Electronic Supplementary Material (ESI) for CrystEngComm.

Supporting Information

A single precursor approach for ZIFs synthesis: Transformation of a new 1D $[Zn(Im)(HIm)_2(OAc)]$ structure to 3D $Zn(Im)_2$ frameworks

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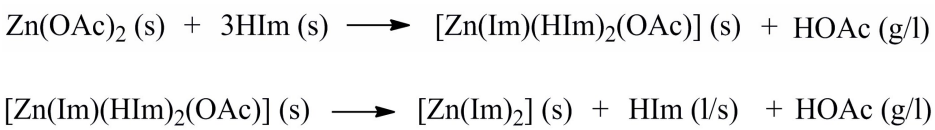
Table S1 Crystallographic data and structure refinement summary for $C_{11}H_{14}N_6O_2Zn$ (CCDC 1044169)

Compound	$Zn(Im)(HIm)_2(OAc)$
Formula	$C_{11}H_{14}N_6O_2Zn$
Formula weight	327.65
Crystal system	Monoclinic
Space group	*P2(1)/c*
Cell parameters	*a = 10.9252(9)* Å *b = 9.3337(6)* Å *c = 14.2595(3)* Å *alpha = 90 deg.* *beta = 98.0093(10) deg.* *gamma = 90 deg.*
Cell volume	1439.89(16) $Å^3$
Z	4
Calculated density	1.511 g/cm^3
Temperature	293(2) K
Absorption coefficient	1.716 mm^{-1}
Crystal size	0.21 x 0.12 x 0.07 mm
Reflections collected/unique	6203
GOF	1.066
Final R indices [I > 2sigma (I)]	R_1 = 0.0560, wR_2 = 0.1271
R indices (all data)	R_1 = 0.1112, wR_2 = 0.1726



Scheme S1 Reaction equation for synthesis of $[Zn(Im)(HIm)_2(OAc)]$ (1) (above) and coi (3) (below) (Im=imidazolate, HIm=imidazole, OAc=carboxylate, HOAc= acetic acid)

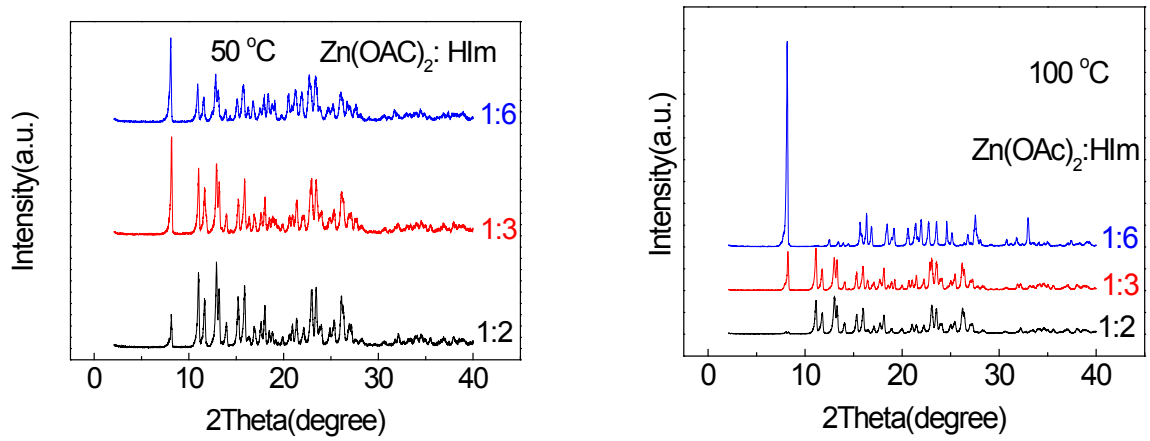


Figure S1. PXRD patterns of the products using a solvent-free synthesis at 50 °C (left) and 100 °C (right) for 24 h with different molar ratios of $Zn(OAc)_2$-HIm mixtures: 1:2, 1:3 and 1:6.

