

Supplementary Information

Oxalic Acid, a Versatile Coformer for Multicomponent Forms with 9-Ethyladenine

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EXPERIMENTAL METHODS

Solution syntheses

Synthesis of 9ETADE-OXA (1:1) salt (1). A mixture of 9ETADE (75.05 mg, 0.46 mmol) and oxalic acid dihydrate (57.97 mg, 0.46 mmol) was suspended in MilliQ water at room temperature for two days. After that, the solid was filtered and air-dried. Single crystals were obtained by slow evaporation of an aqueous solution.

Synthesis of 9ETADE-OXA (1:1) hydrated salt (2). A mixture of 9ETADE (75.06 mg, 0.46 mmol) and oxalic acid dihydrate (57.93 mg, 0.46 mmol) was suspended in acetonitrile at room temperature for two days. After that, the solid was filtered and air-dried.

Synthesis of 9ETADE-OXA (2:1) salt (3). A mixture of 9ETADE (100.02 mg, 0.61 mmol) and oxalic acid dihydrate (38.63 mg, 0.31 mmol) was suspended in MilliQ water at room temperature for two days. After that, the solid was filtered and air-dried. Single crystals were obtained by slow evaporation of a solution in water-acetonitrile (1:1).

Synthesis of 9ETADE-OXA (2:1) hydrated salt (4). A mixture of 9ETADE (100.11 mg, 0.61 mmol) and oxalic acid dihydrate (38.72 mg, 0.31 mmol) was suspended in acetonitrile at room temperature for two days. After that, the solid was filtered and air-dried.

Grinding Screening

Synthesis of 9ETADE-OXA (1:1) hydrated salt (5). A mixture of 9ETADE (100.37 mg, 0.62 mmol) and oxalic acid dihydrate (77.68 mg, 0.62 mmol) and two drops of MilliQ water were ground together for 30 min at 30 Hz.

Synthesis of 9ETADE-OXA (1:1) hydrated salt (6). A mixture of 9ETADE (100.19 mg, 0.61 mmol) and oxalic acid dihydrate (77.39 mg, 0.61 mmol) and two drops of methanol were ground together for 30 min at 30 Hz.

Synthesis of 9ETADE-OXA (2:1) hydrated salt (4). A mixture of 9ETADE (100.23 mg, 0.61 mmol) and oxalic acid dihydrate (38.7 mg, 0.31 mmol) and two drops of MilliQ water were ground together for 30 min at 30 Hz.

Synthesis of 9ETADE-OXA (2:1) hydrated salt (4). A mixture of 9ETADE (100.02 mg, 0.61 mmol) and oxalic acid dihydrate (38.61 mg, 0.31 mmol) and two drops of methanol were ground together for 30 min at 30 Hz.

Figure S1. TGA-DSC traces of 9-ethyladenine-oxalic acid (1:1) salt (**1**).

