ELECTRONIC SUPPLEMENTARY INFORMATION

Water-induced phase transformation of a Cu^{II}-coordination framework with pyridine-2,5-dicarboxylate and di-2-pyridyl ketone: synchrotron radiation analysis

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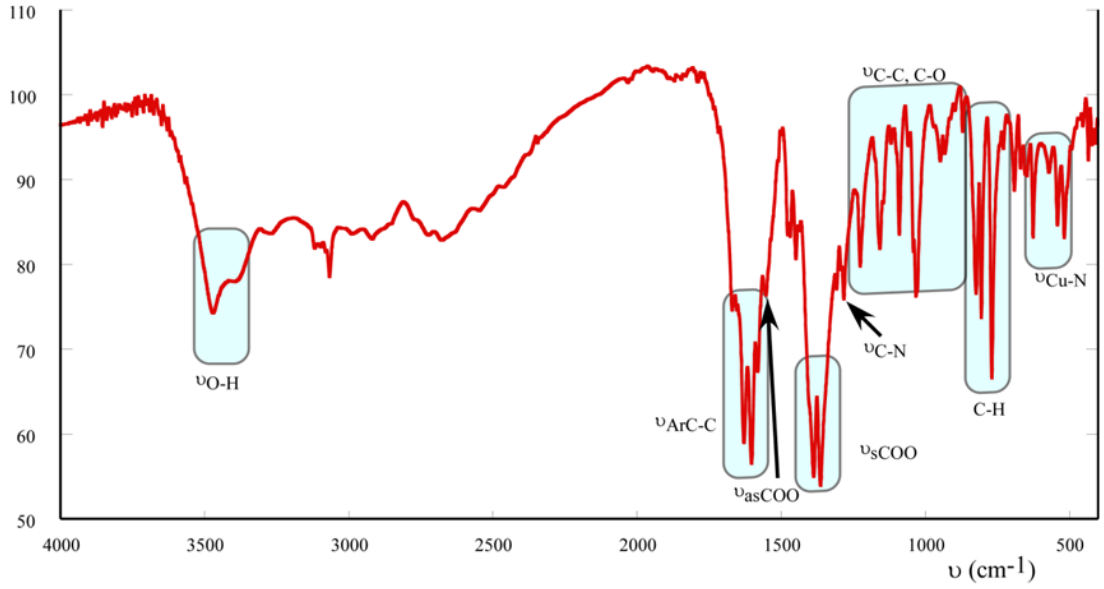

Figure S1. IR spectra for compound **1** ($C_{18}H_{15}N_3O_7Cu$). The following bands (cm^{-1}) are marked 3470 (OH), 1656 and 1604 (aroC-C), 1557 (asCOO), 1390, 1364 and 1453 (sCOO), 1282 (C-N), 826, 774 and 693 (C-H) and 548-514 (Cu-N)

