Supplementary Material (ESI) for CrystEngComm

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

Chih-Chieh Wang,*[a] Wen-Chun Chung,[a] Hui-Wun Lin,[a] Shuen-Chieh Dai,[a] Jia-Shiuan Shiu,[a] Gene-Hsiang Lee,[b] Hwo-Shuenn Sheu[c] and William Lee[d]

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

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

[a]Symmetry 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

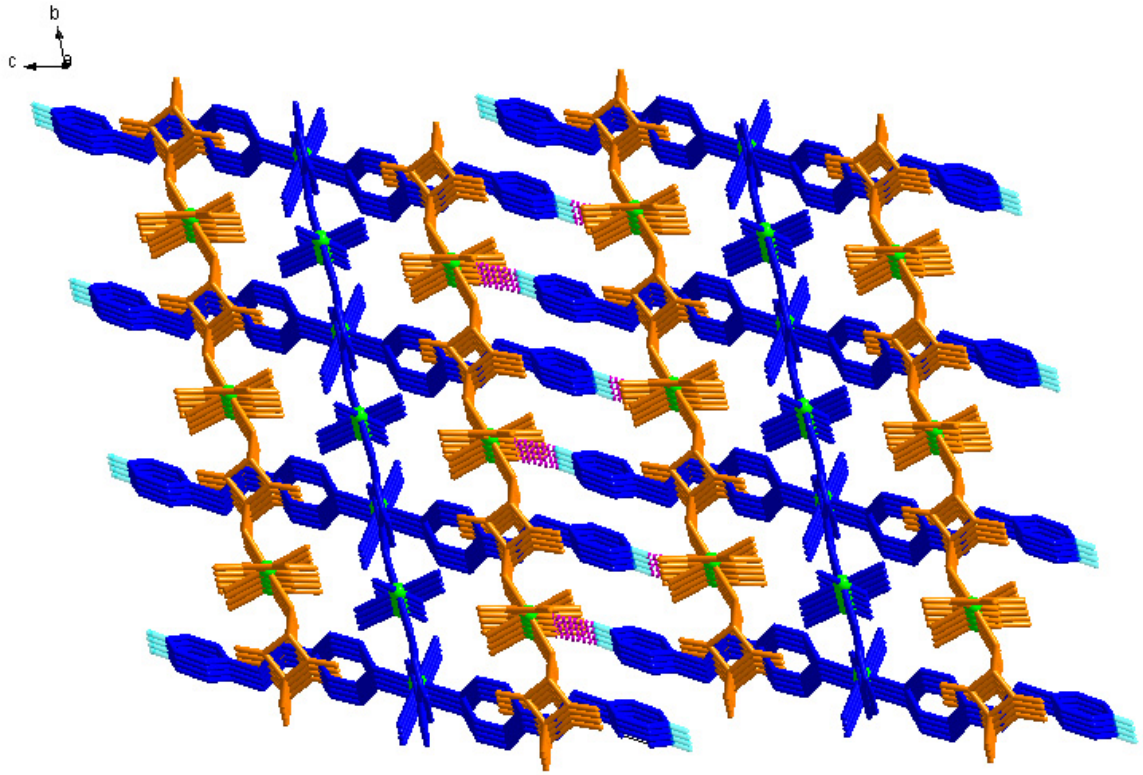
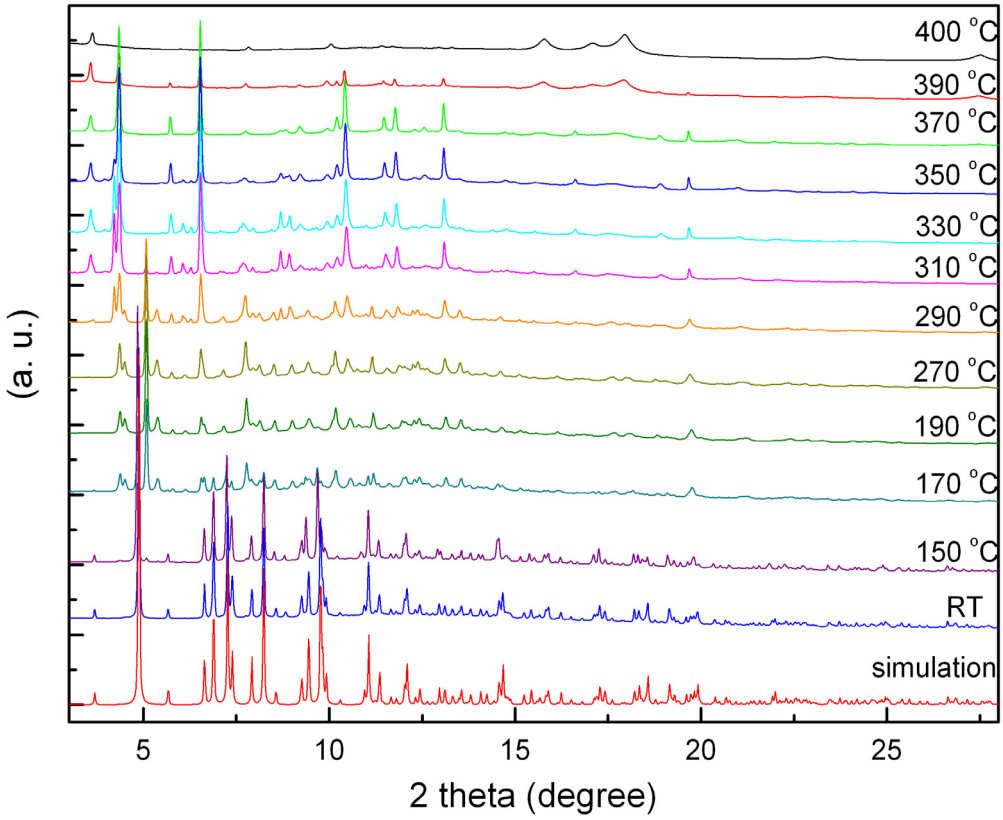
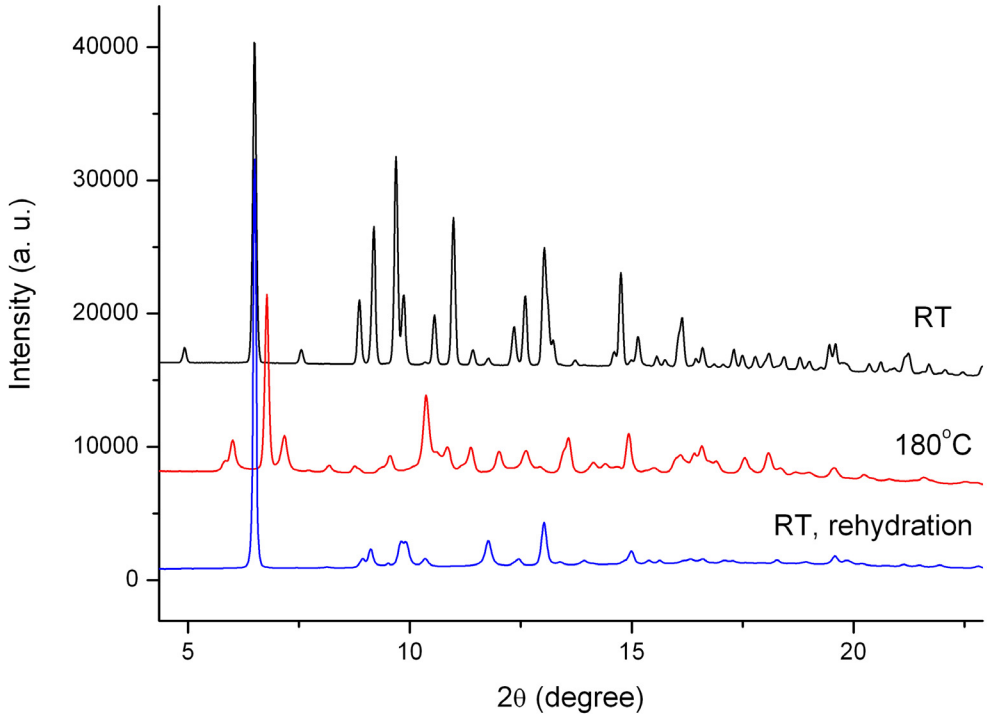