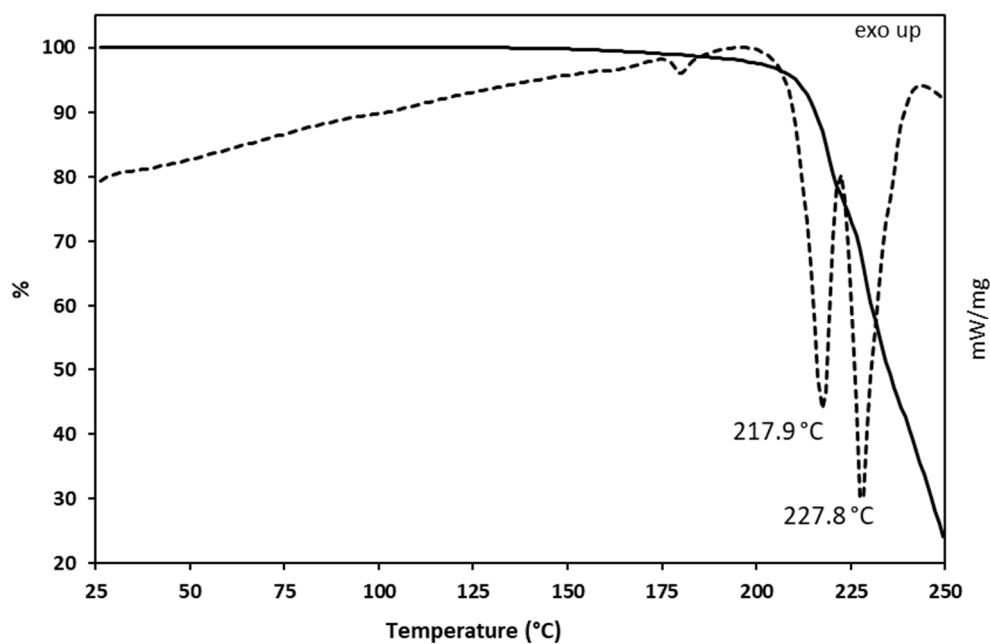


Figure S2. TGA-DSC traces of 9-ethyladenine-oxalic acid (2:1) salt (**3**).

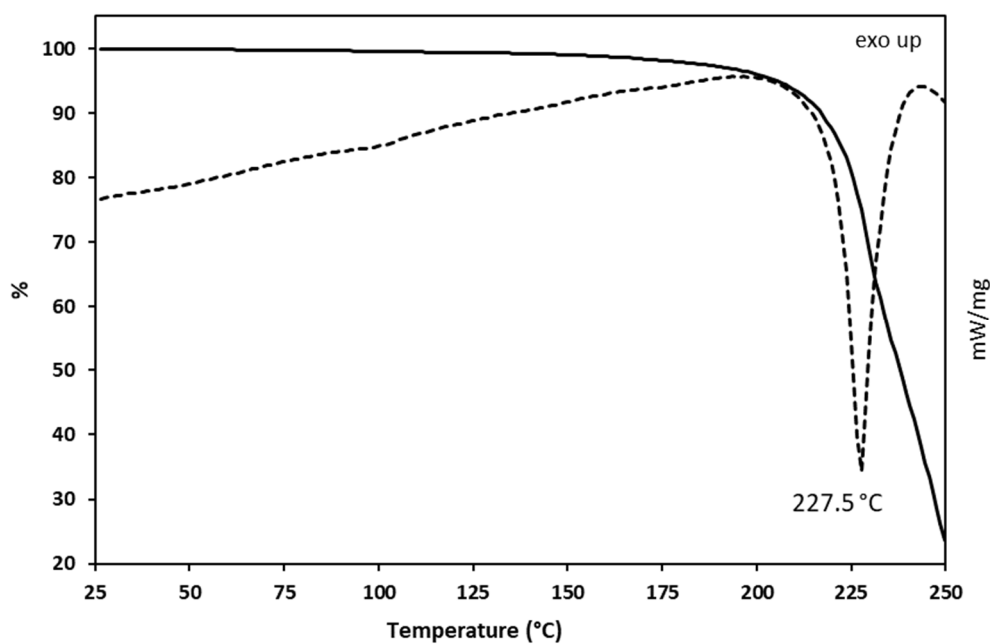


Figure S3. TGA-DSC traces of 9-ethyladenine-oxalic acid hydrated (1:1) salt (**2**).