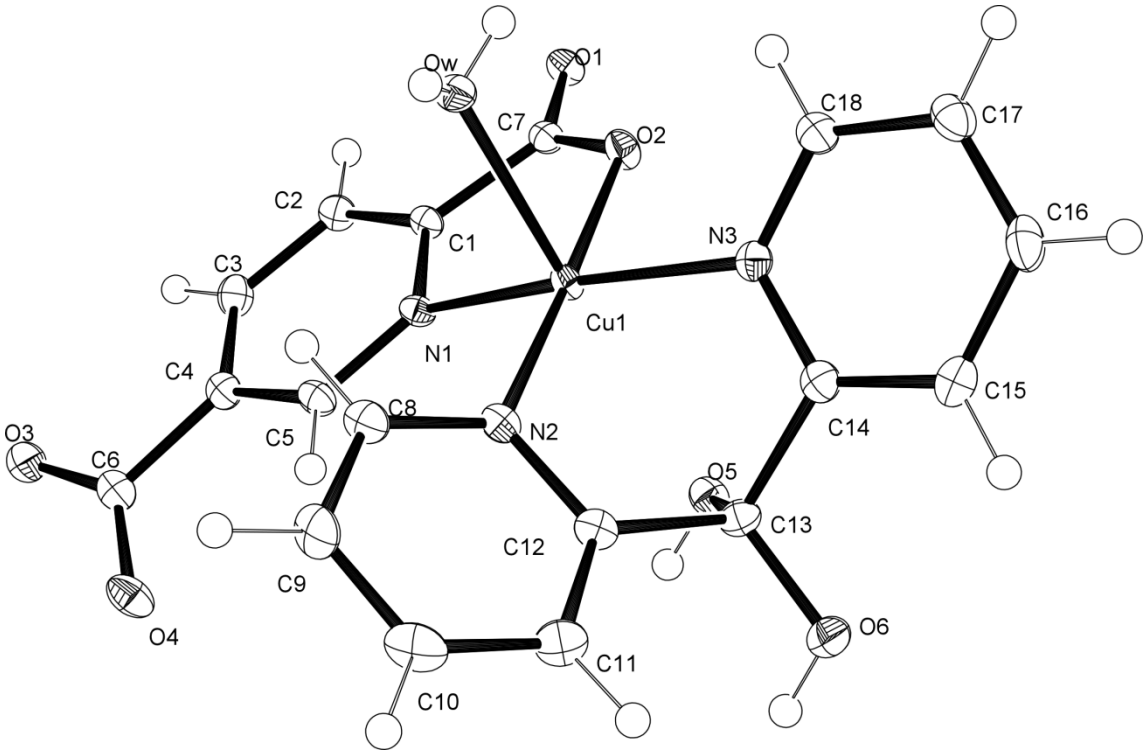

Figure S2. Thermal ellipsoid plot (50% of probability) for compound **1.**

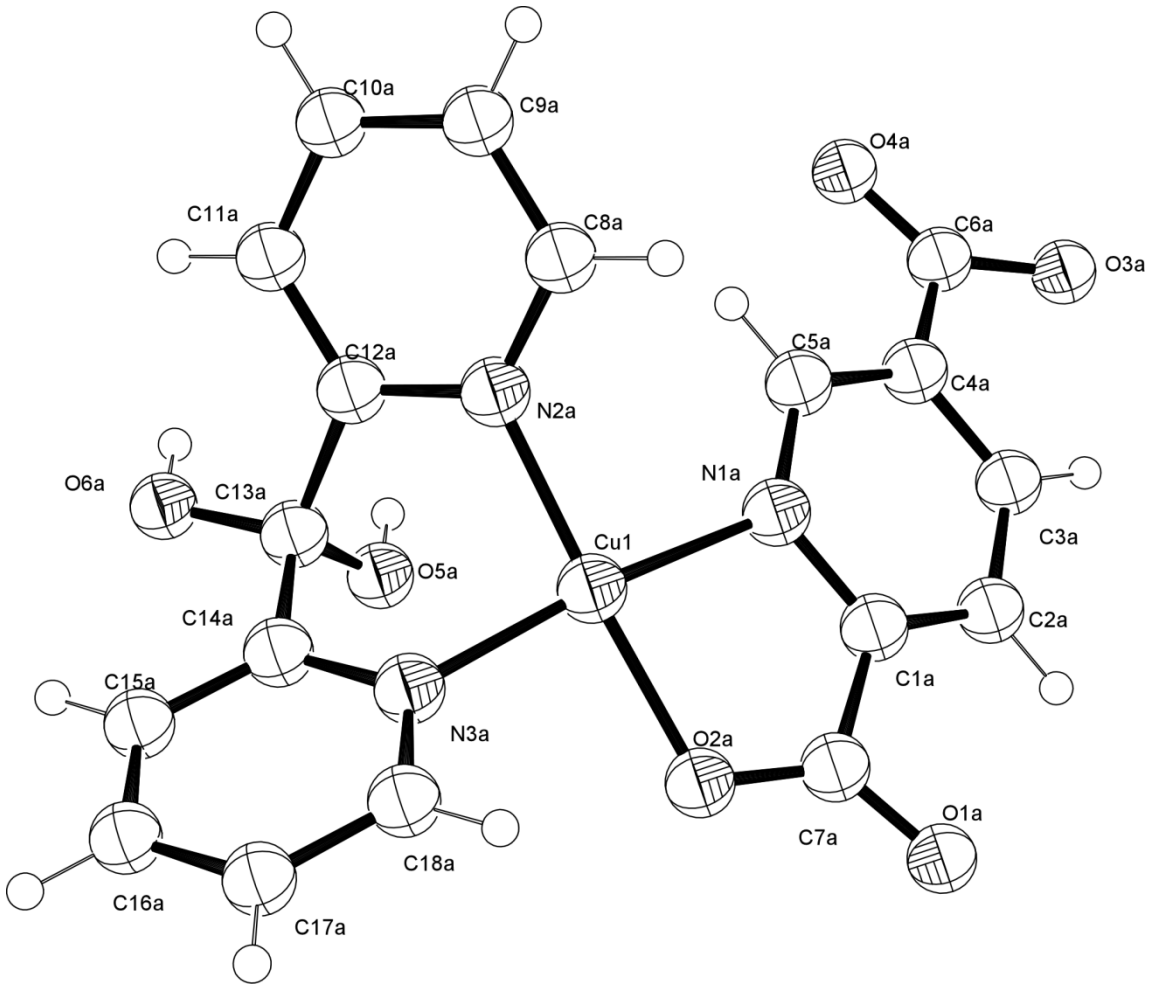

Figure S3. Isotropic ADPs for compound **2**.

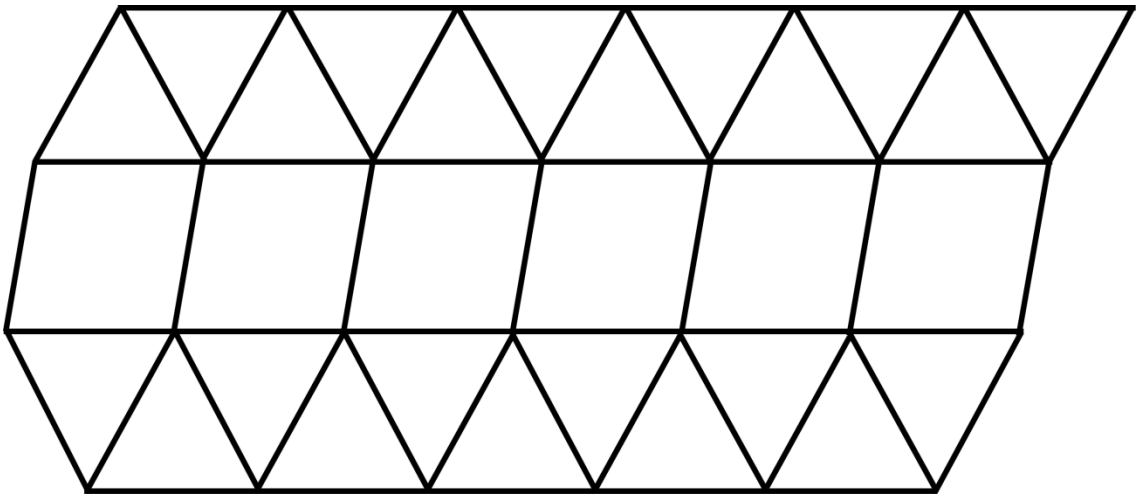

Figure S4. Topological analysis for the 2D supramolecular layer of compound **1.**

