Supporting information

Control over the nucleation process determines the framework topology of porous coordination polymers

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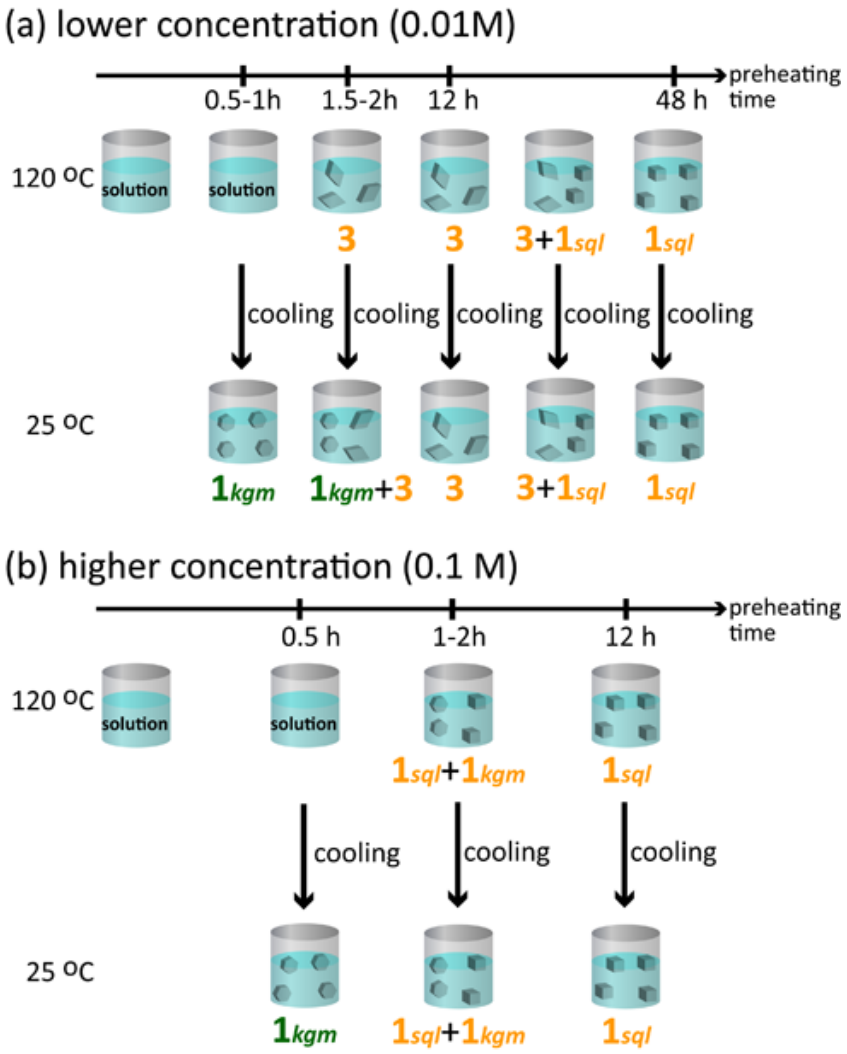

Scheme S1 Summary of the synthetic protocols and the obtained phase at (a) lower and (b) higher concentration. Green and orange indicate crystals obtained after cooling and soon after preheating, respectively.

