

Transformation of a Mother Crystal to a Daughter Crystal through Amorphous phase: De-assembly of Coordination Helices upon Heating and Re-assembly through Aquation

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Dedicated to our beloved colleague Dr. Golam Mostafa [1962-2011]

Table S1: Crystallographic data and refinement parameters of complex **1**

Crystal data	
Formula	C ₇ H ₉ CoNO ₇
Formula Weight	278.08
Crystal System	Orthorhombic
Space group	P2 ₁ 2 ₁ 2 ₁ (No. 19)
a [Å]	9.3953(1)
b [Å]	7.3422(1)
c [Å]	13.9495(2)
V [Å ³]	962.27(2)
Z	4
D(calc) [g/cm ³]	1.919
μ(MoKα)[mm]	1.805
F(000)	564
Crystal Size [mm]	0.15 x 0.17 x 0.20
Temperature (K)	295
Radiation [Å]	MoKα 0.71073
θ Min-Max [°]	2.6, 25.3
Dataset	-11: 11 ; -8: 8 ; -16: 16
Total	7279
Unique Data	1753
R(int)	0.034
Observed[I > 2.0 σ(I)]	1694
Nref	1753
Npar	145
R	0.0281
wR2	0.0746
S	1.11
Max. and Av. σ/esd	0.00, 0.00
Min. and Max. Δρ [e/Å ³]	-0.46, 0.41

$$w = 1/[\sigma^2(F_o^2) + (0.0410P)^2 + 0.5333P] \text{ where } P = (F_o^2 + 2F_c^2)/3$$

Table S2: Selected Bond distances (Å) and angles (°) of complex 1

Bond lengths			
Co1-O1	2.067(2)	Co1-N1	2.149(3)
Co1-O1W	2.046(2)	Co1-O4*	2.147(2)
Co1-O2W	2.041(2)	Co1-O3**	2.170(2)
Bond angles			
O1-Co1-O1W	88.48(10)	O1W-Co1-O3**	88.22(10)
O1-Co1-O2W	171.86(10)	O2W-Co1-N1	95.43(11)
O1-Co1-N1	77.59(10)	O2W-Co1-O4*	86.65(9)
O1-Co1-O4*	97.84(9)	O2W-Co1-O3**	87.22(9)
O1-Co1-O3**	88.08(9)	O4*-Co1-N1	93.42(10)
O1W-Co1-O2W	98.01(11)	O3**-Co1-N1	85.68(10)
O1W-Co1-N1	164.95(11)	O3**-Co1-O4*	173.68(9)
O1W-Co1-O4*	94.11(10)		

Symmetry: * = x, 1+y, z; ** = -1/2+x, 1/2-y, 1-z

Table S3: Hydrogen bond dimensions of the complex 1

D-H...A	D-H	H...A	D...A	<D-H...A	Symmetry
O1W-H1W1...O2W	0.86	2.600	3.215(3)	130.0	-1/2+x, 3/2-y, 1-z
O1W-H1W1...O4	0.86	2.180	2.688(3)	118.0	-1/2+x, 1/2-y, 1-z
O1W-H2W1...O3W	0.86	2.330	2.626(4)	101.0	x, 1+y, z
O3W-H1W3...O1W	0.85	2.080	2.626(4)	121.0	x, -1+y, z
O3W-H1W3...O2	0.85	2.570	3.016(4)	114.0	1/2+x, 1/2-y, 1-z
O2W-H1W2...O1	0.85	2.140	2.680(3)	121.0	1/2+x, 3/2-y, 1-z
O2W-H2W2...O1	0.85	2.379	2.701(3)	103.01	1/2-x, 1-y, -1/2+z

Table S4: Crystallographic data and refinement parameters of phase 3

Crystal data	
	Phase 3
Formula	C ₇ H ₃ CoNO ₆ , 4H ₂ O
Formula Weight	332.03
Crystal System	Monoclinic
Space group	P21/a (No. 14)
a [Å]	10.898(3)
b [Å]	14.146(5)
c [Å]	9.730(3)
β [°]	96.01(3)
V [Å ³]	1491.8(8)
Z	4
D(calc) [g/cm ³]	1.425
μ(CuKα)[mm]	9.450
F(000)	636
Temperature (K)	293
Radiation [Å]	CuK _α 1.54180
θ Min-Max [°]	5, 60
Dataset	999:-99 ; 999:-99 ; 999:-99
Unique Data	812
R	0.0245
wR2	0.0395

Table S5: Selected bond lengths (Å) and bond angles (°) of complex **3**

Bond lengths			
Co1 -O1W	2.2162	Co1 -N1	2.3269
Co1 -O3*	2.2395	Co1 -O2W	2.2092
Co1 -O1	2.2381		
Bond angles			
O1-Co1-O1W	88.58	O1-Co1-O3*	87.86
O1W-Co1-O2W	97.94	O2W-Co1-N1	95.51
O1W-Co1-N1	164.97	O2W-Co1-O3*	89.61
O1W-Co1-O3*	70.57	O3*-Co1-N1	102.92
O1-Co1-O2W	171.79	O1-Co1-N1	77.47