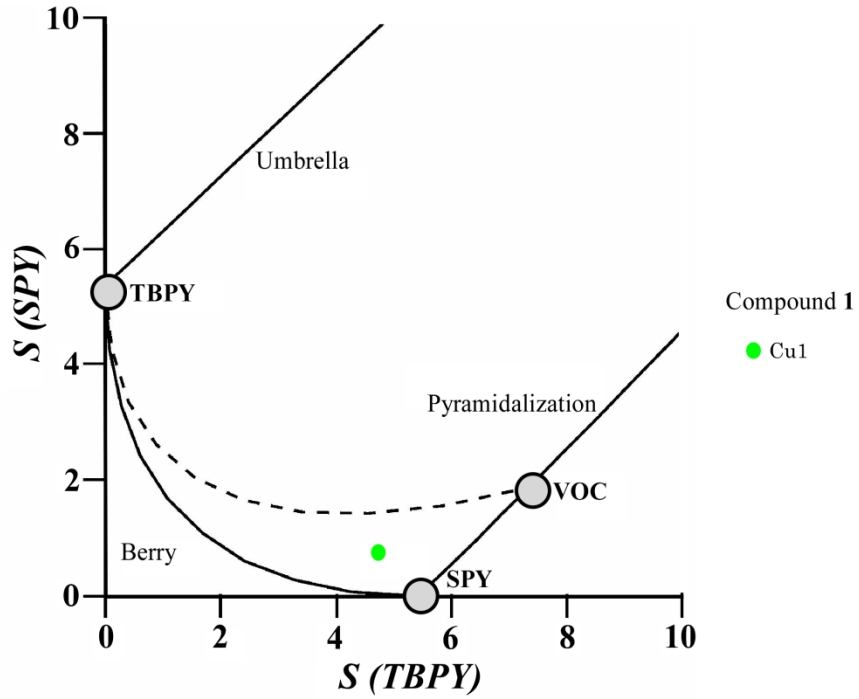

Figure S5. Distortion modes diagram of a pyramidal based squared coordination environment for compound **1**, Cu1 is colored in green.

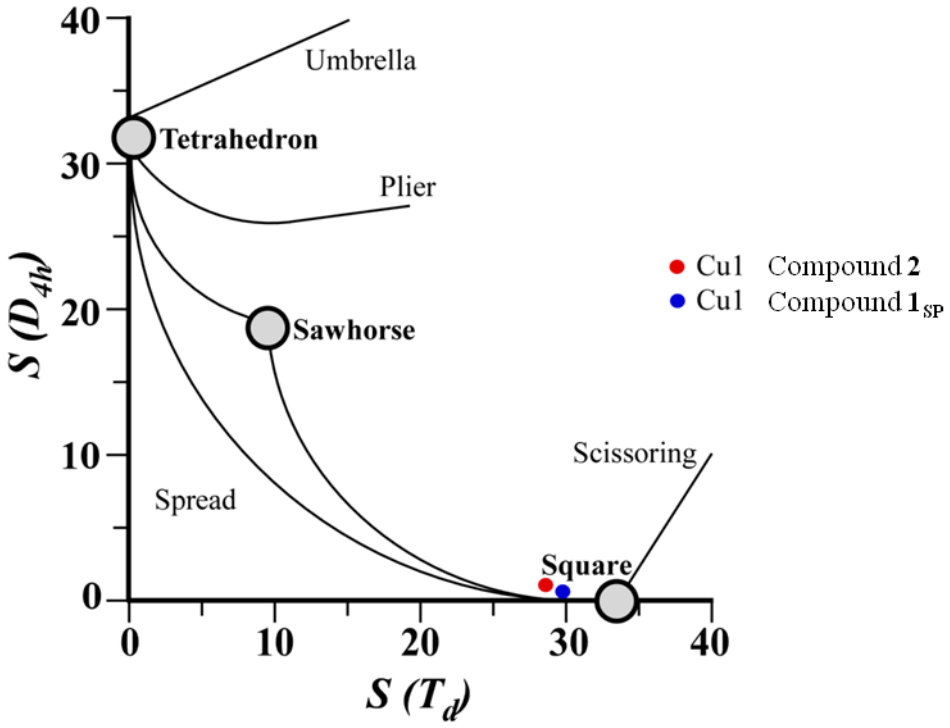

Figure S6. Distortion modes diagram of a pyramidal based squared coordination environment for compound **2** and compound **1** after eliminate the water molecule (**1**$_{SP}$).