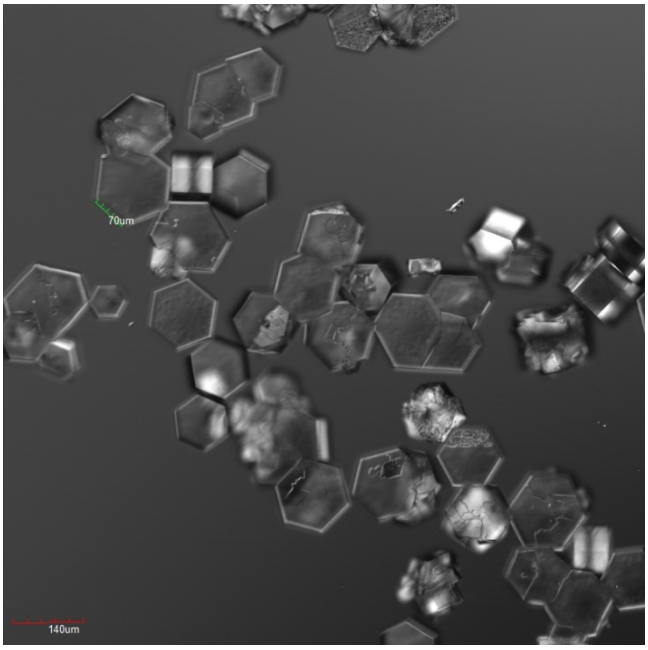

Figure S1 A picture of single crystals of $\mathbf{1}_{kgm}$.

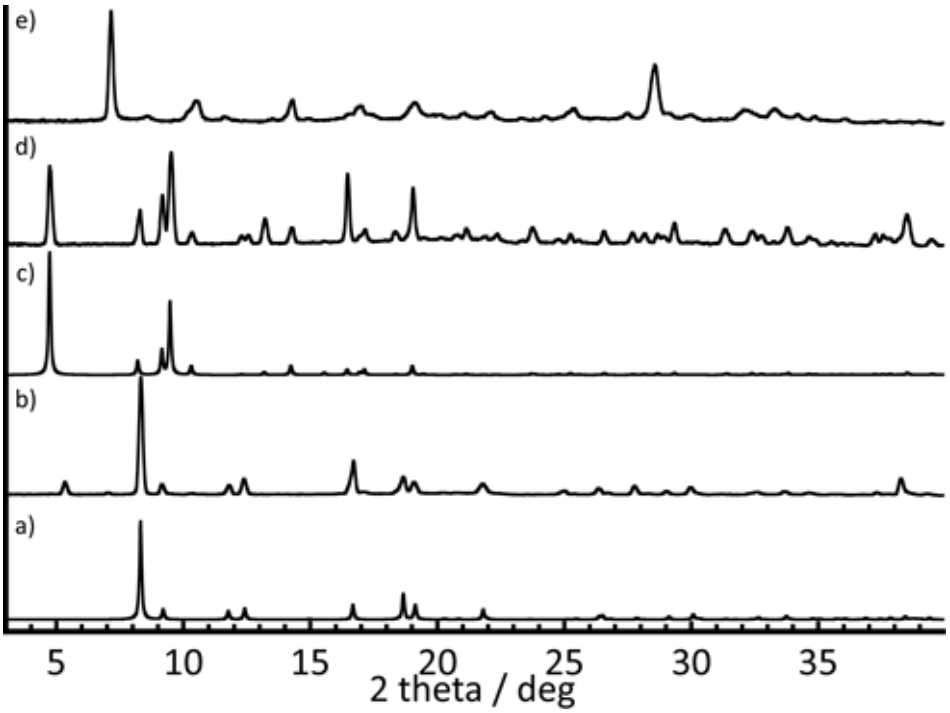

Figure S2 PXRD patterns of**1**$_{sql}$ (b), **1**$_{kgm}$ (d), and **3** (e) and simulated patterns of **1**$_{sql}$ (a), **1**$_{kgm}$ (c).