Symmetry * = 3/2-x, 1/2+y, 1-z

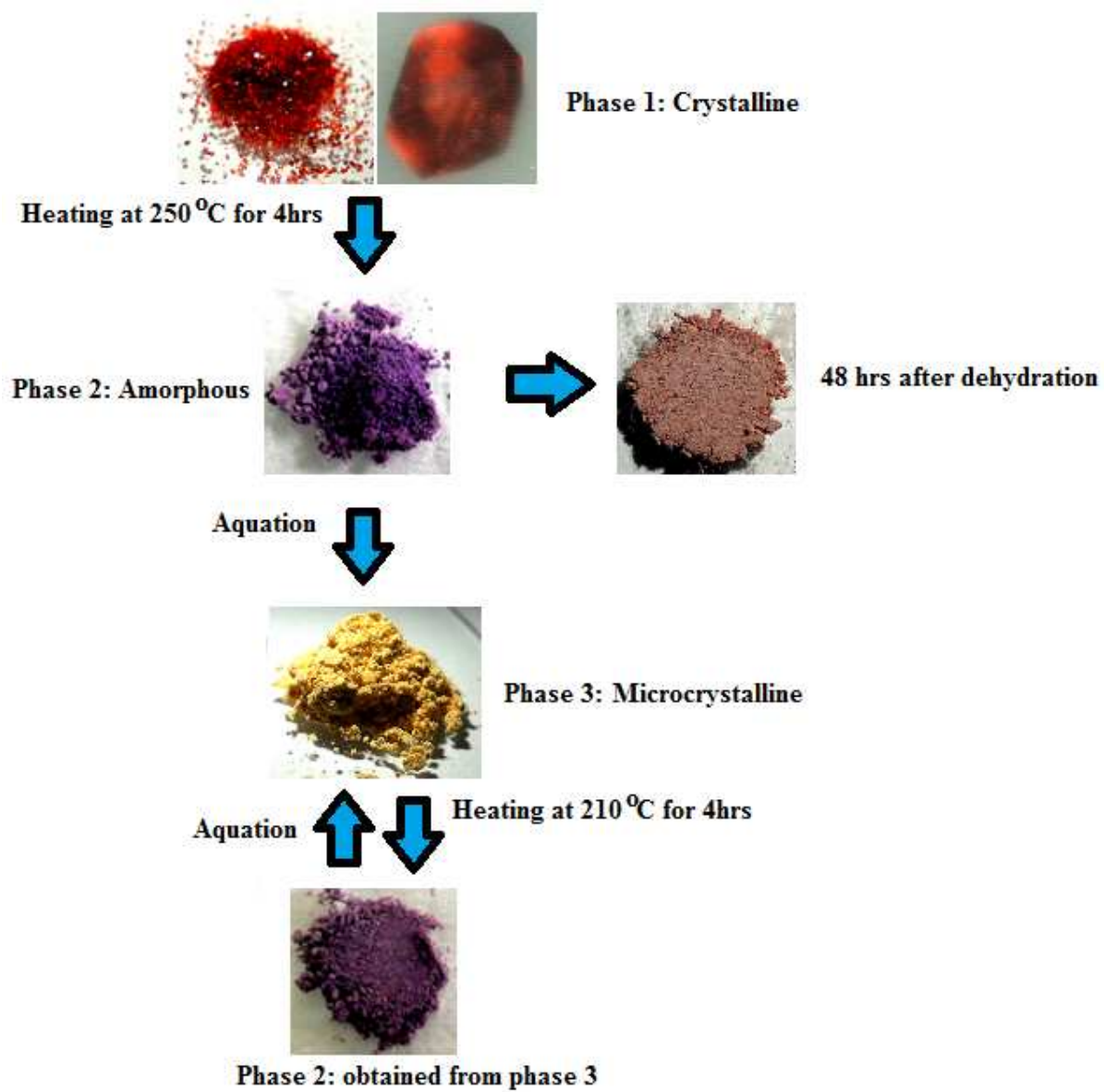


Figure S1. Picture of all phases

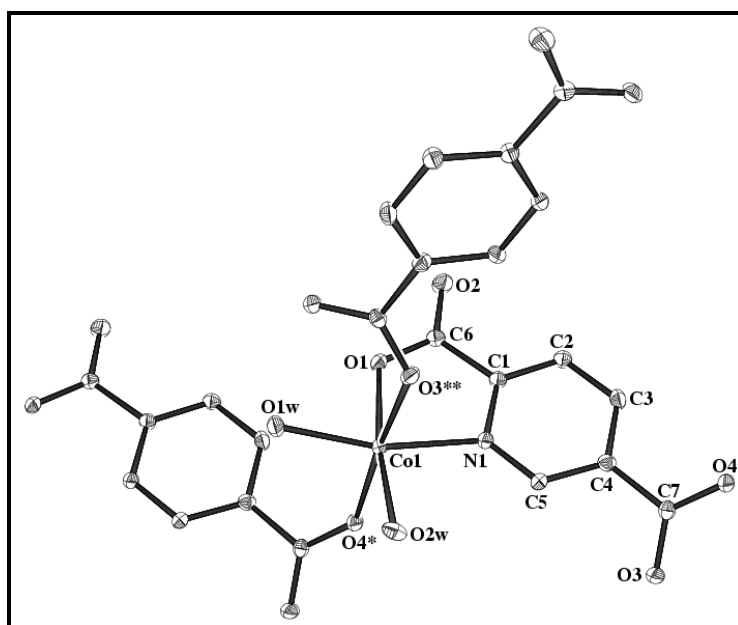


Figure S2. The ORTEP diagram of the complex with 30% probability of **complex 1**
 (* = $x, 1+y, z$; ** = $-1/2+x, 1/2-y, 1-z$)

