

Assembly of Two Zinc(II)-Squarate Coordination Polymers with Noncovalent and Covalent Bonds Derived from Flexible Ligands, 1,2-Bis(4-pyridyl)ethane (dpe)

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Table S1. The O–H...O hydrogen bonds for **1**

Table S2. The O–H...O and N–H...O hydrogen bonds for **2**

Figure S1 Representation of the 3D supramolecular architecture for **2**.

Figure S2 (a) Temperature-dependent powder X-ray diffraction patterns of **1** from room temperature to 400 °C and its simulation from single-crystal diffraction data. The baselines for each temperature were shifted for clarity. (b) The powder patterns of compound **1** at RT, 180°C and re-hydrated samples at RT.

Figure S3 (a) Temperature-dependent powder X-ray diffraction patterns of **2** from room temperature to 450 °C and its simulation from single-crystal diffraction data. The baselines for each temperature were shifted for clarity. (b) The powder patterns of compound **2** at RT, 250°C and re-hydrated samples at RT.

Table S1. The O–H...O hydrogen bonds for **1**^a

D–H (Å)	D...A(Å)	H...A(Å)	∠ D–H...Acceptor(°)
O(5)–H(5A) 0.86(4)	O(5)...O(2) _i 2.656	H(5A)...O(2) _i 1.82	∠ O(5)–H(5)...O(2) _i 165(4)
O(5)–H(5B) 0.81(4)	O(5)...O(4) _{ii} 2.714	H(5B)...O(4) _{ii} 1.91	∠ O(5)–H(5B)...O(4) _{ii} 173(4)
O(6)–H(6A) 0.87(3)	O(6)...O(4) 2.651	H(6A)...O(4) 1.79	∠ O(6)–H(6A)...O(4) 169(3)
O(6)–H(6B) 0.78(4)	O(6)...O(2) _{iii} 2.685	H(6B)...O(2) _{iii} 1.91	∠ O(6)–H(6B)...O(2) _{iii} 176(4)

^aSymmetry operations used to generate equivalent atoms: (i) x, –1+y, z (ii) –1+x, 1+y, z (iii) 1+x, –1+y, z

Table S2. The O–H...O and N–H...O hydrogen bonds for **2**^a

D–H (Å)	D...A(Å)	H...A(Å)	∠ D–H...Acceptor(°)
N(2)–H(2A) 0.860(4)	N(2)...O(12) _{iv} 2.721	H(2A)...O(12) _{iv} 1.87	∠ N(2)–H(2A)...O(12) _{iv} 171.3(2)
O(3)–H(3) 0.790(2)	O(3)...O(2) 2.782	H(3)...O(2) 2.01	∠ O(3)–H(3)...O(2) 167.1(2)
O(4)–H(4) 0.809(2)	O(4)...O(9) _i 2.695	H(4)...O(9) _i 1.99	∠ O(4)–H(4)...O(9) _i 145.7(2)
O(4)–H(4') 0.805(3)	O(4)...O(6) _i 2.920	H(4)...O(6) _i 2.92	∠ O(4)–H(4)...O(6) _i 126.6(2)
O(5)–H(5) 0.927(3)	O(5)...O(13) _{iii} 2.764	H(5)...O(13) _{iii} 1.87	∠ O(5)–H(5)...O(13) _{iii} 161.4(2)
O(5)–H(5') 0.798(2)	O(5)...O(1) _i 2.792	H(5')...O(1) _i 2.03	∠ O(5)–H(5')...O(1) _i 159.4(2)
O(14)–H(14) 0.721(2)	O(14)...O(11) 2.707	H(14)...O(11) 1.99	∠ O(14)–H(14)...O(11) 172.3(2)
O(14)–H(14') 0.879(2)	O(14)...O(7) 2.682	H(14')...O(7) 1.80	∠ O(14)–H(14')...O(7) 176.1(2)
O(15)–H(15) 0.814(2)	O(15)...O(7) _{ii} 2.670	H(15)...O(7) _{ii} 1.86	∠ O(15)–H(15)...O(7) _{ii} 174.1(2)
O(15)–H(15') 0.703(2)	O(15)...O(13) _i 2.700	H(15')...O(13) _i 2.01	∠ O(15)–H(15')...O(13) _i 169.0(2)