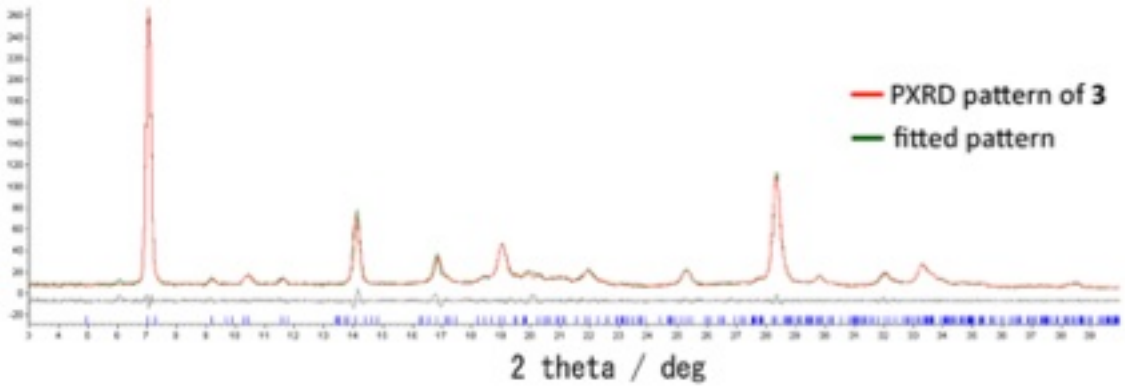

Figure S3 A PXRD pattern of **3** (red line) and a fitted pattern (green line).

Peak fitting of 3: Peak fitting analysis was performed using TOPAS (Bruker) program. The unit cell parameters obtained from SCXRD measurement (monoclinic, *a* = 12.94(2), *b* =9.60(1), *c* = 18.72(3) Å, and β = 106.52(3)) were used as a initial model. Unit cell parameters obtained from the peak fitting were *a* = 13.165(2), *b* =9.6113(7), *c* = 18.3747(2) Å, and β = 107.13(1) deg, R_{wp} = 7.267%.

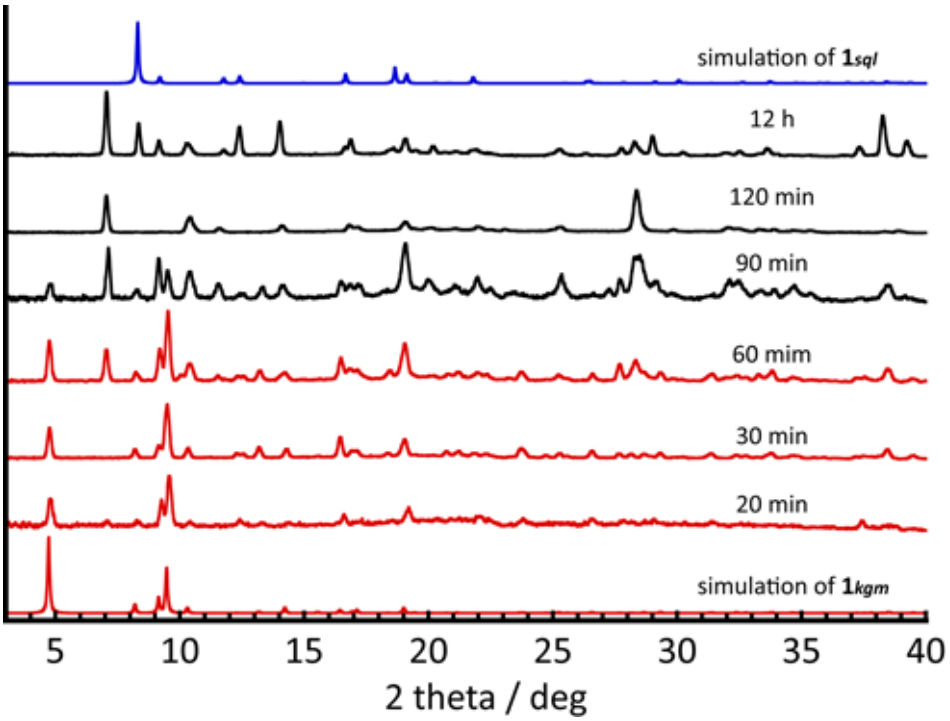

Figure S4 PXRD patterns of the products with various preheating time (20 min, 0.5, 1, 1.5, 2, and 12 h) after cooling process and simulated patterns of $\mathbf{1}_{kgm}$ and $\mathbf{1}_{sql}$. The concentration of zinc ions is 0.03 M.