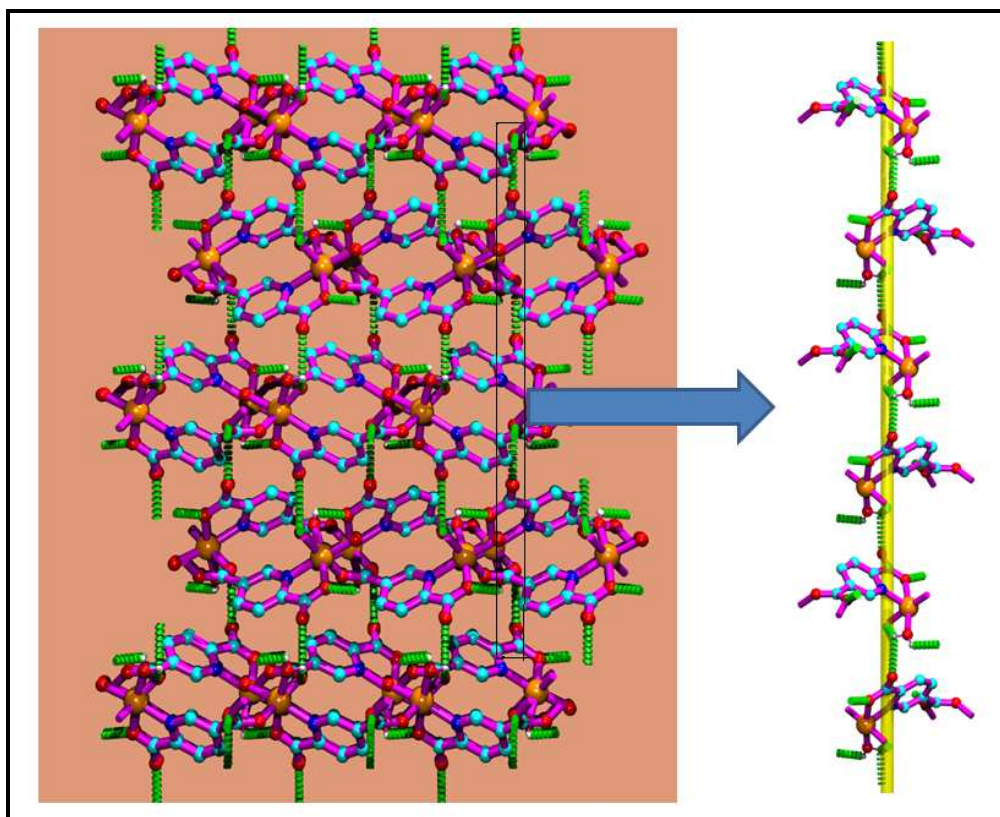


Figure S3. The 2D coordination sheets are converted to 3D supramolecular framework by helical O2W-H2W2...O2 hydrogen bonding interactions in **complex 1**

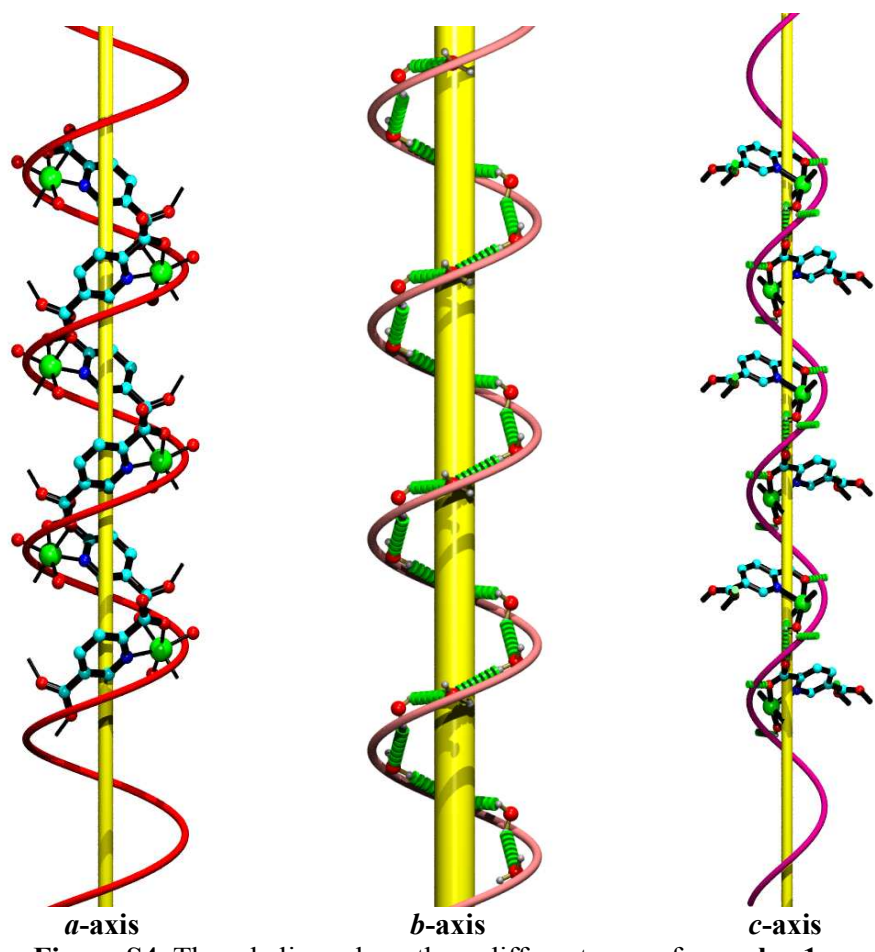
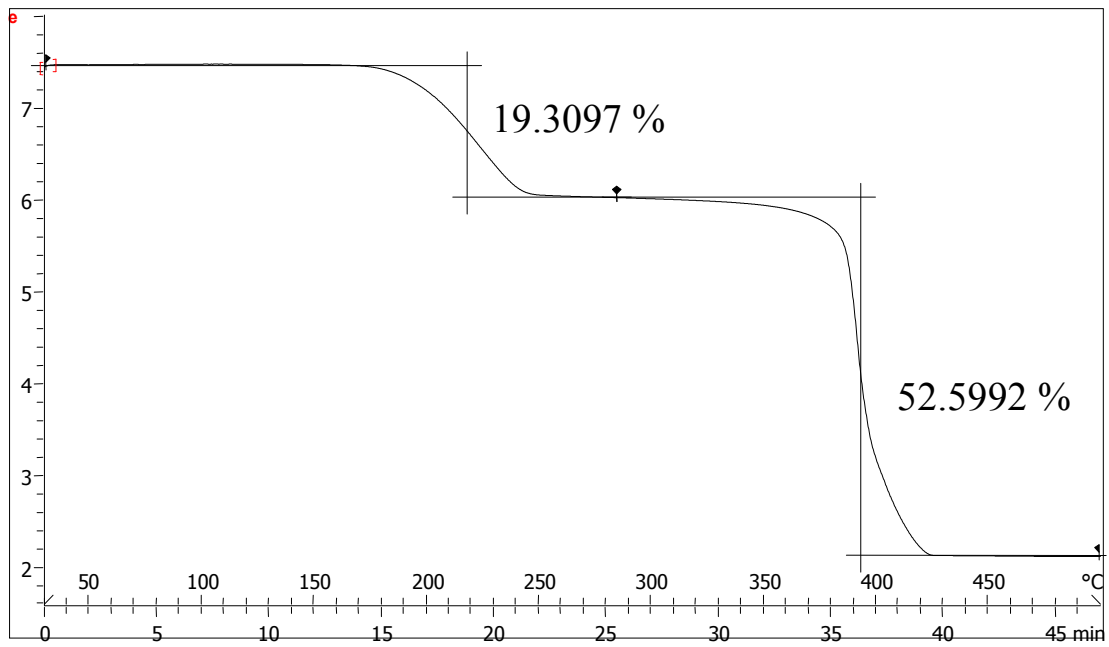
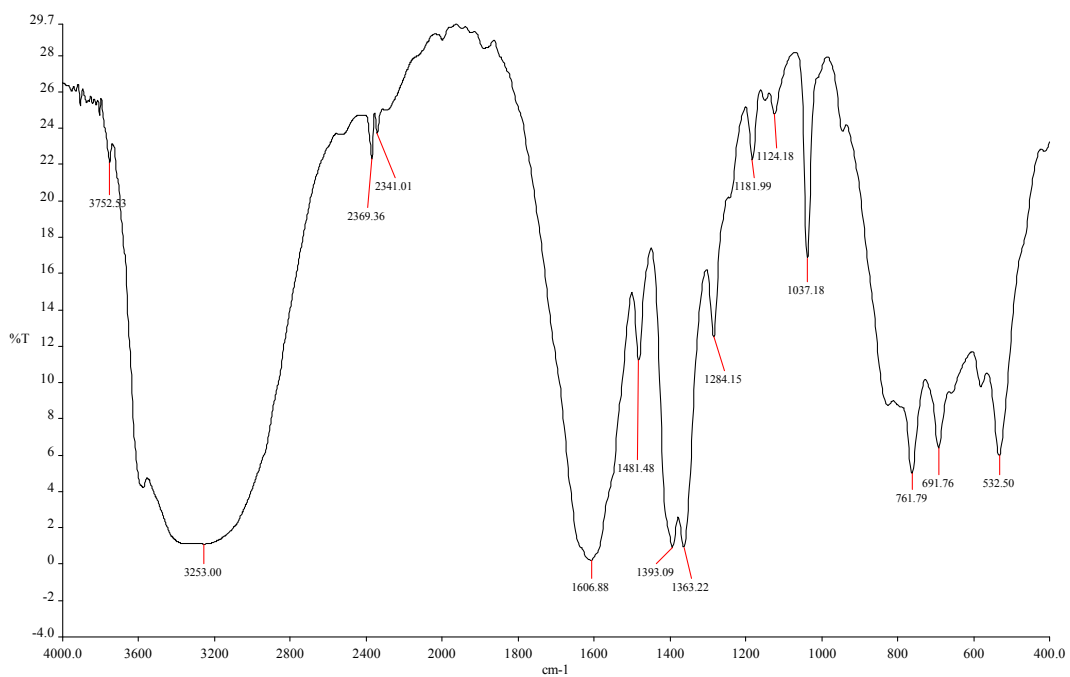