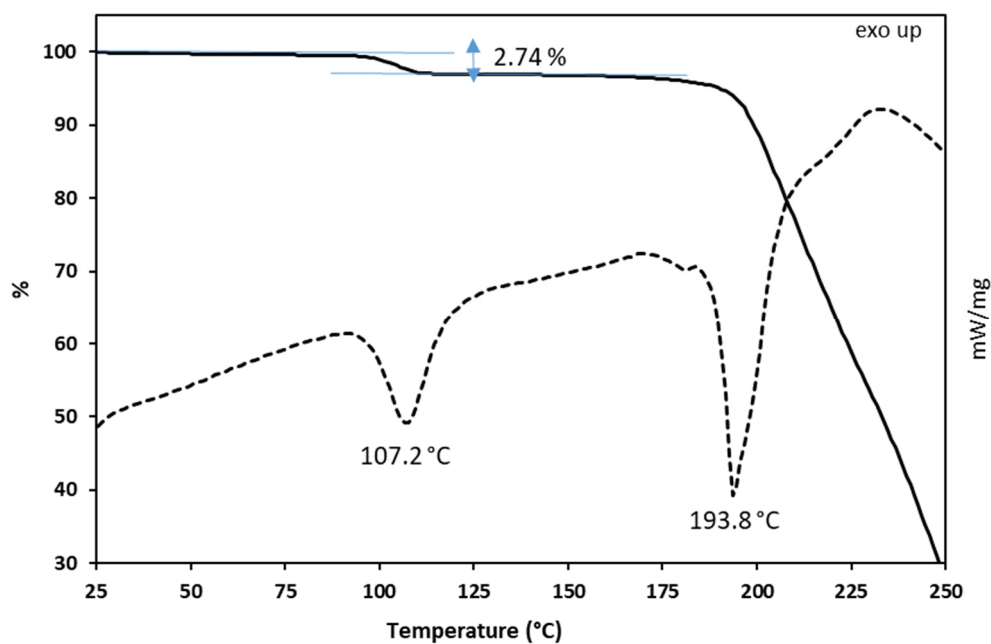


Figure S4. TGA-DSC traces of 9-ethyladenine-oxalic acid hydrated (2:1) salt (**4**).

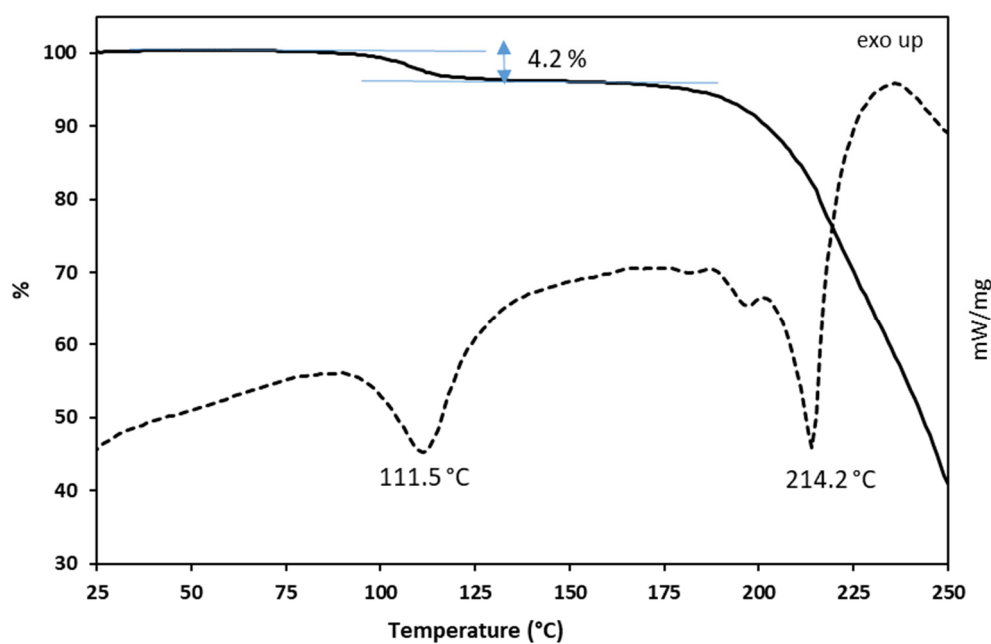


Figure S5. TGA-DSC traces of 9-ethyladenine-oxalic acid hydrated (1:1) salt (**5**).