^aSymmetry operations used to generate equivalent atoms: (i) x, 1+y, z (ii) 1+x, y, z (iii) –x, 1–y, 1–z (iv) 1–x, –y, –z

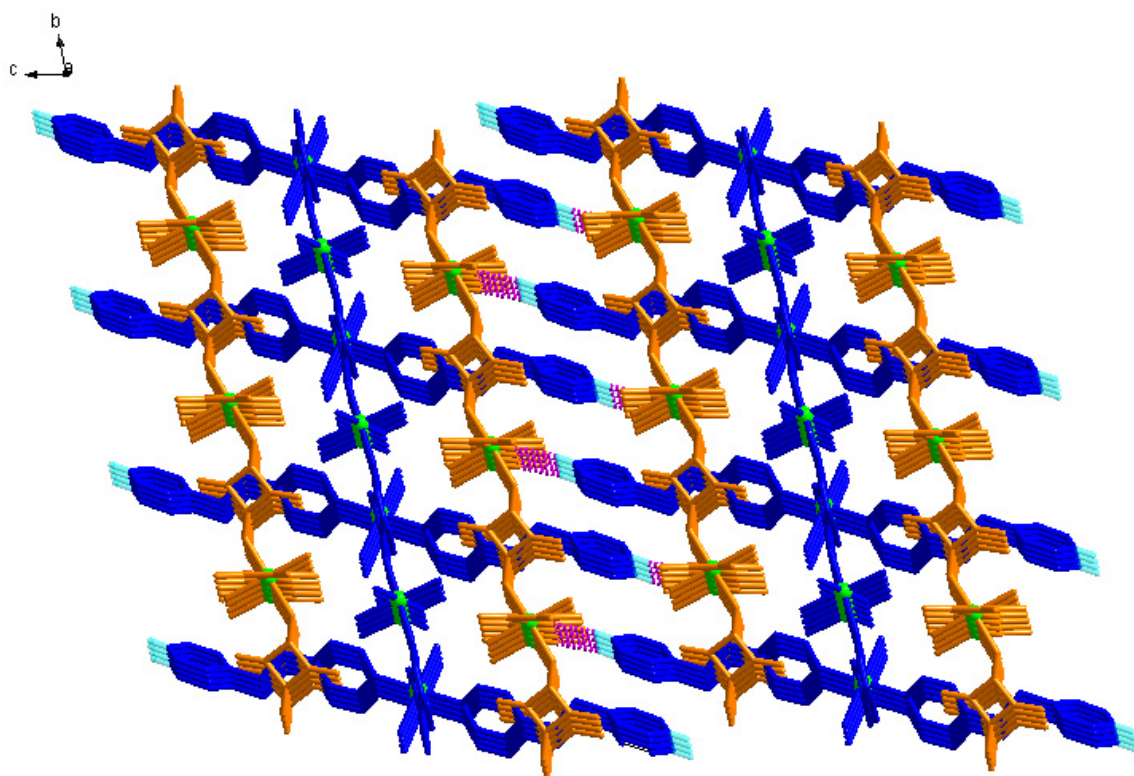
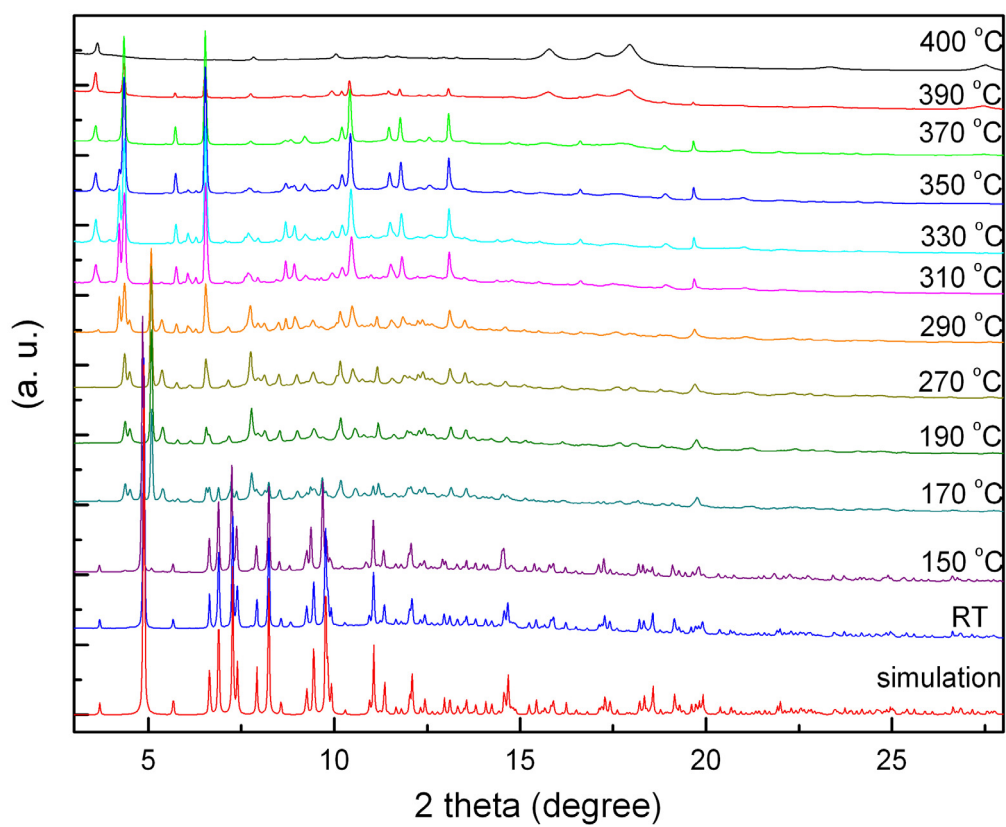
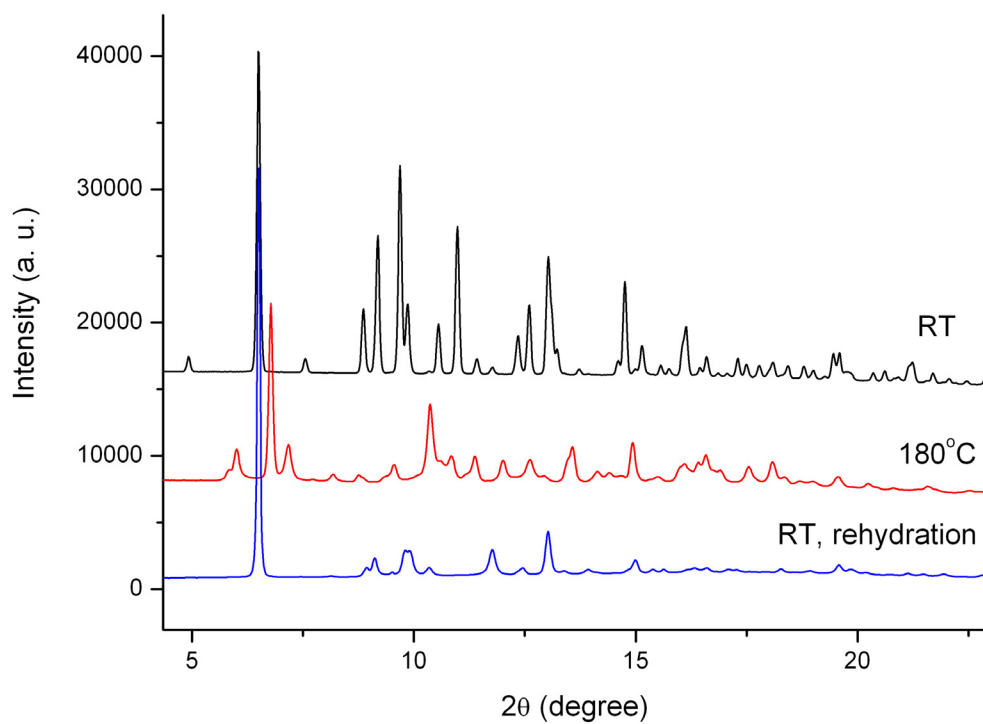