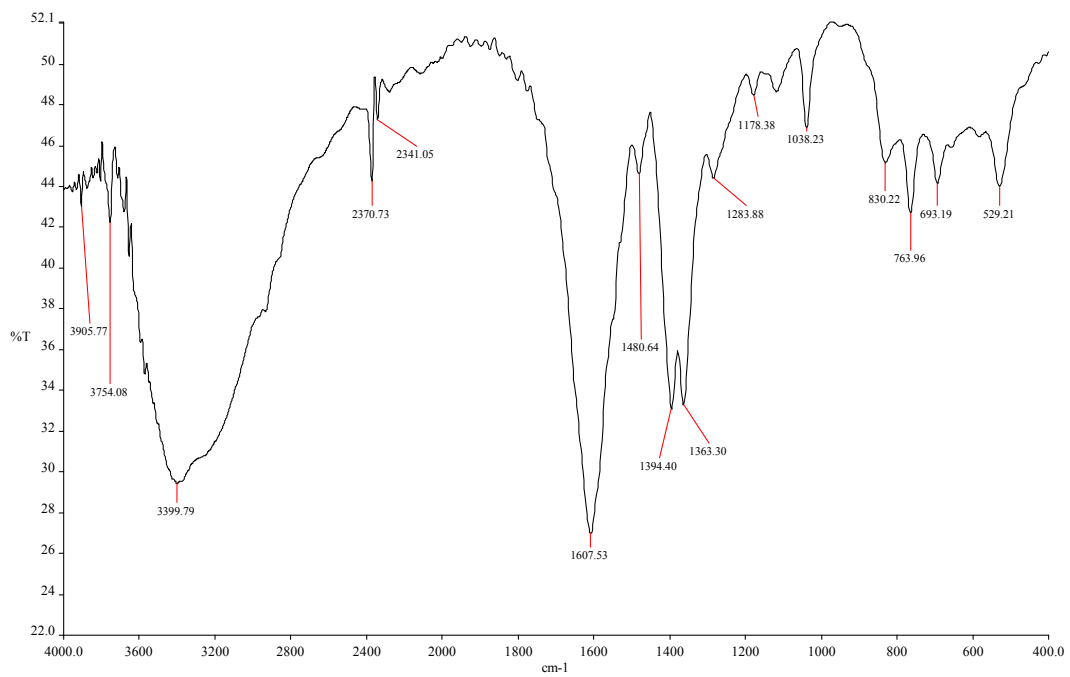
Figure S4. Three helices along three different axes of **complex 1**