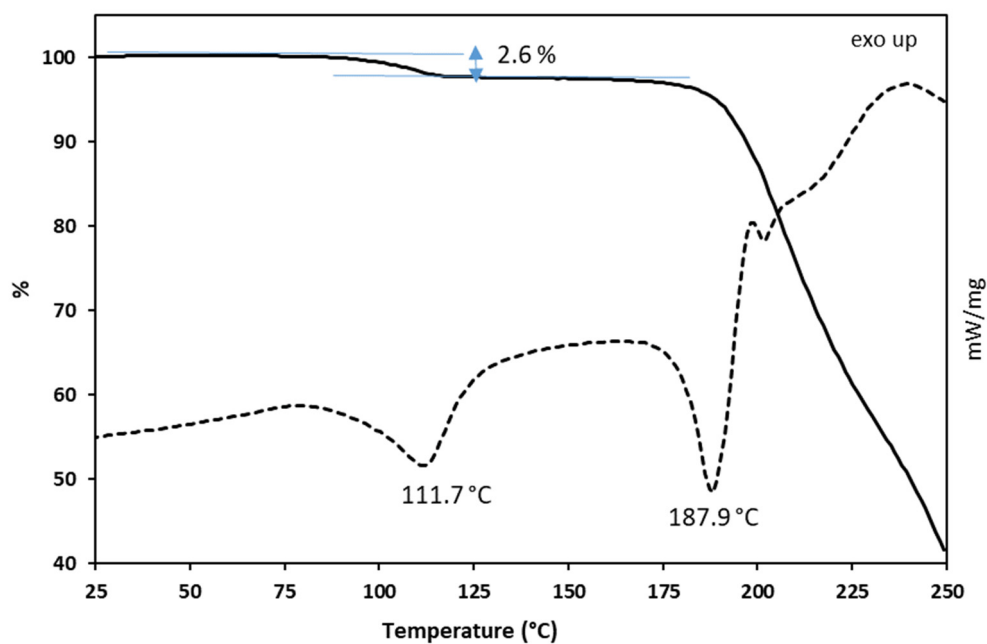
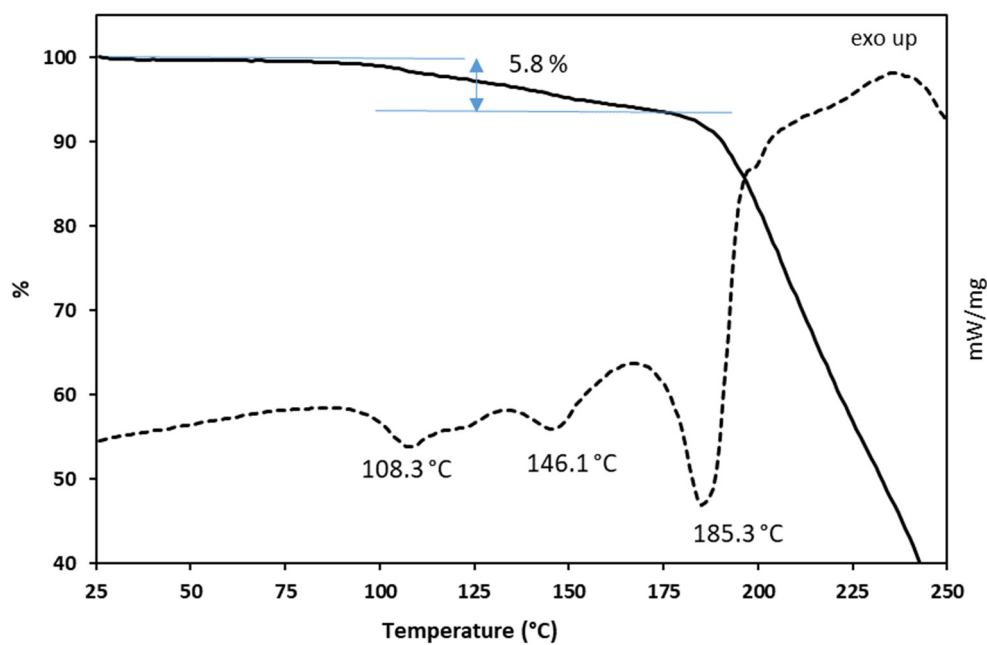
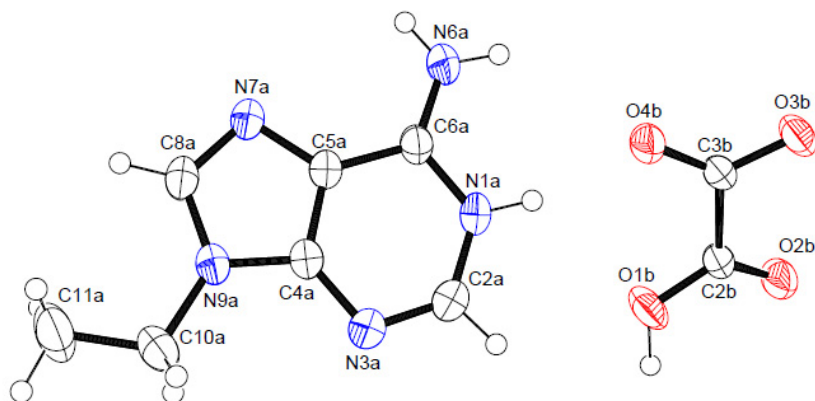