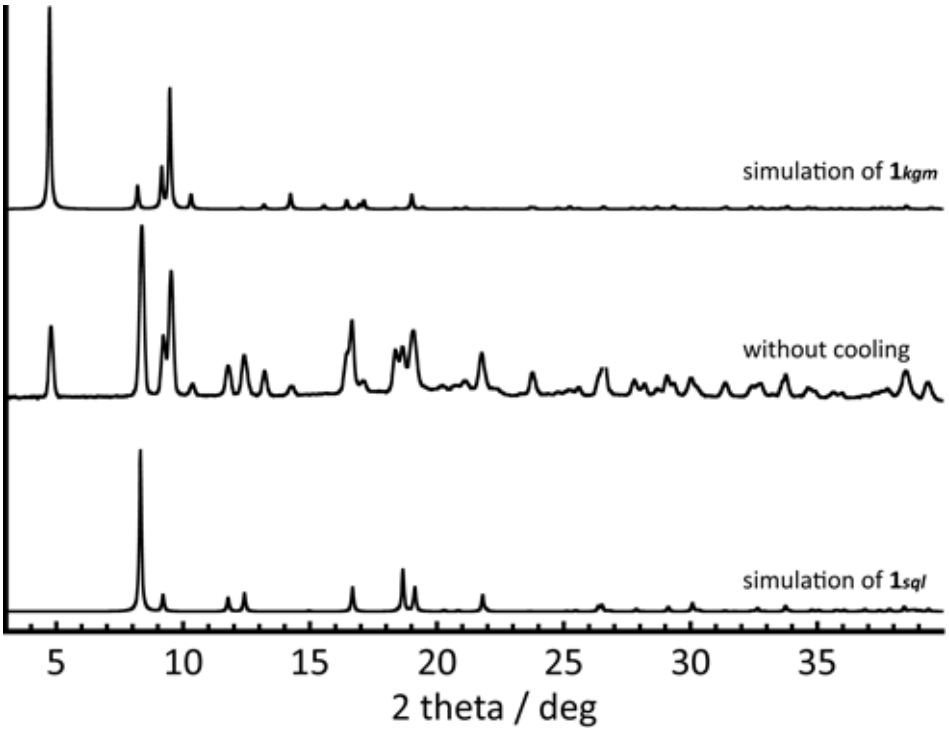

Figure S5 A PXRD pattern of the products soon after the preheating process (60 min) and simulated patterns of $\mathbf{1}_{kgm}$ and $\mathbf{1}_{sql}$. The concentration of zinc ions is 0.1 M.