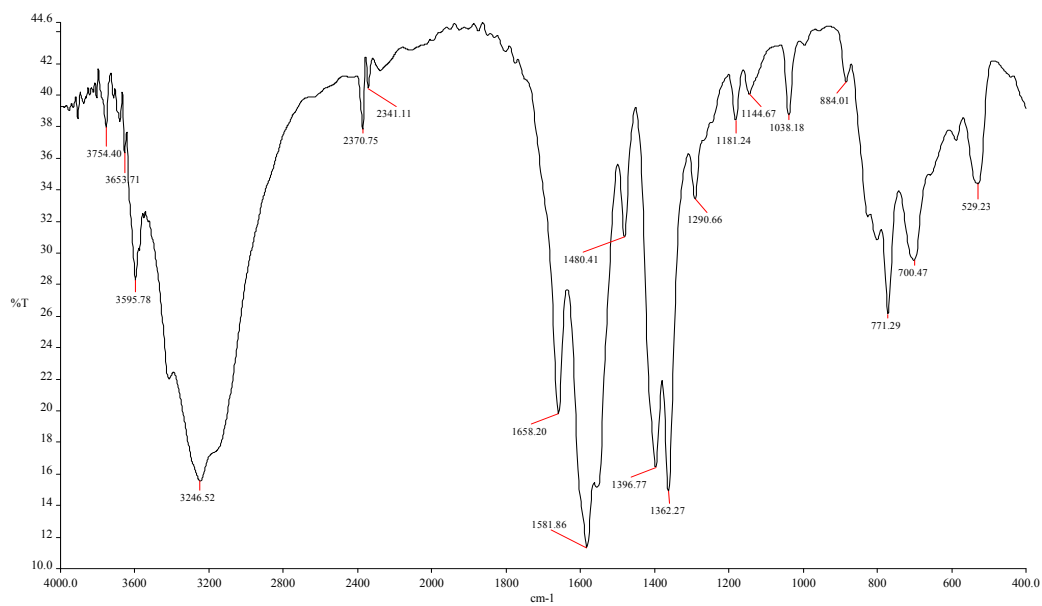
Phase 1
Figure S5. Thermal plot of phase 1



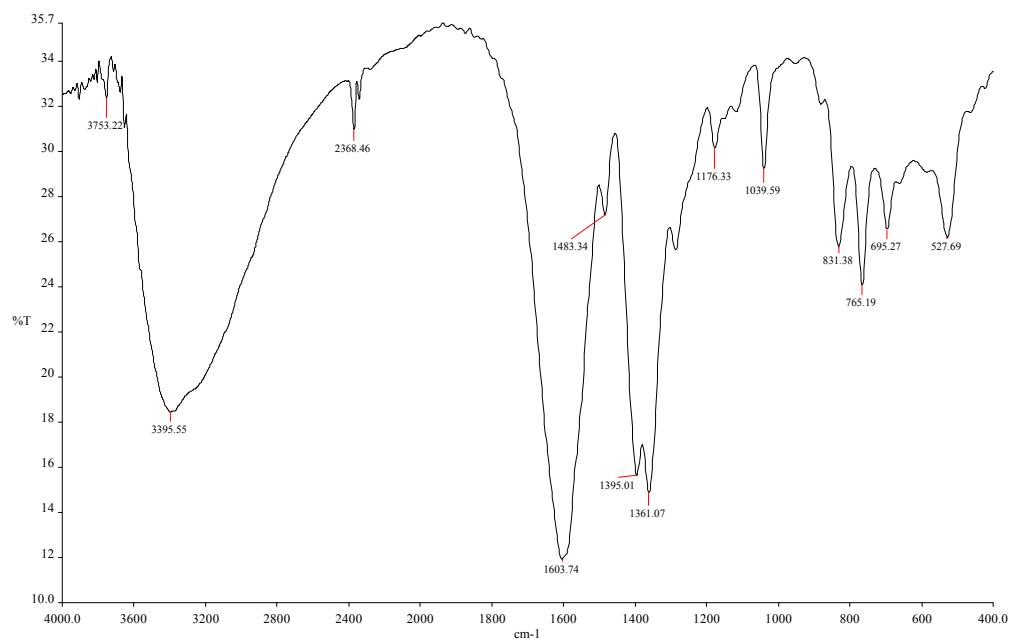
Phase 1



Phase 2



Phase 3



Phase 2 obtained by dehydration of 3

Figure S6. IR spectra of three different phases

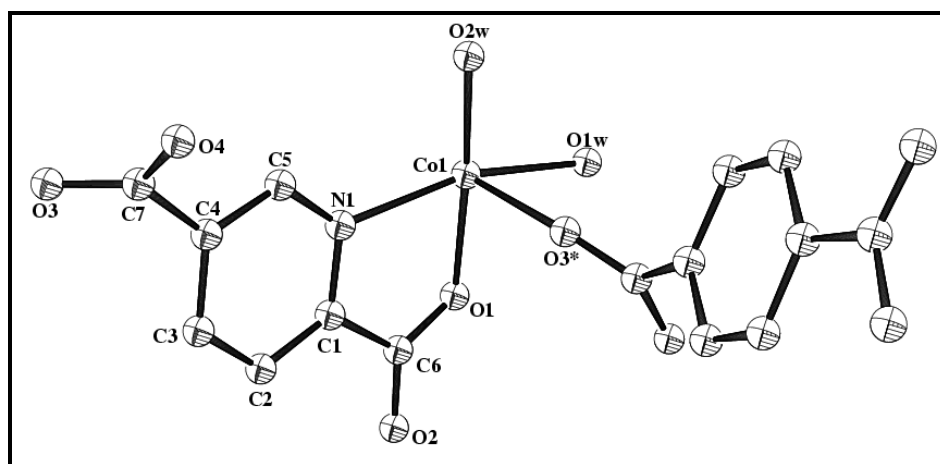


Figure S7. ORTEP diagram of phase 3 ($*=3/2-x, 1/2+y, 1-z$) (O1W and O2W are two coordinated water molecules)