Figure S1

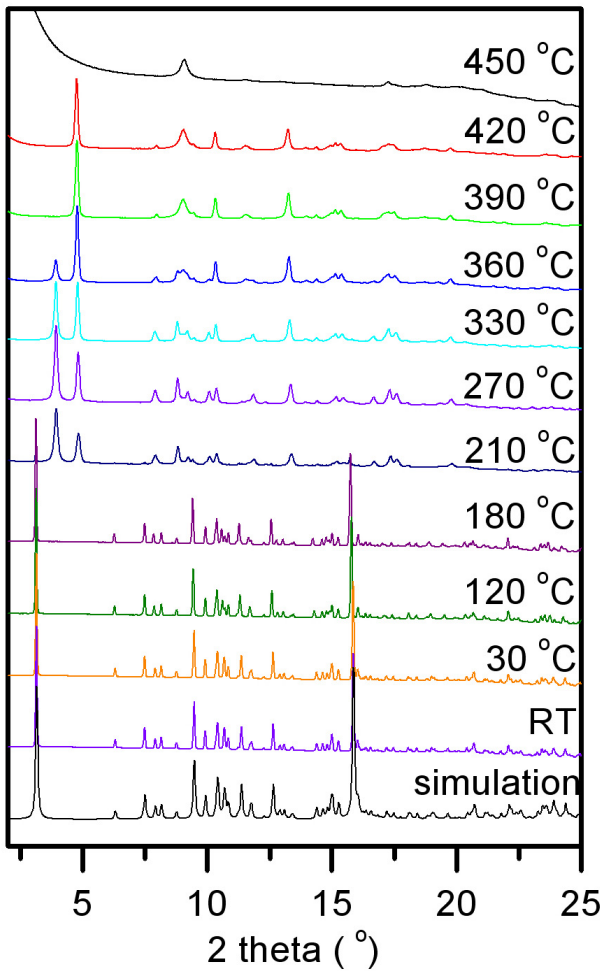


(a)

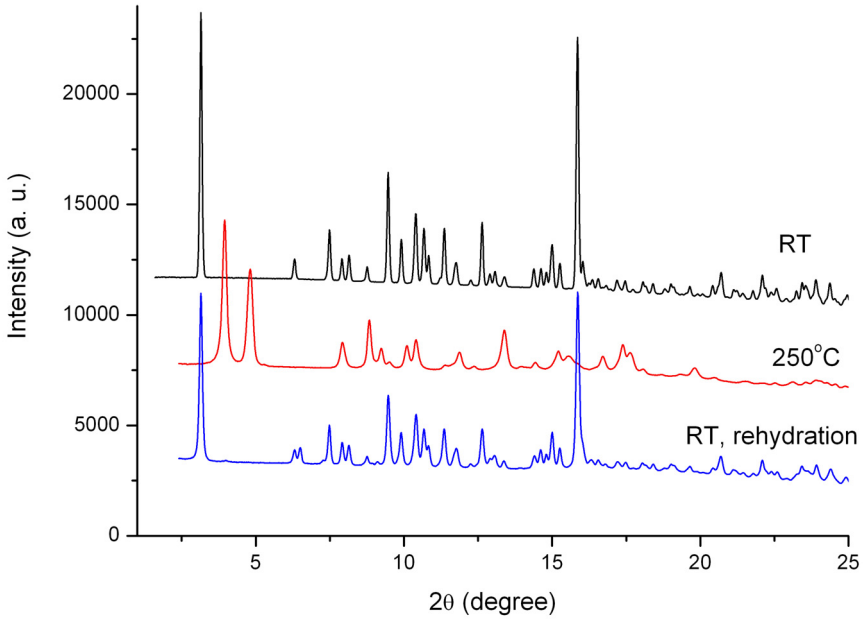


(b)

Figure S2



(a)



(b)

Figure S3