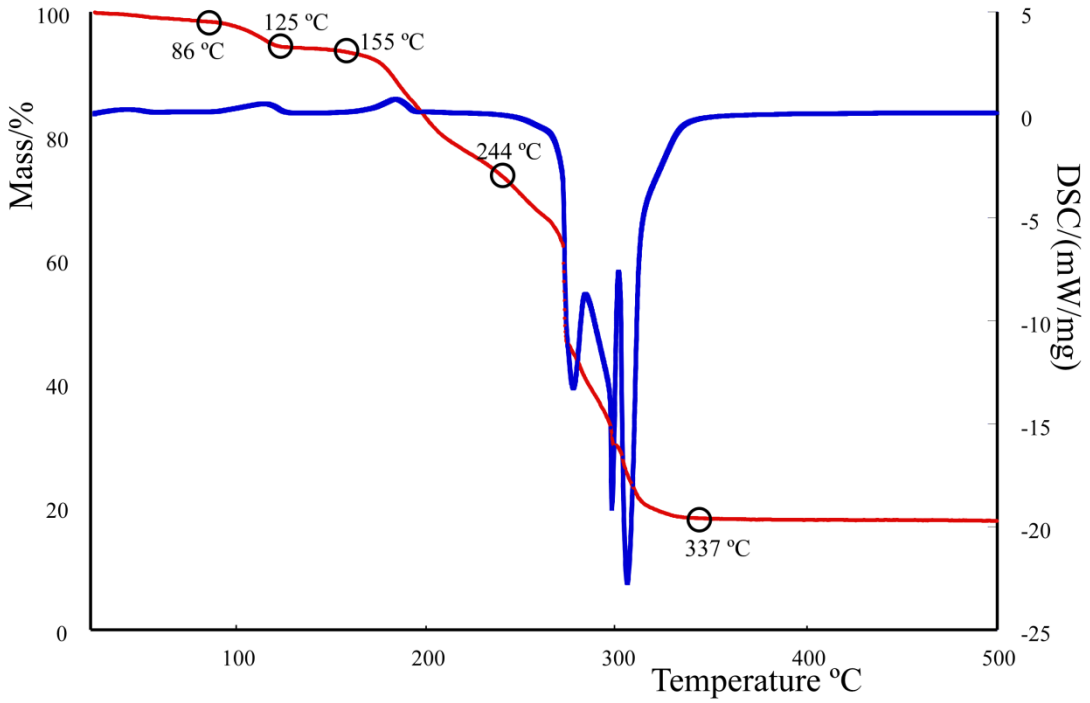

Figure S7. Thermogravimetric analysis of compound **1.**

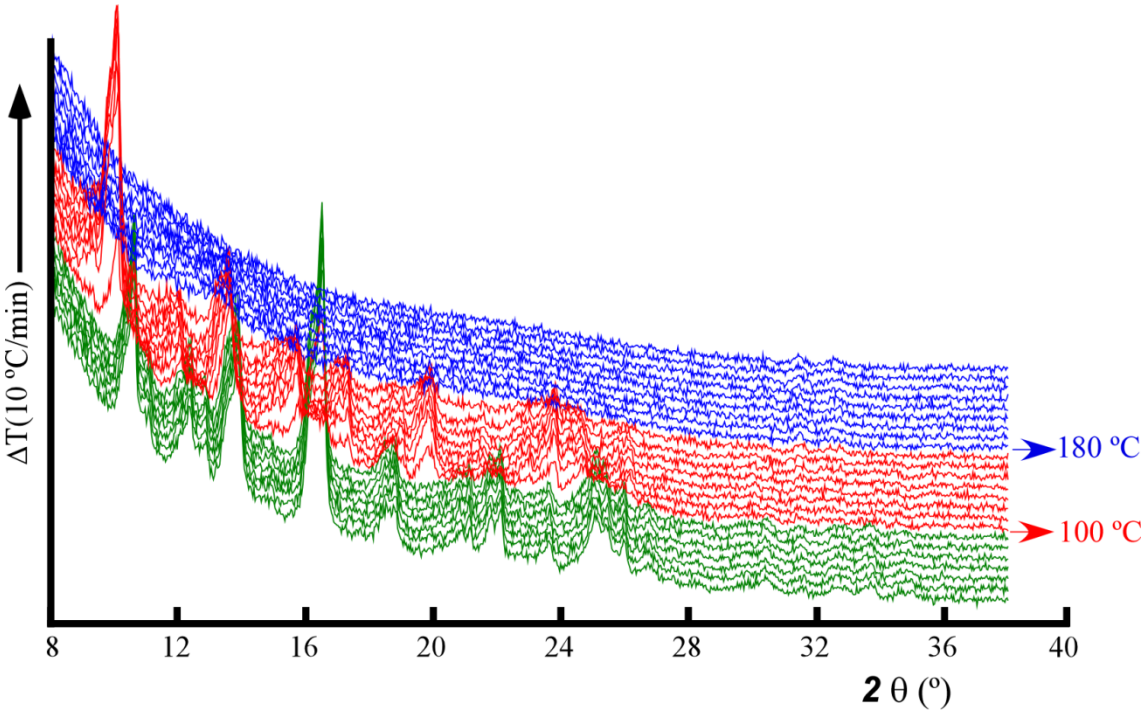

Figure S8. Thermodiffractogram for compound **1** up to 300 ºC in 10 ºC steps.

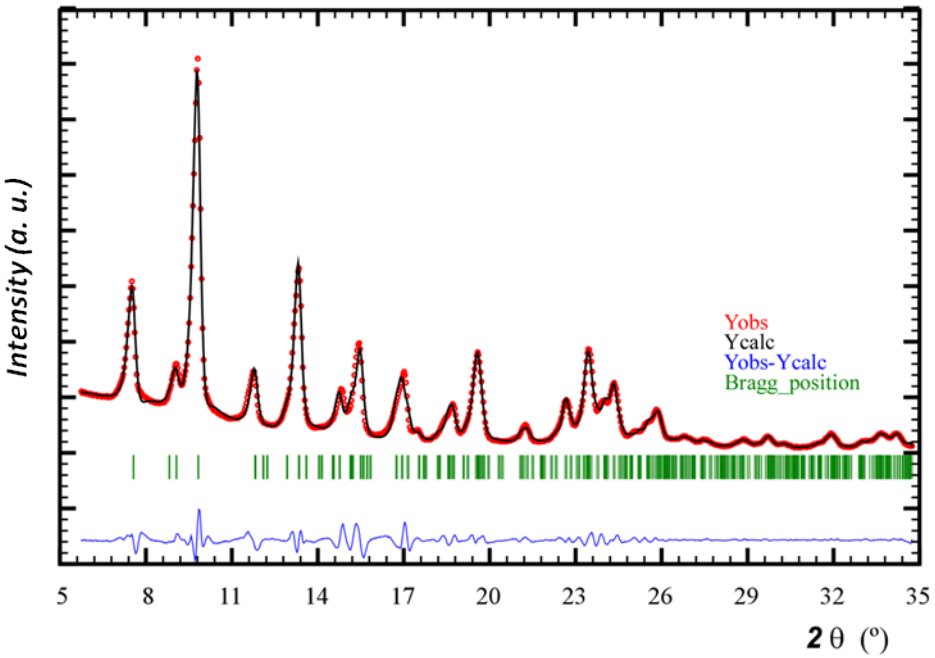

Figure S9. Pattern-Mattching of compound **2** from a pattern obtained in the TDX at 130 °C with CuKα radiation.