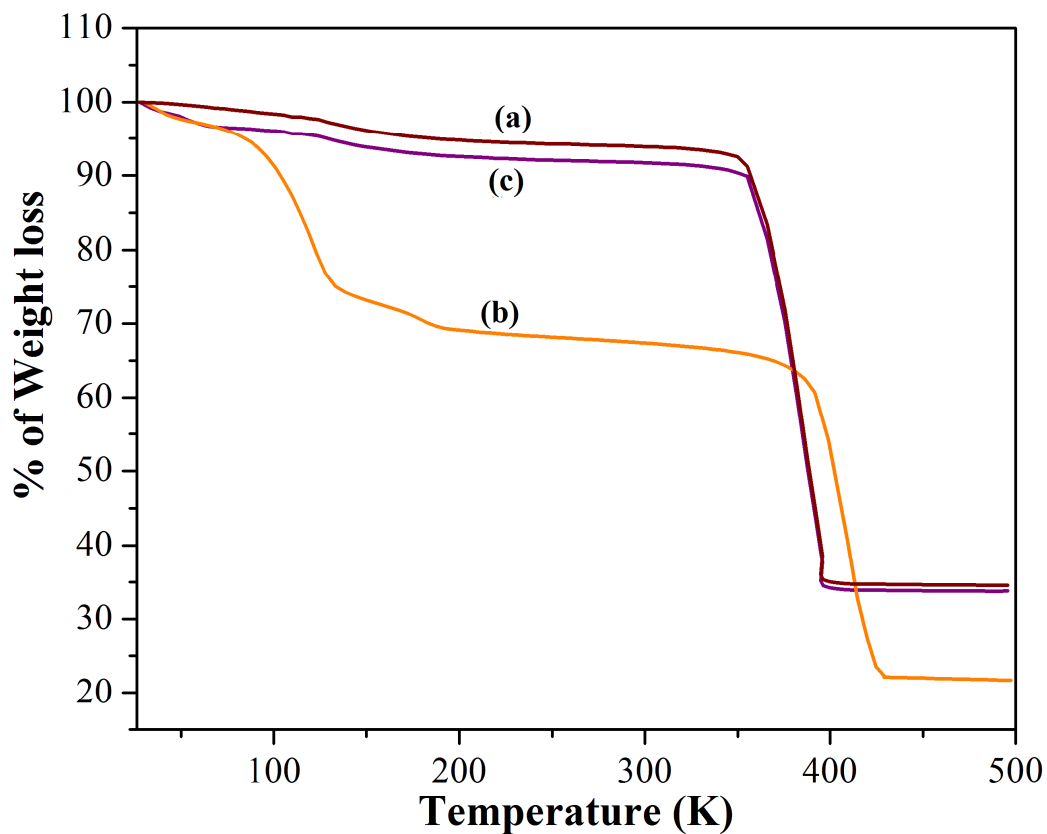


Figure S8. Thermal plots of (a) phase 2, (b) phase 3 and (c) phase obtained by dehydration of 3

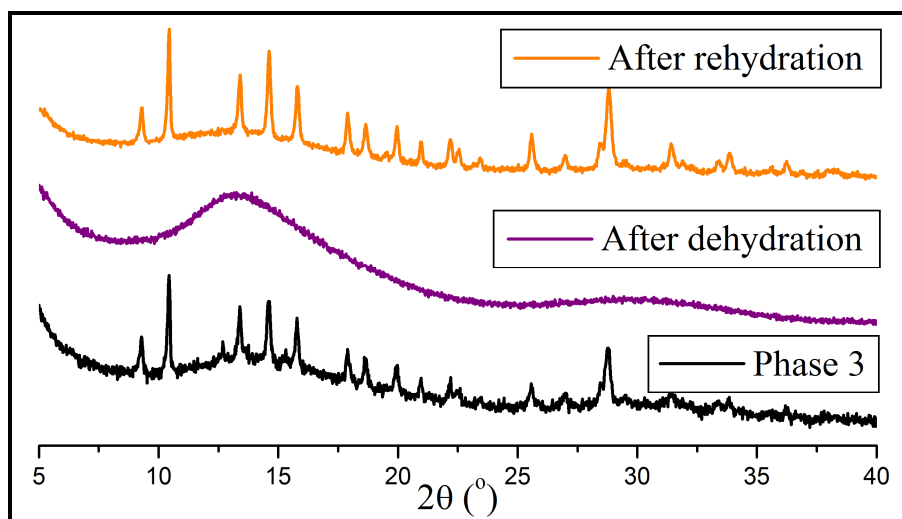


Figure S9. Reversible crystalline to amorphous to crystalline transformation of phase 3