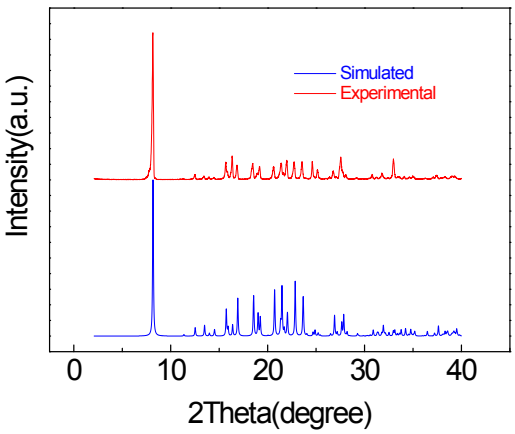


Figure S2. Experimental XRD pattern for the sample and the XRD pattern simulated from the crystal structure data for $Zn(Im)(HIm)_2(OAc)$ (**1**) (CCDC 1044169).

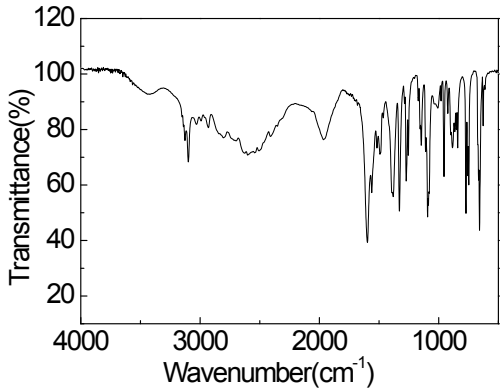


Figure S3. FT-IR spectrum of $Zn(Im)(HIm)_2(OAc)$ (**1**)

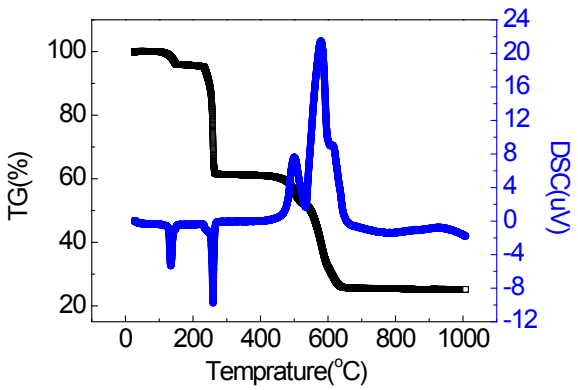


Figure S4. TG-DSC curves for $Zn(Im)(HIm)_2(OAc)$ (**1**).

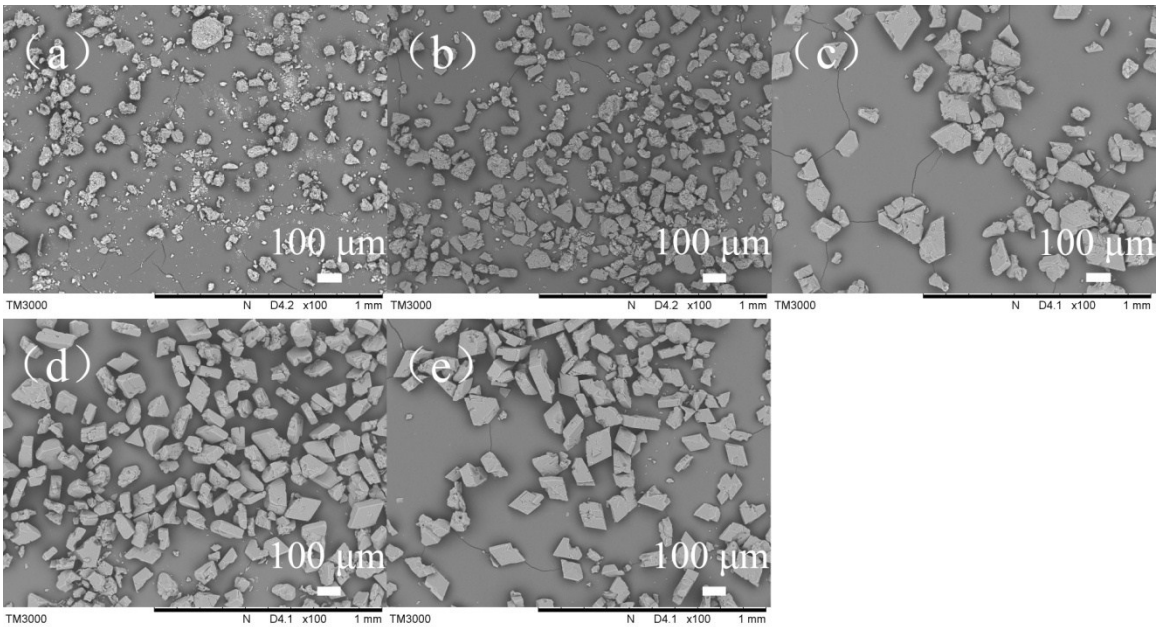


Figure S5. SEM images illustrating the crystallization process of [Zn(Im)(Him)2OAc] (1) at 100 °C (heated to the reaction temperatures at a rate of 5 °C min^{-1}) as a function of reaction time: (a) 1 h; (b) 3 h; (c) 6 h; (d) 12 h; (e) 24 h.