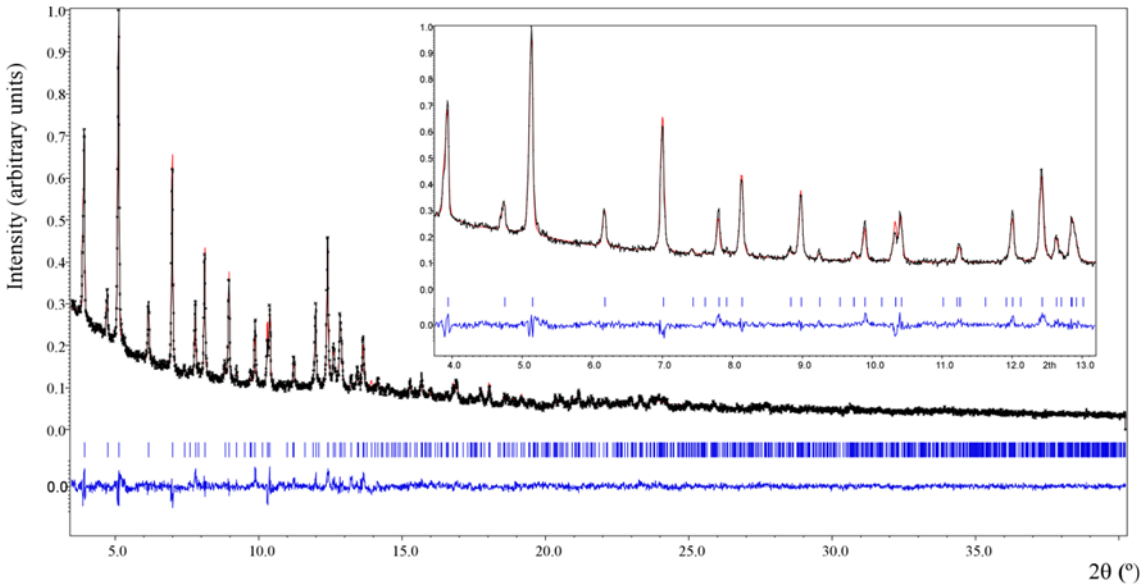

Figure S10. Structural refinement of compound **2** using a pattern obtained by synchrotron radiation at 130 °C.

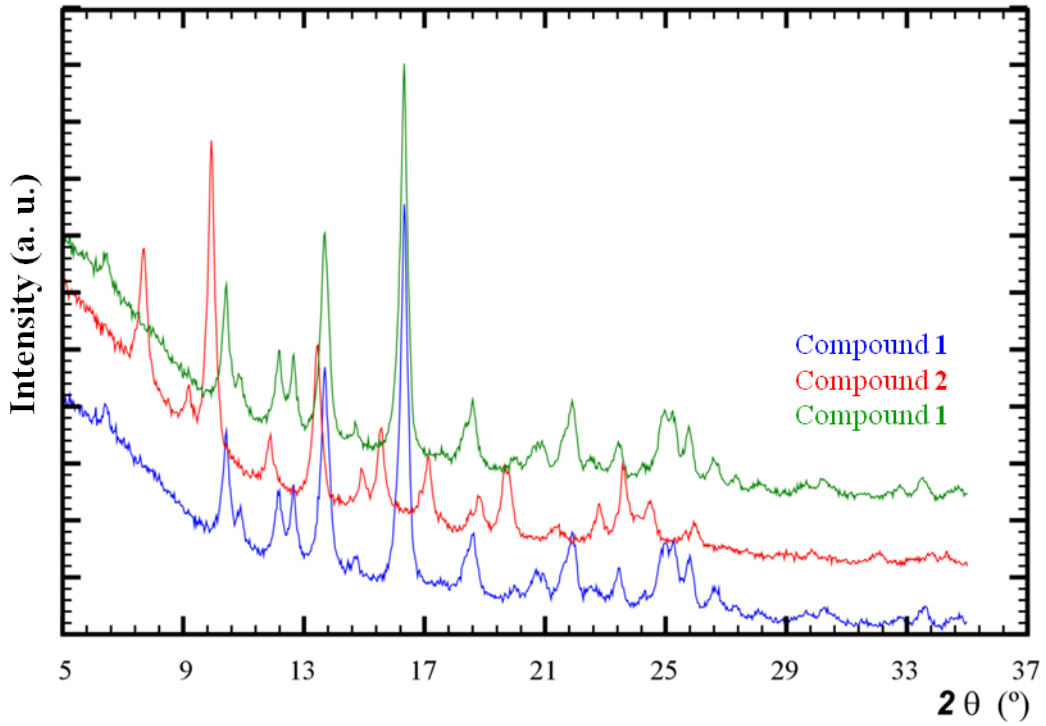

Figure S11. Reversible structural transformation observed from compound **1** to-compound **2** to-compound **1.** The pattern colored in red was collected at 130 °C.