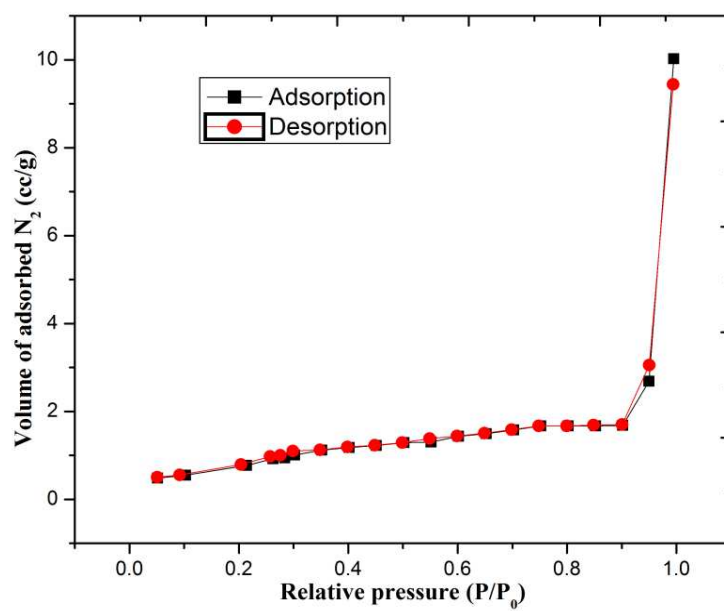


Figure S10. N_2 adsorption isotherm of phase 2

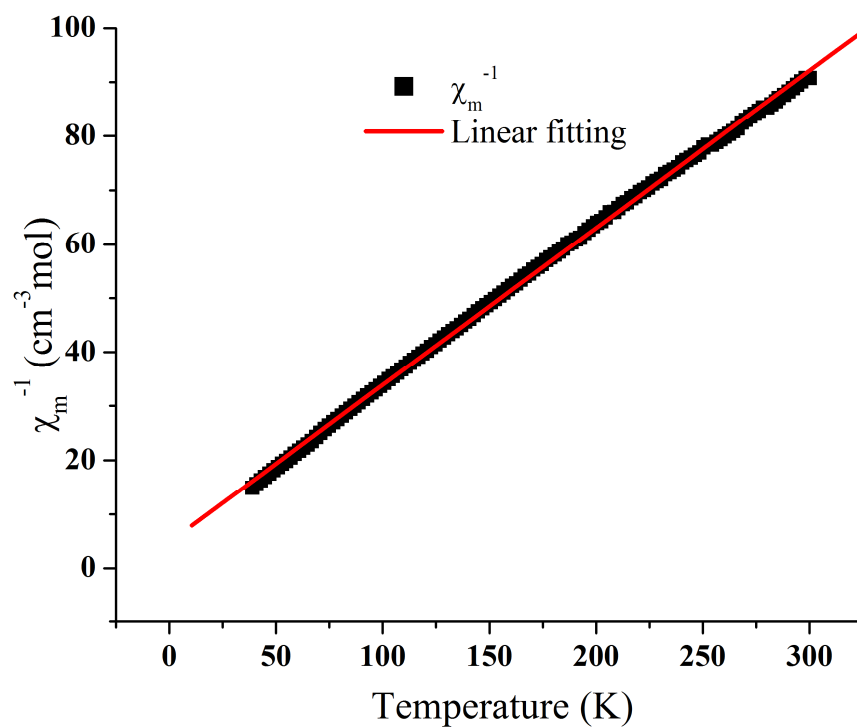


Figure S11. χ_m^{-1} vs T plot of phase 1

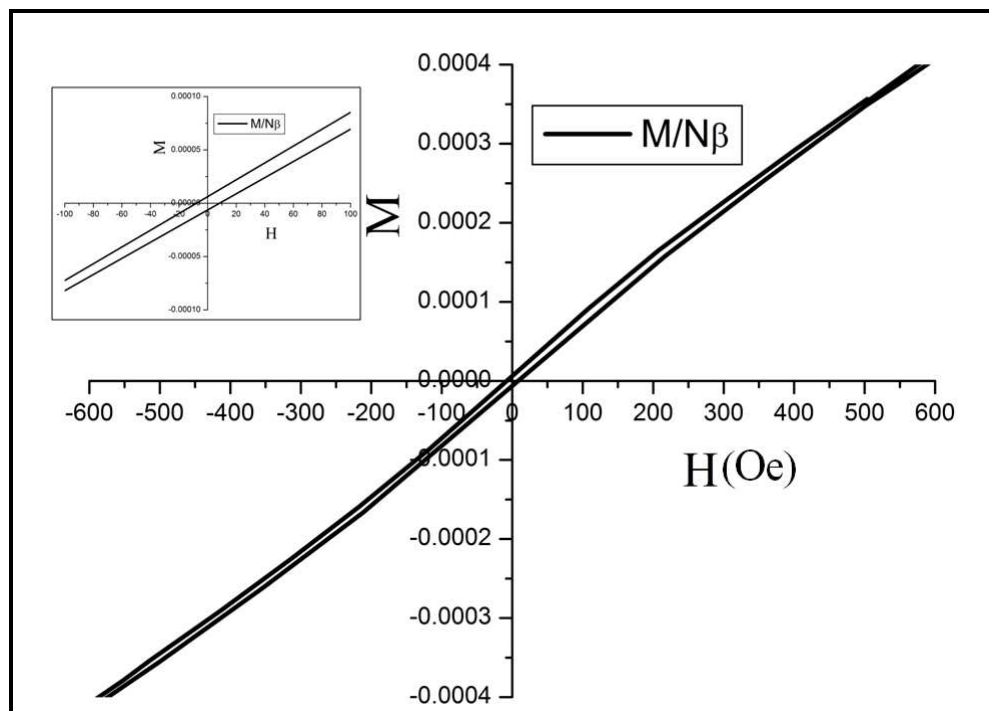


Figure S12. M vs H plot of phase 1

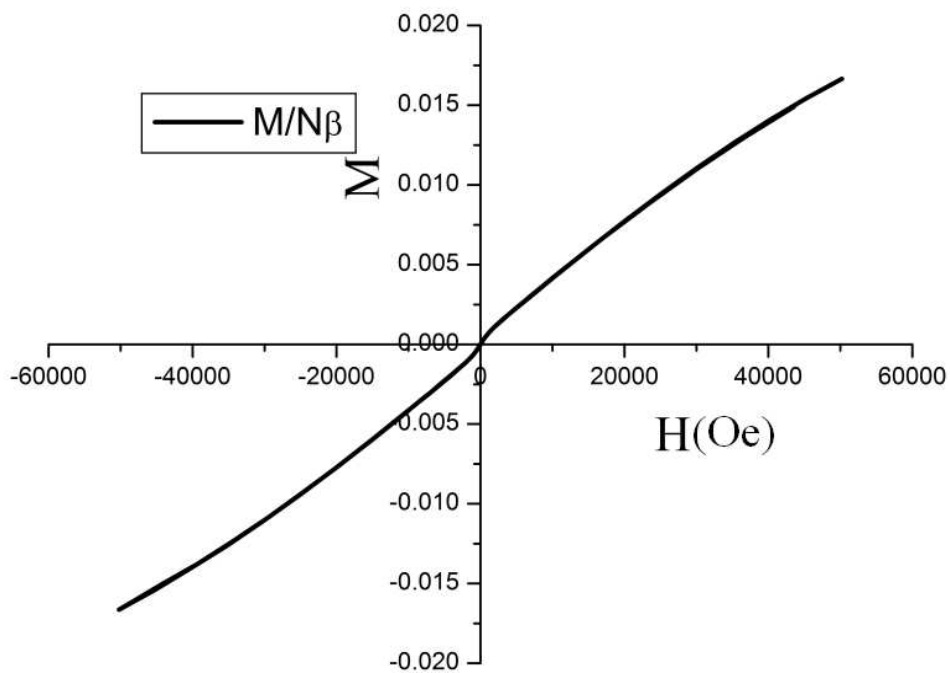


Figure S13. Unsaturation of magnetization even at 5T

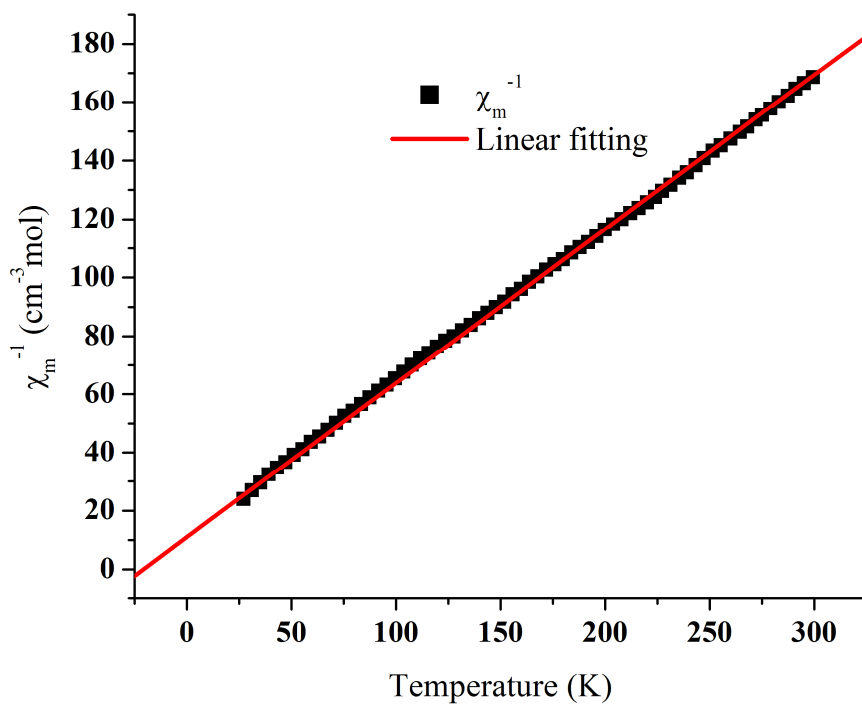