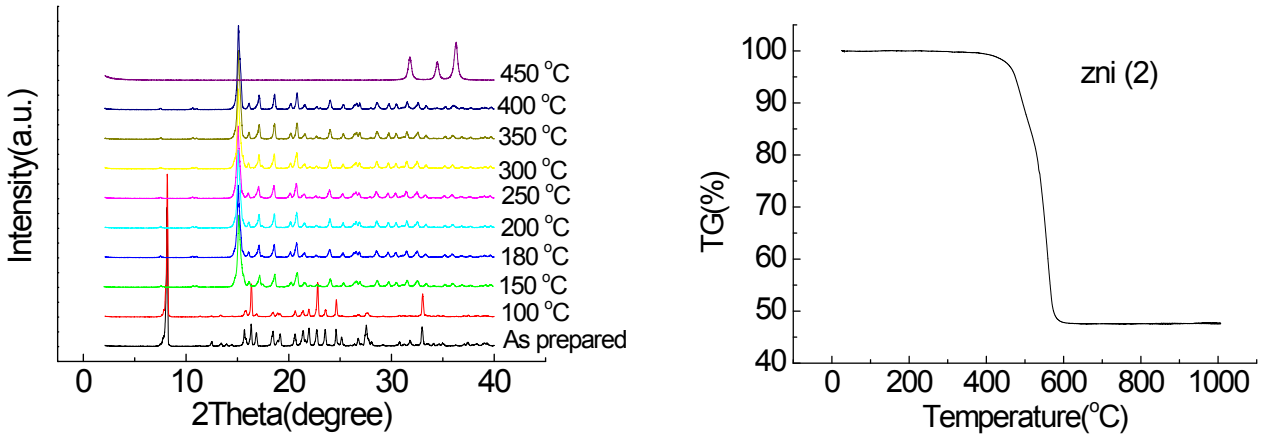


Figure S6. (left) Zn(Im)(HIm)$_2$(OAc) (**1**) heated in air at a heating rate of 5 °C min^{-1} to a set temperature (100–450 °C) and maintained at this temperature for 24 h; (right) TG curves for zni (**2**) obtained at 350 °C.

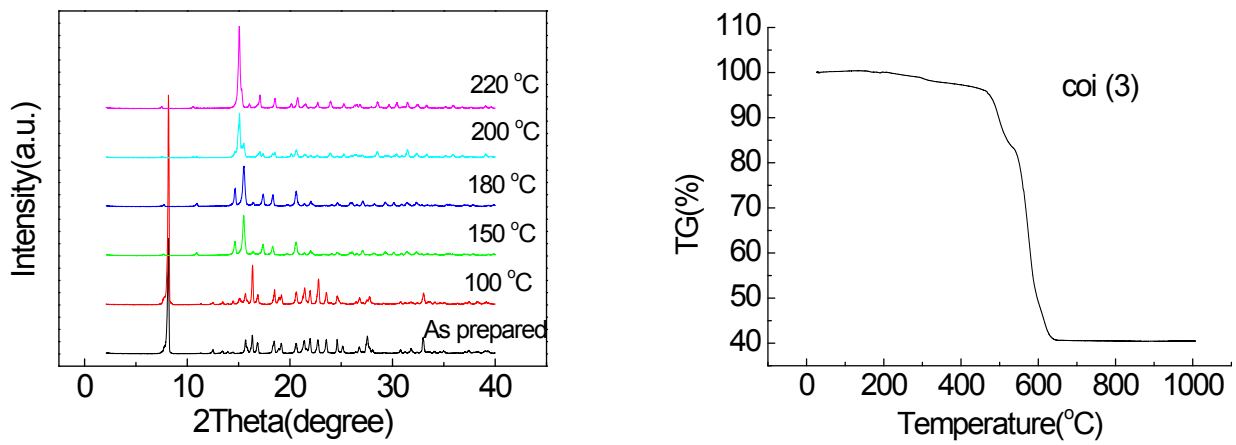


Figure S7. (left) Zn(Im)(HIm)$_2$(OAc) (**1**) was sealed in a Teflon-lined stainless steel autoclave, heated at a heating rate of 5 °C min^{-1} to a set temperature (100–220 °C) and maintained at this temperature for 24 h; (right) TG curves for coi (**3**) obtained at 180 °C.