Figure S6. TGA-DSC traces of 9-ethyladenine-oxalic acid hydrated (1:1) salt (**6**).



a)



b)

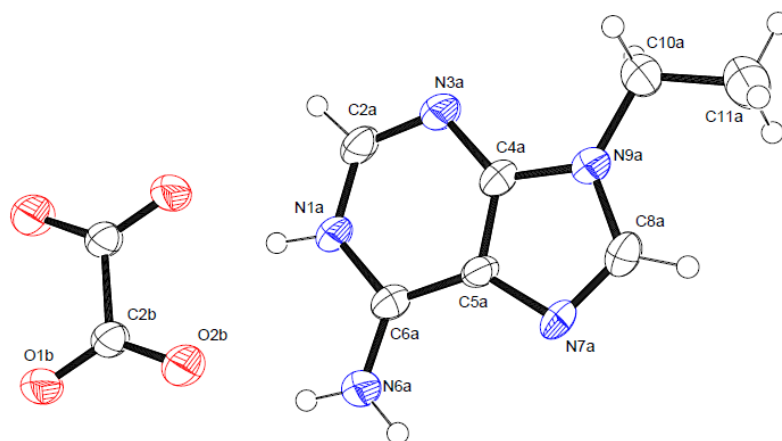


Table S1. Hydrogen bond details for 9-ethyladenine-oxalic acid (1:1) salt (**1**).

D–H···A	D–H (Å)	H···A (Å)	D···A (Å)	<(DHA) (°)	Symmetry code
N(1A)–H(1A)···O(1B)	0.86(2)	2.47(2)	3.0412(17)	124.0(16)	
N(1A)–H(1A)···O(4B)	0.86(2)	1.92(2)	2.7449(16)	158.7(18)	
C(2A)–H(2A)···O(1B)	0.93	2.56	3.1379(19)	120.3	
N(6A)–H(6A1)···O(2B)	0.86	2.23	2.9438(17)	139.9	-x,-y+1,-z+2
N(6A)–H(6A1)···O(3B)	0.86	2.41	3.0271(18)	128.7	-x,-y+1,-z+2
N(6A)–H(6A2)···N(7A)	0.86	2.12	2.9469(18)	161.6	-x,-y+2,-z+1
C(8A)–H(8A)···O(2B)	0.93	2.25	3.1197(18)	155.5	x,y+1,z-1
C(10A)–H(10A)···O(4B)	0.97	2.66	3.410(2)	134.3	-x+1,-y+1,-z+1
O(1B)–H(1B)···O(3B)	1.06(2)	1.41(2)	2.4728(15)	177(2)	x+1,y,z

Table S2. Hydrogen bond details for 9-ethyladenine-oxalic acid (2:1) salt (**3**).

D–H···A	D–H (Å)	H···A (Å)	D···A (Å)	<(DHA) (°)	Symmetry code
N(1A)–H(1)···O(1B)	0.91(3)	1.93(4)	2.746(3)	148(3)	-x+2,-y,-z+1
N(1A)–H(1)···O(2B)	0.91(3)	2.28(3)	2.968(3)	133(3)	
C(2A)–H(2A)···N(7A)	0.93	2.40	3.224(4)	148.0	x,y-1,z
N(6A)–H(6A1)···O(2B)	0.86	1.95	2.743(3)	152.7	
N(6A)–H(6A2)···O(1B)	0.86	2.06	2.873(3)	156.4	-x+2,-y+1,-z+1
C(11A)–H(11A)···O(2B)	0.96	2.64	3.576(5)	163.8	-x+1,-y+1,-z+1

Figure S8. Diffractograms of initial and undissolved solids for compounds 9ETADE-OXA (2:1) (**3**), 9ETADE-OXA (1:1) (**1**) and 9ETADE-SUC (1:1) salt.