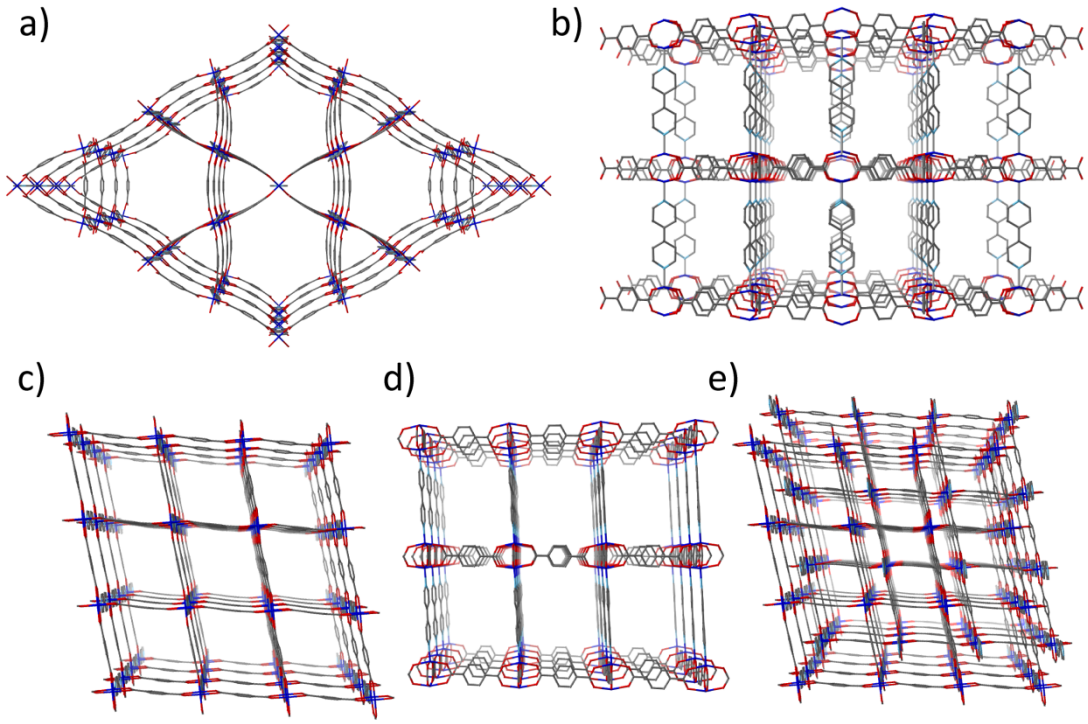

Figure S6 Crystal structures of $\mathbf{2}_{kgm}$ and $\mathbf{2}_{sql}$ along *c* axis (a), (c) and *a* axis (b), (d), respectively. Two-fold interpenetrations observed in $\mathbf{2}_{sql}$ (e). Hydrogen atoms and disordered guest molecules are omitted for clarity.

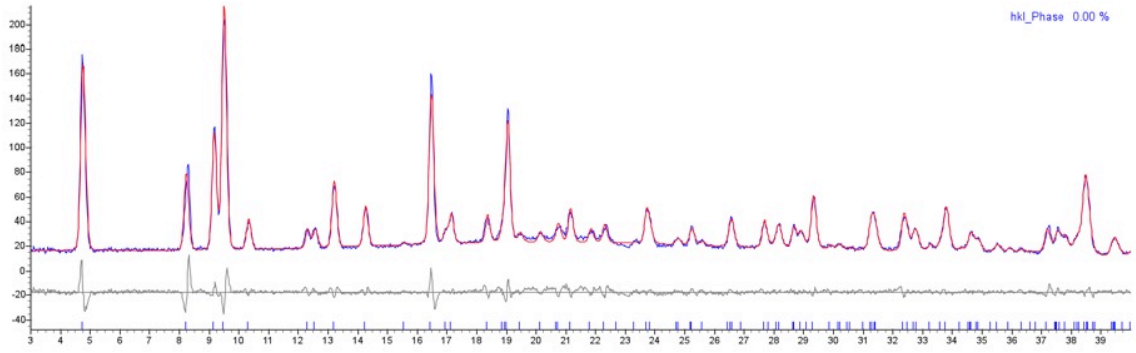

Figure S7 A PXRD pattern of the products with 1h of preheating time after cooling process (blue line) and a fitted pattern (red line).

Peak fitting: Peak fitting analysis was performed using TOPAS (Bruker) program. The unit cell parameters of $\mathbf{1}_{kgm}$ obtained from SCXRD measurement (hexagonal, a = 21.6195(13), and c = 9.6282(8) Å) were used as a initial model. Unit cell parameters obtained from the peak fitting were a = 21.558(1), and b =9.675(5), R_{wp} = 7.587%.