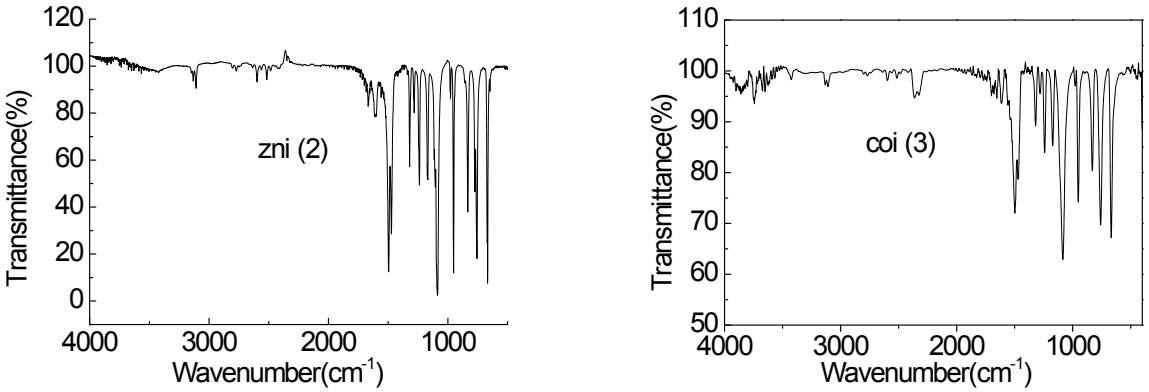


Figure S8. (left) FT-IR spectrum of zni (**2**) obtained at 150 °C; (right) FT-IR spectrum of coi (**3**) obtained at 150 °C.

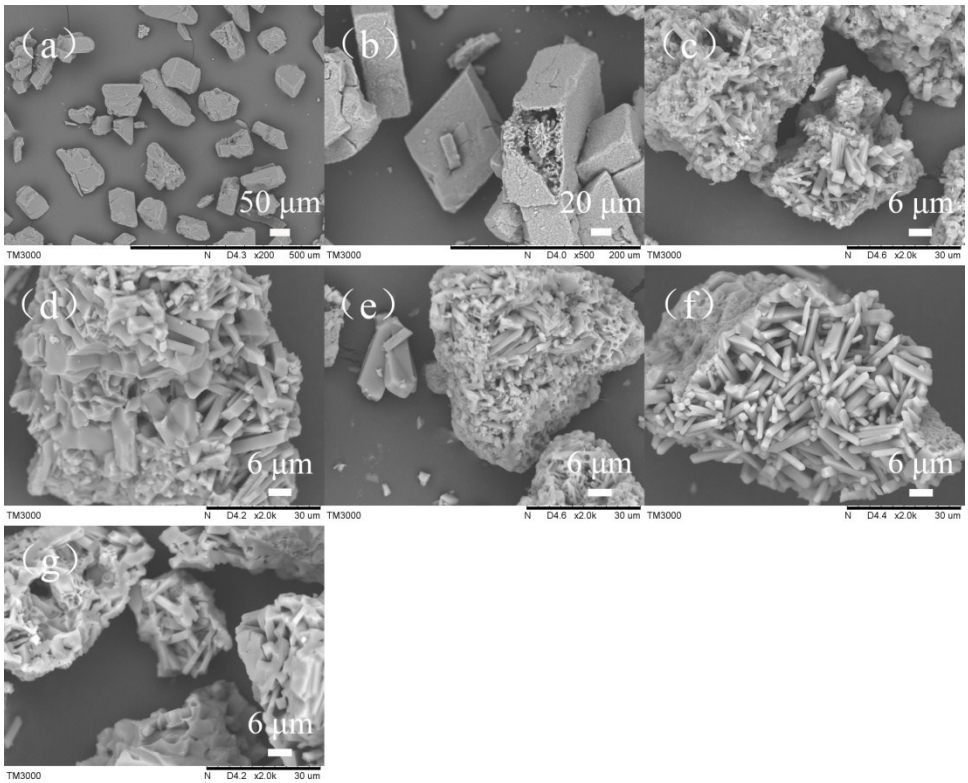


Figure S9. SEM images of (1) after heat treatment in open atmosphere as a function of temperature which was increased at a rate of 5 °C min^{-1}: (a) 100 °C; (b) 125 °C; (c) 150 °C; (d) 200 °C; (e) 250 °C; (f) 300 °C; (g) 350 °C