Figure S1

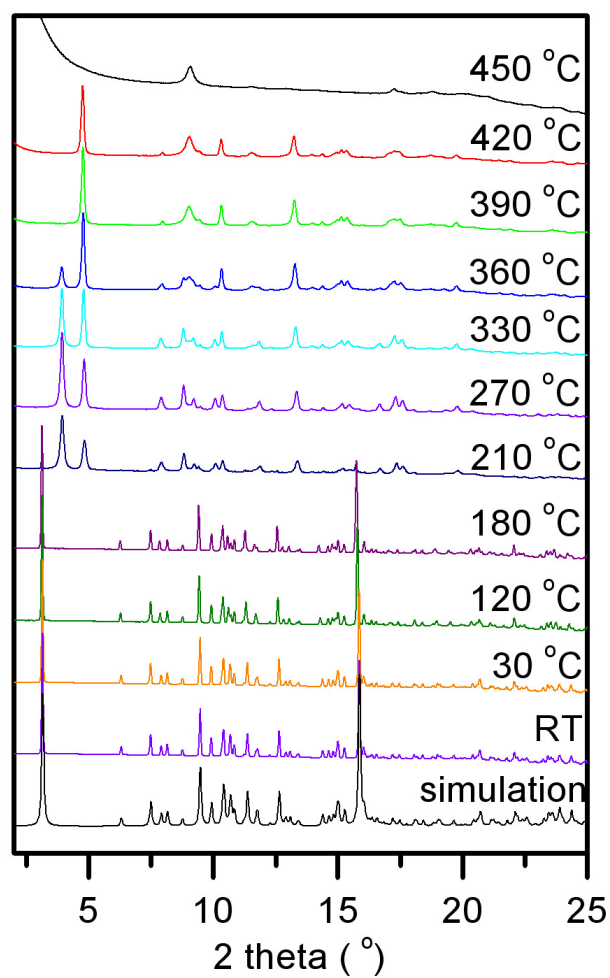


(a)

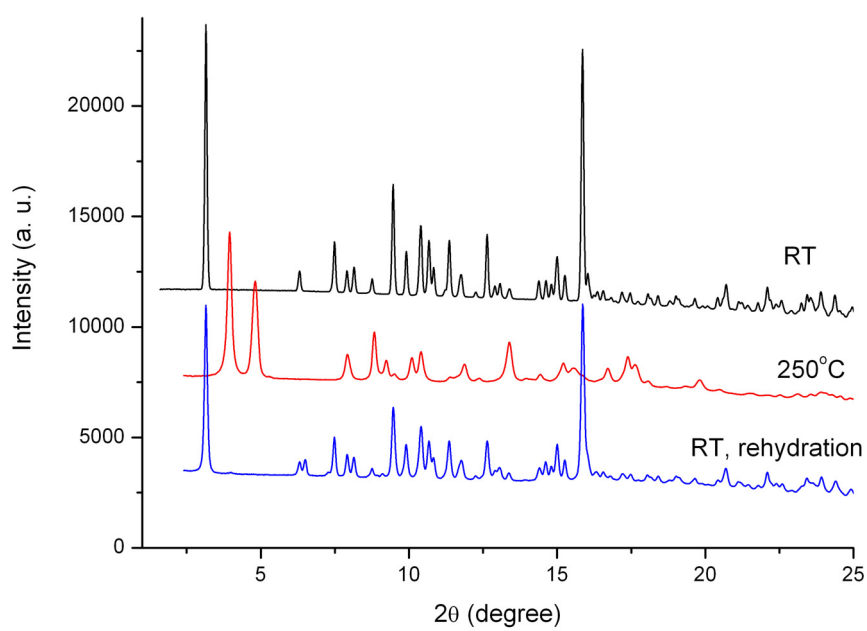


(b)

Figure S2



(a)



(b)

Figure S3