 %	99.8 %	θ = 25.00°: 100.0 %
Absorption correction	multi-scan	multi-scan	multi-scan
Max. and min. transmission	0.8608 and 0.8771	0.8226 and 0.8451	0.8496and 0.9122
Refinement method	Full-matrix least-squares on F^2	Full-matrix least-squares on F^2	Full-matrix least-squares on F^2
Data / restraints / parameters	5104/6/401	3576/0/198	2701/0/198
Goodness-of-fit on F^2	1.128	1.195	1.065
Final R. [I>2sigma(I)]	R1 = 0.0621, wR2 = 0.1346	R1 = 0.0632, wR2 = 0.2025	R1 =0.0312, wR2 = 0.0697
R indices (all data)	R1 = 0.0718, wR2 = 0.1402	R1 =0.0739, wR2 = 0.2069	R1 =0.0492, wR2 = 0.0735