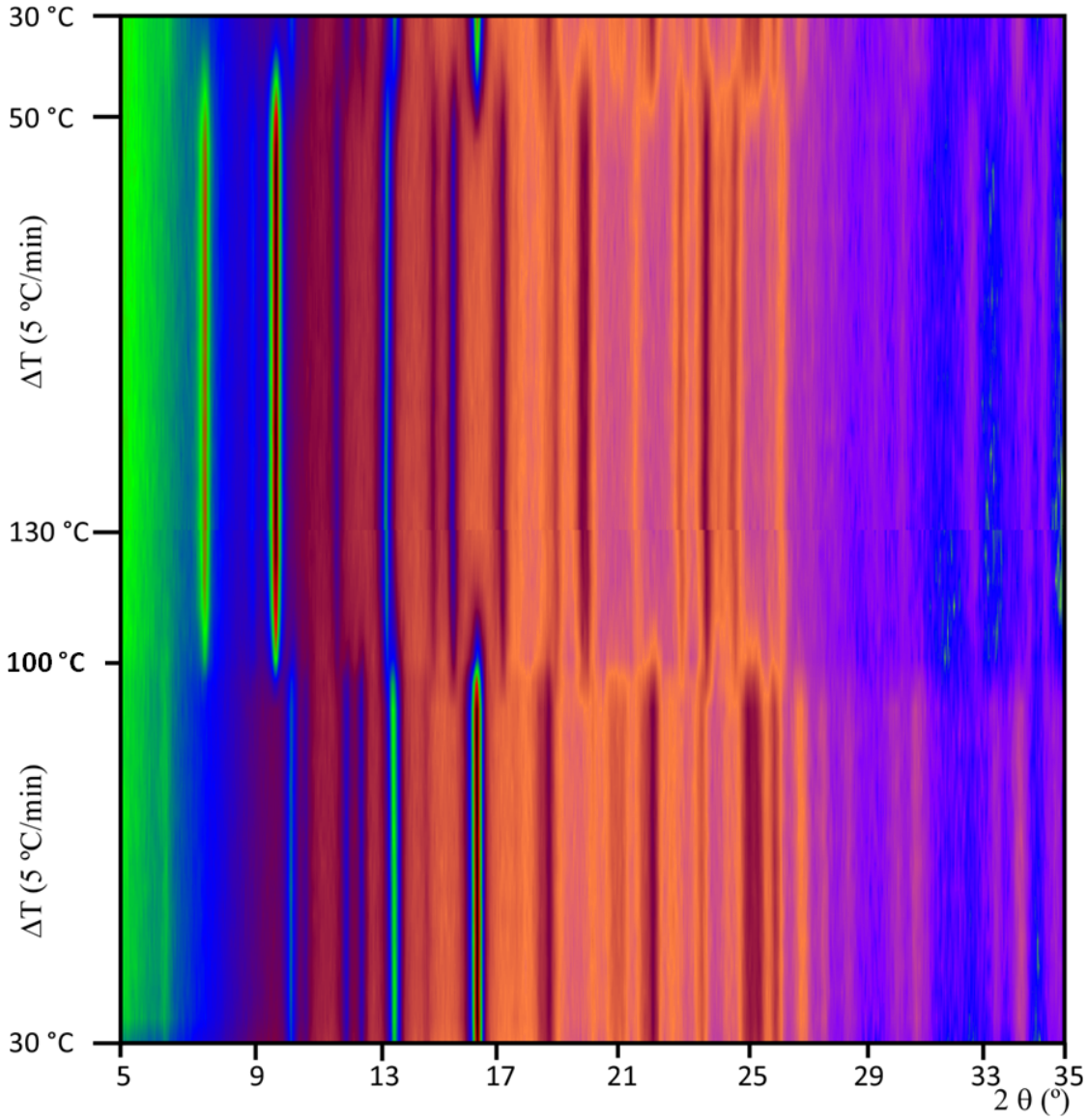

Figure S12. TDX from 30 to 130 °C, and 130 to 30 °C, confirming the reversibility of the structural transformation.

Table S1. Selected bond angles (º) and distances (Å) for compound **1** (distances in bold).

Cu	N1	N2	N3	O2	OW
OW	94.83(7)	91.88(8)	95.07(7)	85.92(7)	**2.322(2)**
O2	82.48(8)	177.78(8)	90.59(8)	**1.949(2)**	
N3	167.47(9)	89.83(8)	**2.008(2)**		
N2	97.50(8)	**2.001(2)**			
N1	**2.021(2)**				

Table S2. Selected bond angles (º) and distances (Å) for compound **2** (distances in bold).

Cu1	N1a	N2a	N3a	O2a
O2a	83.6(8)	175.0(9)	92.8(9)	**1.96(2)**
N3a	170.7(9)	92.1(9)	**1.92(2)**	
N2a	91.8(7)	**2.00(2)**		
N1a	**2.03(2)**			

Table S3. Hydrogen bonds for compound **1**.

O-H	A(O)	O-H(Å)	H···A (Å)	O···A (Å)	O-H···A (°)
O(W)-H(2OW)	O(1) 1+x, y, z	0.818(11)	2.066(12)	2.877(3)	171(3)
O(W)-H(1OW)	O(1) 1/2+x, y, 1/2-z	0.814(19)	2.032(19)	2.840(2)	172(3)
O(5)-H(5O)	O(4) –x, -y, -z	0.84	1.80	2.606(2)	161
O(6)-H(6)	O(3) –x, -y, -z	0.84	1.81	2.645(2)	170

Table S4. Hydrogen bonds for compound **2**.

O-H	A(O)	O-H(Å)	H···A (Å)	O···A (Å)	O-H···A (°)
O(5a)-H(1o5)	O(4a) –x, -y, -z	0.84(2)	1.83(3)	2.59(3)	150(2)
O(6a)-H(1o6)	O(3a) –x, -y, -z	0.84(3)	2.09(3)	2.90(3)	160(4)