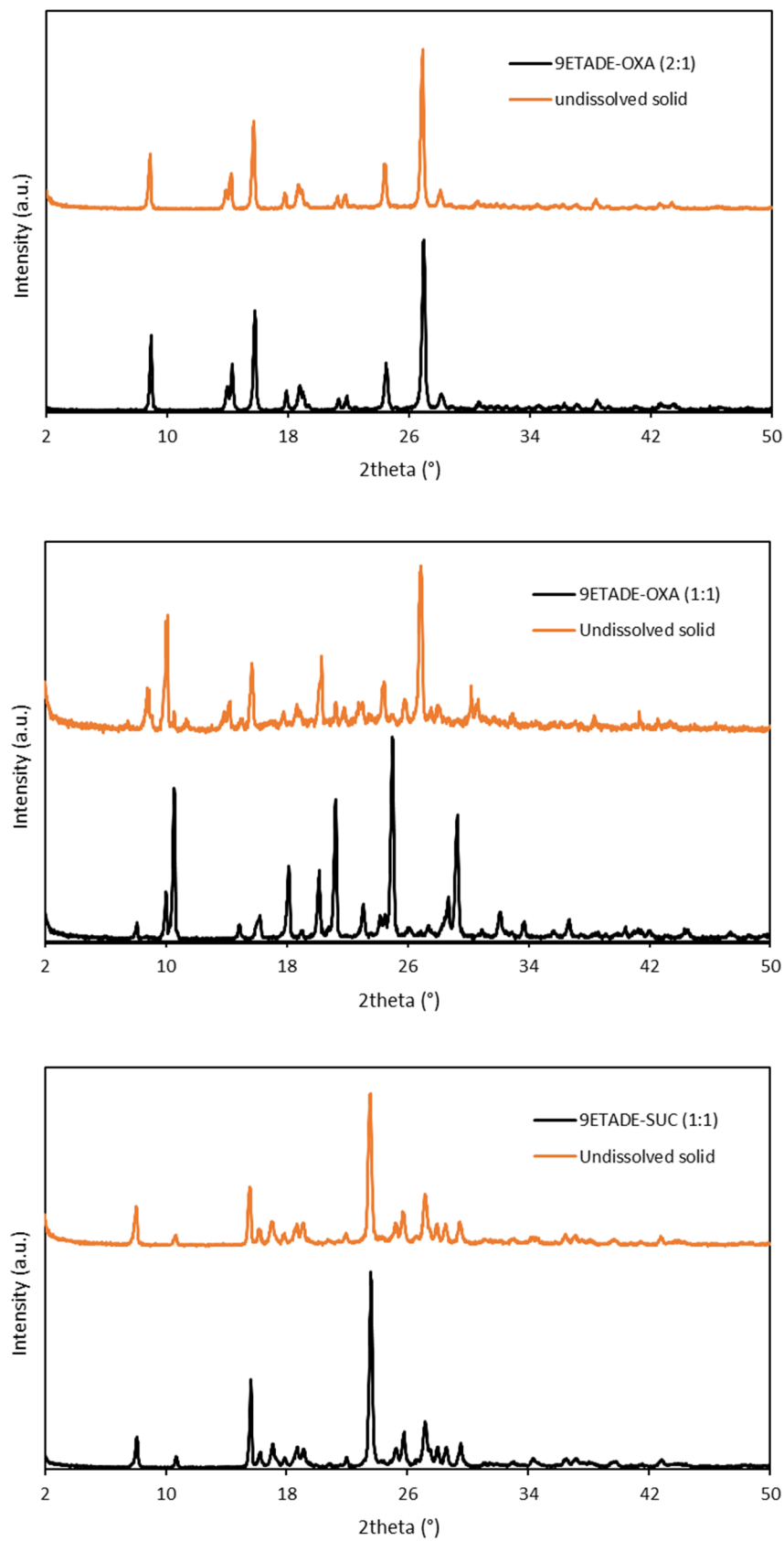


Figure S9. PXRD patterns of the anhydrous 9ETADE-OXA salts under different temperature and relative humidity conditions.