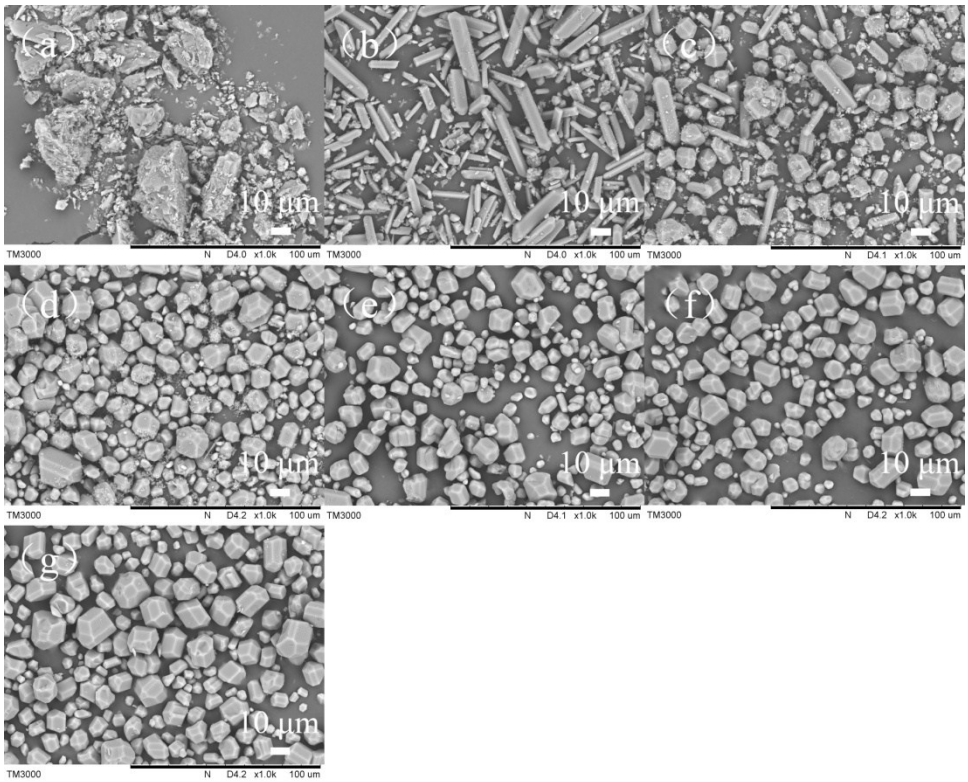


Figure S10. SEM images of (1) after heat treatment in a closed vessel at 150 °C (heated to the reaction temperatures at a rate of 5 °C min^{-1}) as a function of reaction time, the reaction times were: (a) 0 h; (b) 0.5 h; (c) 1.5 h; (d) 3 h; (e) 6 h; (f) 12 h; (c) 24 h.

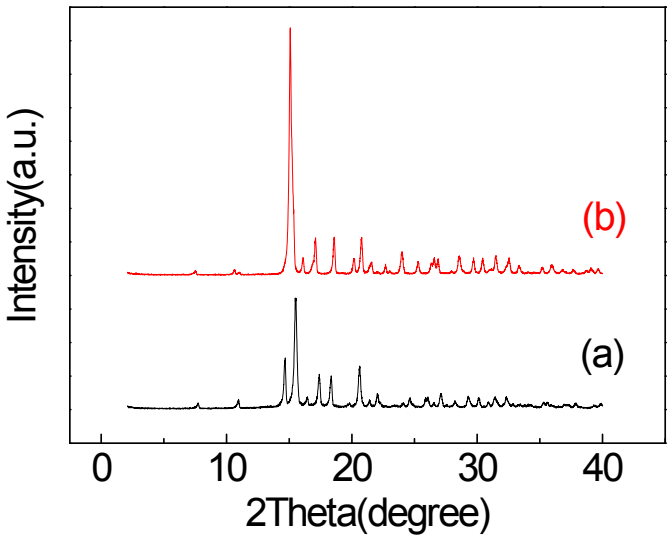


Figure S11. coi (3) (a) transforms into zni (b) when heated in air at a heating rate of 5 °C min^{-1} to 375 °C.