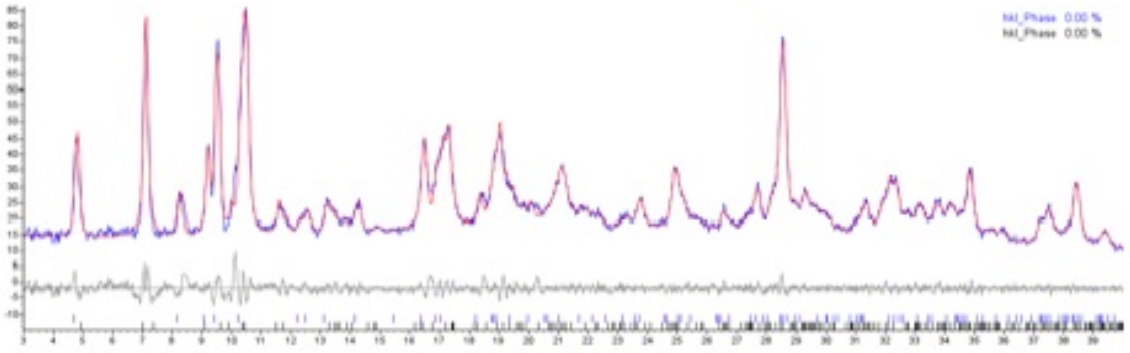

Figure S8 A PXRD pattern of the products with 1.5h of preheating time after cooling process (blue line) and a fitted pattern (red line).

Peak fitting: Peak fitting analysis was performed using TOPAS (Bruker) program. The unit cell parameters of **1**$_{kgm}$ and **3** obtained from SCXRD measurement (**1**$_{kgm}$: hexagonal, a = 21.6195(13), and c = 9.6282(8) Å, **3**: monoclinic, a = 12.94(2), b =9.60(1), c = 18.72(3) Å, and β = 106.52(3)) were used as a initial model. Unit cell parameters obtained from the peak fitting were a = 21.609(2), and c = 9.697(1) Å for **1**$_{kgm}$ and a = 13.100(2), b =9.7102(1), c = 18.480(3) Å, and β = 106.44(1) deg for **3**, R_{wp} = 5.47%.

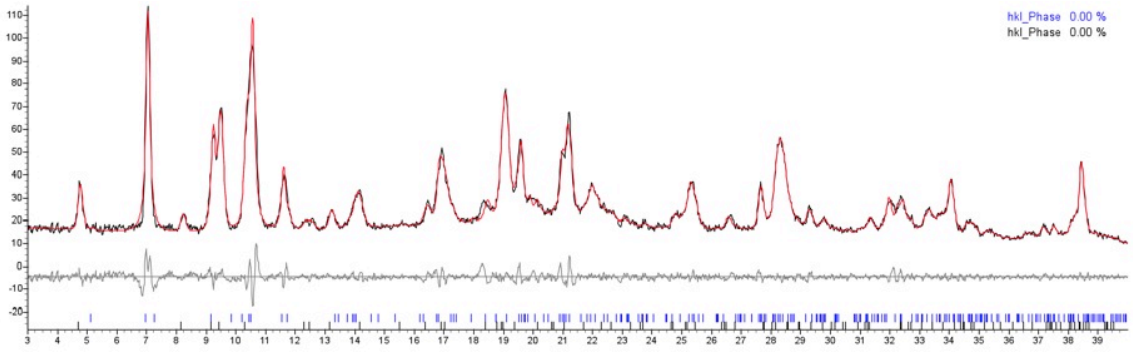

Figure S9 A PXRD pattern of the products with 2.0 h of preheating time after cooling process (blue line) and a fitted pattern (red line).

Peak fitting: Peak fitting analysis was performed using TOPAS (Bruker) program. The unit cell parameters of $\mathbf{1}_{kgm}$ and **3** obtained from SCXRD measurement ($\mathbf{1}_{kgm}$: hexagonal, a = 21.6195(13), and c = 9.6282(8) Å, **3**: monoclinic, a = 12.94(2), b =9.60(1), c = 18.72(3) Å, and β = 106.52(3)) were used as a initial model. Unit cell parameters obtained from the peak fitting were a = 21.607(3), and c = 9.6032(8) Å for $\mathbf{1}_{kgm}$ and a = 13.294(2), b =9.6849(1), c = 18.614(3) Å, and β = 107.94(1) deg for **3**, R_{wp} = 6.38%.