Figure S14. χ_m^{-1} vs T plot of phase 2

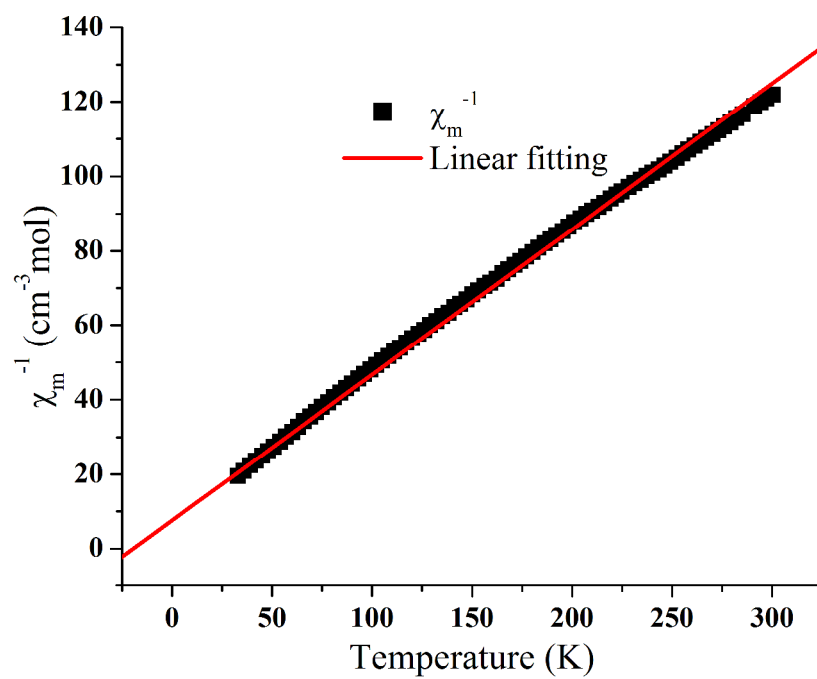


Figure S15. χ_m^{-1} vs T plot of phase 3

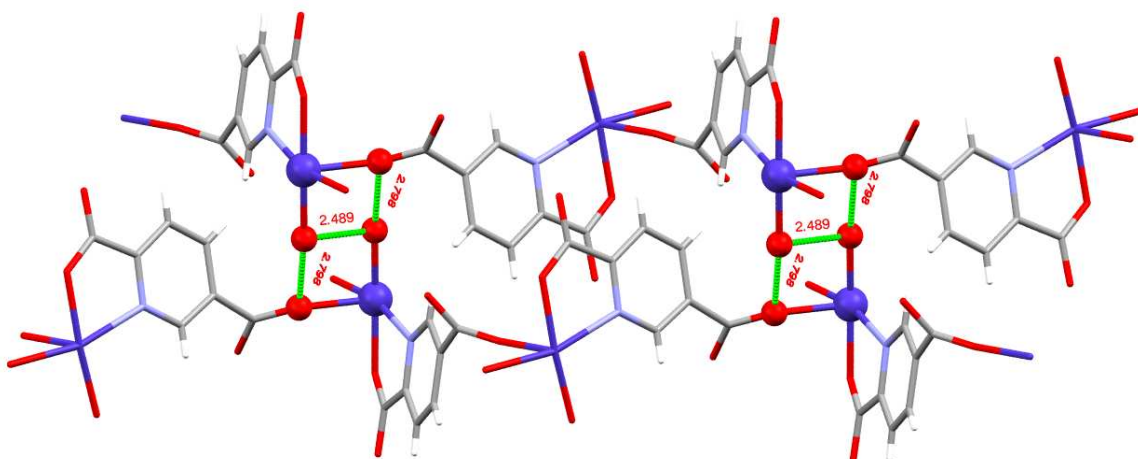


Figure S16. Formation of cyclic hydrogen bonding synthon motif of phase 3

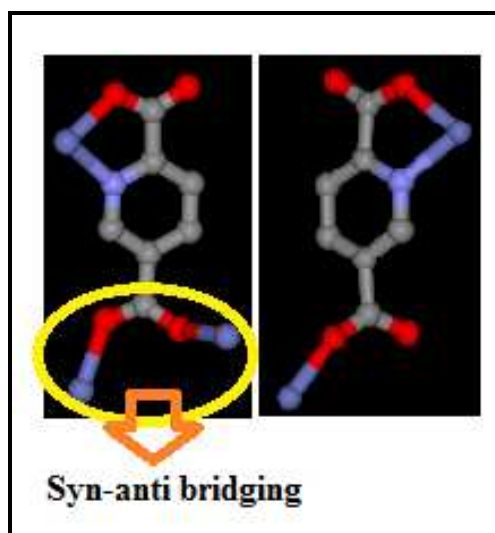


Figure S17. Syn-anti bridging of 2,5-pdc ligand get collapsed in phase 3