Table S5. Bond distances (Å) and angles (º) for compound **1.**

Distances			
C(1)-C(2)	1.384(3)	**N(1)-C(5)**	1.341(3)
C(1)-C(7)	1.515(3)	**N(1)-C(1)**	1.348(3)
C(2)-C(3)	1.391(3)	**N(2)-C(8)**	1.336(3)
C(2)-H(2)	0.95	**N(2)-C(12)**	1.353(3)
C(3)-H(3)	0.95	**N(3)-C(18)**	1.341(4)
C(4)-C(3)	1.387(4)	**N(3)-C(14)**	1.343(3)
C(4)-C(6)	1.515(3)	**O(1)-C(7)**	1.232(3)
C(5)-C(4)	1.393(4)	**O(2)-C(7)**	1.272(3)
C(5)-H(5C)	0.95	**O(3)-C(6)**	1.256(3)
C(8)-C(9)	1.385(4)	**O(4)-C(6)**	1.257(3)
C(8)-H(8)	0.95	**O(5)-C(13)**	1.419(3)
C(9)-H(9)	0.95	**O(5)-H(5O)**	0.84
C(10)-C(9)	1.380(4)	**O(6)-C(13)**	1.393(3)
C(10)-H(10)	0.95	**O(6)-H(6)**	0.84
C(11)-C(12)	1.375(4)	**OW-H(2OW)**	0.82(1)
C(11)-C(10)	1.387(4)	**OW-H(1OW)**	0.81(1)
C(11)-H(11)	0.95	**Cu(1)-O(2)**	1.949(2)
C(13)-C(14)	1.520(3)	**Cu(1)-N(2)**	2.001(2)
C(13)-C(12)	1.538(3)	**Cu(1)-N(3)**	2.008(2)
C(14)-C(15)	1.376(4)	**Cu(1)-N(1)**	2.021(2)
C(15)-H(15)	0.95	**Cu(1)-OW**	2.322(2)
Angles			
N(1)-C(1)-C(2)	123.0(2)	**O(6)-C(13)-O(5)**	113.2(2)
N(1)-C(1)-C(7)	114.5(2)	**O(6)-C(13)-C(14)**	108.6(2)
C(2)-C(1)-C(7)	122.5(2)	**O(5)-C(13)-C(14)**	105.5(2)
C(1)-C(2)-C(3)	118.3(2)	**O(6)-C(13)-C(12)**	111.4(2)
C(1)-C(2)-H(2)	120.9	**O(5)-C(13)-C(12)**	109.2(2)
C(3)-C(2)-H(2)	120.9	**C(14)-C(13)-C(12)**	108.8(2)
C(4)-C(3)-C(2)	119.1(2)	**N(3)-C(14)-C(15)**	122.6(2)
C(4)-C(3)-H(3)	120.4	**N(3)-C(14)-C(13)**	113.9(2)
C(2)-C(3)-H(3)	120.4	**C(15)-C(14)-C(13)**	123.5(2)
C(3)-C(4)-C(5)	118.9(2)	**C(14)-C(15)-C(16)**	118.0(2)
C(3)-C(4)-C(6)	120.9(2)	**C(14)-C(15)-H(15)**	121.0
C(5)-C(4)-C(6)	120.1(2)	**C(16)-C(15)-H(15)**	121.0
N(1)-C(5)-C(4)	122.2(2)	**C(17)-C(16)-C(15)**	119.5(2)
N(1)-C(5)-H(5C)	118.9	**C(17)-C(16)-H(16)**	120.2
C(4)-C(5)-H(5C)	118.9	**C(15)-C(16)-H(16)**	120.2
O(3)-C(6)-O(4)	127.3(2)	**C(16)-C(17)-C(18)**	119.0(2)
O(3)-C(6)-C(4)	116.6(2)	**C(16)-C(17)-H(17)**	120.5
O(4)-C(6)-C(4)	116.1(2)	**C(18)-C(17)-H(17)**	120.5
O(1)-C(7)-O(2)	125.3(2)	**N(3)-C(18)-C(17)**	121.5(2)
O(1)-C(7)-C(1)	119.6(2)	**N(3)-C(18)-H(18)**	119.2
O(2)-C(7)-C(1)	115.1(2)	**C(17)-C(18)-H(18)**	119.2
N(2)-C(8)-C(9)	121.5(2)	**O(2)-Cu(1)-N(2)**	177.78(8)
N(2)-C(8)-H(8)	119.2	**O(2)-Cu(1)-N(3)**	90.59(8)
C(9)-C(8)-H(8)	119.2	**N(2)-Cu(1)-N(3)**	89.83(8)
C(10)-C(9)-C(8)	119.2(2)	**O(2)-Cu(1)-N(1)**	82.48(8)
C(10)-C(9)-H(9)	120.4	**N(2)-Cu(1)-N(1)**	97.50(8)
C(8)-C(9)-H(9)	120.4	**N(3)-Cu(1)-N(1)**	167.47(8)
C(9)-C(10)-C(11)	119.1(2)	**O(2)-Cu(1)-OW**	85.92(7)
C(9)-C(10)-H(10)	120.5	**N(2)-Cu(1)-OW**	91.88(8)
C(12)-C(11)-C(10)	119.1(3)	**N(3)-Cu(1)-OW**	95.07(7)
C(12)-C(11)-H(11)	120.4	**N(1)-Cu(1)-OW**	94.83(7)
C(10)-C(11)-H(11)	120.4	**C(5)-N(1)-C(1)**	118.3(2)
N(2)-C(12)-C(11)	121.5(2)	**C(5)-N(1)-Cu(1)**	130.6(2)
N(2)-C(12)-C(13)	114.5(2)	**C(1)-N(1)-Cu(1)**	111.0(1)
C(11)-C(12)-C(13)	123.9(2)	**C(8)-N(2)-C(12)**	119.5(2)

Table S6. Fractional atomic coordinates and equivalent thermal factors for compound **1**.

Atoms	X	Y	Z	U_{iso}, Å^2
H(2)	-3709	-1854	1372	14
H(3)	-2936	-2285	617	16
H(5O)	-460	1418	866	17
H(5C)	736	-562	535	13
H(6)	1567	2507	765	23
H(8)	3800	-581	1035	16
H(9)	6143	-227	532	20
H(10)	6467	1061	318	22
H(11)	4468	1977	635	19
H(15)	2627	2875	1846	18
H(16)	2859	2786	2670	21
H(17)	2112	1633	3038	19
H(18)	1153	588	2587	14
H(2OW)	3603(17)	-760(30)	1954(13)	23
H(1OW)	2070(50)	-770(30)	2223(7)	23

$$U_{eq} = \frac{1}{3}\left[U_{11}\left(aa^*\right)^2 + U_{22}\left(bb^*\right)^2 + U_{33}\left(cc^*\right)^2 + 2U_{13}aca^*c^*\cos\beta\right]$$

Table S7. Anisotropic displacement parameters (A^2 x 10^3) for compound **1**.

Atoms	U11	U22	U33	U23	U13	U12
C(1)	5(1)	12(1)	8(1)	0(1)	2(1)	1(1)
C(2)	10(2)	13(1)	12(1)	0(1)	1(1)	-1(1)
C(3)	13(2)	12(1)	16(1)	-4(1)	-2(1)	-2(1)
C(4)	7(1)	15(1)	11(1)	-1(1)	-1(1)	3(1)
C(5)	9(2)	15(2)	10(1)	0(1)	2(1)	0(1)
C(6)	9(1)	19(2)	11(1)	-3(1)	-1(1)	1(1)
C(7)	8(1)	12(1)	8(1)	1(1)	-1(1)	3(1)
C(8)	10(2)	18(2)	13(1)	1(1)	1(1)	2(1)
C(9)	8(2)	22(2)	20(2)	-1(1)	4(1)	8(1)
C(10)	5(1)	31(2)	19(2)	5(1)	6(1)	-2(1)
C(11)	11(2)	17(2)	19(1)	3(1)	1(1)	-4(1)
C(12)	6(1)	14(1)	10(1)	0(1)	-2(1)	-3(1)
C(13)	10(2)	11(1)	12(1)	3(1)	-1(1)	1(1)
C(14)	9(1)	12(1)	12(1)	-1(1)	1(1)	1(1)
C(15)	16(2)	11(1)	19(2)	-1(1)	0(1)	0(1)
C(16)	19(2)	16(2)	17(2)	-8(1)	-6(1)	3(1)
C(17)	16(2)	20(2)	12(1)	-3(1)	-4(1)	5(1)
C(18)	9(2)	16(2)	11(1)	-1(1)	-3(1)	5(1)
Cu(1)	16(1)	19(1)	17(1)	-2(1)	2(1)	-2(1)
N(1)	6(1)	11(1)	7(1)	1(1)	1(1)	-1(1)
N(2)	6(1)	13(1)	8(1)	-1(1)	-1(1)	-2(1)
N(3)	6(1)	10(1)	11(1)	-1(1)	0(1)	2(1)
O(1)	6(1)	15(1)	10(1)	0(1)	3(1)	-2(1)
O(2)	11(1)	13(1)	10(1)	-3(1)	2(1)	-4(1)
O(3)	24(1)	15(1)	13(1)	-2(1)	-1(1)	0(1)
O(4)	13(1)	23(1)	12(1)	-3(1)	3(1)	-6(1)
O(5)	9(1)	15(1)	10(1)	-1(1)	-2(1)	0(1)
O(6)	22(1)	10(1)	14(1)	2(1)	-2(1)	1(1)
OW	9(1)	13(1)	10(1)	2(1)	0(1)	3(1)

Table S9. Bond distances (Å) and angles (º) for compound **2.**

Distances			
O1a-C7a	1.24(3)	**C18a-C17a**	1.39(3)
O3a-C6a	1.26(3)	**C16a-C17a**	1.39(3)
O2a-C7a	1.26(3)	**C16a-C15a**	1.39(3)
O4a-C6a	1.25(3)	**O5a-C13a**	1.11(3)
N1a-C1a	1.38(2)	**O6a-C13a**	1.48(4)
N1a-C5a	1.39(2)	**C5a-H1c5a**	0.9599
C1a-C7a	1.51(2)	**C2a-H1c2a**	0.9596
C1a-C2a	1.39(2)	**C3a-H1c3a**	0.9603
C5a-C4a	1.39(2)	**C8a-H1c8a**	0.958
C2a-C3a	1.39(2)	**C11a-H1c11a**	0.9608
C4a-C3a	1.38(2)	**C10a-H1c10a**	0.9618
C4a-C6a	1.32(2)	**C9a-H1c9a**	0.9573
N2a-C8a	1.39(3)	**C18a-H1c18a**	0.9614
N2a-C12a	1.39(2)	**C16a-H1c16a**	0.9622
C8a-C9a	1.40(3)	**C17a-H1c17a**	0.9601
C11a-C10a	1.40(2)	**C15a-H1c15a**	0.9593
C11a-C12a	1.39(2)	**O5a-H1o5**	0.84(3)
C10a-C9a	1.39(3)	**O6a-H1o6**	0.84(3)
C12a-C13a	1.56(2)	**Cu(1)-N(1a)**	2.03 (2)
N3a-C14a	1.39(2)	**Cu(1)-N(2a)**	2.00 (2)
N3a-C18a	1.39(2)	**Cu(1)-N(3a)**	1.92 (2)
C14a-C15a	1.39(2)	**Cu(1)-O(2a)**	1.96 (2)
C14a-C13a	1.51(2)		
Angles			
Cu1-O2a-C7a	113.6(15)	**C10a-C11a-C12a**	119.8(16)
Cu1-N1a-C1a	109.5(10)	**C11a-C10a-C9a**	120.1(17)
Cu1-N1a-C5a	130.0(11)	**N2a-C12a-C11a**	120.2(15)
C1a-N1a-C5a	120.0(13)	**N2a-C12a-C13a**	117.1(14)
N1a-C1a-C7a	113.3(11)	**C11a-C12a-C13a**	122.7(12)
N1a-C1a-C2a	120.1(12)	**C8a-C9a-C10a**	119.8(18)
C7a-C1a-C2a	126.6(11)	**Cu1-N3a-C14a**	116.0(12)
O1a-C7a-O2a	132.2(18)	**Cu1-N3a-C18a**	123.9(13)
O1a-C7a-C1a	109.4(14)	**C14a-N3a-C18a**	120.0(15)
O2a-C7a-C1a	117.0(14)	**N3a-C14a-C15a**	120.1(14)
N1a-C5a-C4a	119.9(13)	**N3a-C14a-C13a**	117.1(12)
C1a-C2a-C3a	119.9(14)	**C15a-C14a-C13a**	122.7(13)
C5a-C4a-C3a	120.1(12)	**N3a-C18a-C17a**	120.1(16)
C5a-C4a-C6a	123.3(11)	**C17a-C16a-C15a**	120.2(17)
C3a-C4a-C6a	116.6(12)	**C18a-C17a-C16a**	119.7(14)
C2a-C3a-C4a	120.0(15)	**C14a-C15a-C16a**	119.9(15)
O3a-C6a-O4a	138.2(18)	**C12a-C13a-C14a**	107.1(10)
O3a-C6a-C4a	104.9(15)	**C12a-C13a-O5a**	109.5(16)
O4a-C6a-C4a	116.6(14)	**C12a-C13a-O6a**	108.6(14)
Cu1-N2a-C8a	125.7(14)	**C14a-C13a-O5a**	108.7(15)
Cu1-N2a-C12a	113.7(13)	**C14a-C13a-O6a**	109.9(16)
C8a-N2a-C12a	120.1(18)	**O5a-C13a-O6a**	112.8(18)
N2a-C8a-C9a	120.0(17)		

Table S10. Calculated energies for compound $\mathbf{1_{SP}}$ and **2**.

	Energy (Hartree)
$\mathbf{1_{SP}}$	-41290.5014599
2	-41295.9223092

The quantum-mechanical DFT calculations (Gaussian 03 program) have been performed using Becke´s three parameter hybrid functional with the correlation functional of Lee, Yang and Parr (B3LYP) and a split-valence basis set of 6-31G.