Supporting Information

Dynamic Crystal-to-Crystal Transformation of 1D to 2D Lead(II) Coordination Polymer by De- and Rehydration with No Change in Nano-Particles Morphology

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Materials and physical measurements

All chemicals were of reagent grade from Merck Company and were used as commercially obtained without further purification. IR spectra were recorded on a SHIMADZU- IR460 spectrometer in a KBr matrix. Microanalyses were carried out using a Heraeus CHN-O-Rapid analyzer. Melting points were measured on an Electrothermal 9100 apparatus and are uncorrected. The thermal behavior was measured with PL-STA 1500 apparatus. Crystallographic measurements were made at 170(2) K using a Bruker AXS SMART APEX CCD diffractometer. The intensity data were collected using graphite monochromated Mo–K_α radiation (λ=0.71073Å). Accurate unit cell parameters and orientation matrices were obtained from least–squares refinements using the programs Smart and Saint, and the data were integrated using Saint. The structures have been solved by direct methods and refined by full–matrix least–squares techniques on F^2 using SHELXTL. The molecular structure plots were prepared using the ORTEP and Mercury programs. Crystallographic data and details of the data collection and structure refinements are listed in Table S1.

Owing to the low resolution and disorder, the oxygen atoms of one of the NO_3 group were refined by using following restraints:

The N-O distances and O…O separations in one of the NO_3 group has been restrained using the '*DFIX*' command as 1.21Å and 2.19Å, with the deviations of 0.02, respectively. The N2 O21 O22 O23 atoms are restrained to be coplanar using '*FLAT*' command. These restraints are primarily a means to stabilize the refinement. Therefore, the final model is the best one for the current data set.

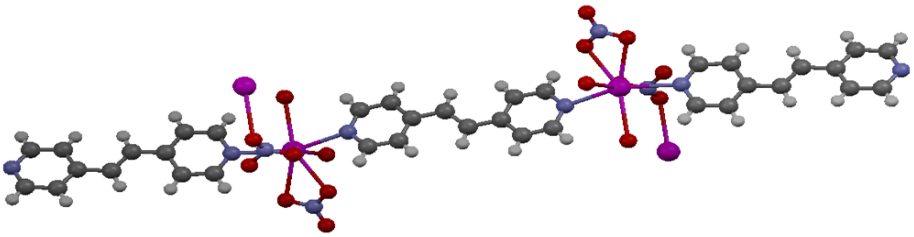
Crystal to Crystal Transformation:

When crystals of 1 are heated in air to 110-120°C for one day they reversibly loose the coordinated water molecule to yield $[Pb_2(\mu\text{-bpe})_3(\mu\text{-}NO_3)_2(NO_3)_2]_n$ (2). The transformation occurs without destruction of the single crystalline character of the material by crystal to crystal transformation. To confirm the transformation of compound 1 to compound 2 upon heating and dehydration of the sample, thermal gravimetric and differential thermal analyses (TGA and DTG) were recorded. The most important feature of the crystal of 1 is that it undergoes a reversible crystal-to-crystal structural transformation driven by dehydration and rehydration. However, when a dehydrated sample is exposed to a water vapor, (i.e., the dry sample is placed in a glass desiccators, beside a water filled beaker) it reabsorbs the lost water.

Table S1 Crystal data and structure refinement for $[Pb(\mu\text{-bpe})_{1.5}(\mu\text{-}NO_3)(NO_3)(H_2O)]_n$ (**1**)

Identification code	**1**
Empirical formula	$C_{18}H_{17}N_5O_7Pb$
Formula weight	622.55
Temperature(K)	170(2)
Wavelength	0.71073
Crystal system	Triclinic
Space group	Pī
Unit cell dimensions	a= 9.3542(14)Å
	b= 11.1933(16)Å
	c= 11.9630(18)Å
	alpha= 62.314(11)° beta = 68.905(12)° gamma= 73.544(11) °
Volume	1024.6(3)Å^3
Z	2
Density (calculated)	2.018 Mg/m^3
Absorption coefficient	8.285
F(000)	596
Theta range for data collection	2 to 27.33 °
Index ranges	$-12 \le h \le 12$
	$-14 \le k \le 13$
	$-15 \le l \le 14$
Reflections collected	4500
Independent reflections	3845*(R*(int) = 0.0662)
Absorption correction	multi-scan
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	4500 / 7 / 281
Goodness-of-fit on F^2	1.088
Final *R* indices [$I>2\sigma(I)$]	R_1= 0.0484 and wR_2= 0.1311
R Indices (all data)	R_1= 0.0569 and wR_2= 0.1403

a



b

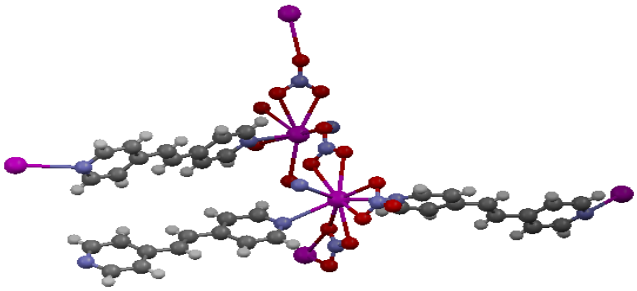


Figure S1. Ball-and-stick plots of the **a**) compound $[Pb_2(\mu\text{-bpe})_3(\mu\text{-}NO_3)_2(NO_3)_2(H_2O)_2]_n$ (**1**) and **b**) compound $[Pb_2(\mu\text{-bpe})_3(\mu\text{-}NO_3)_2(NO_3)_2]_n$ (**2**)

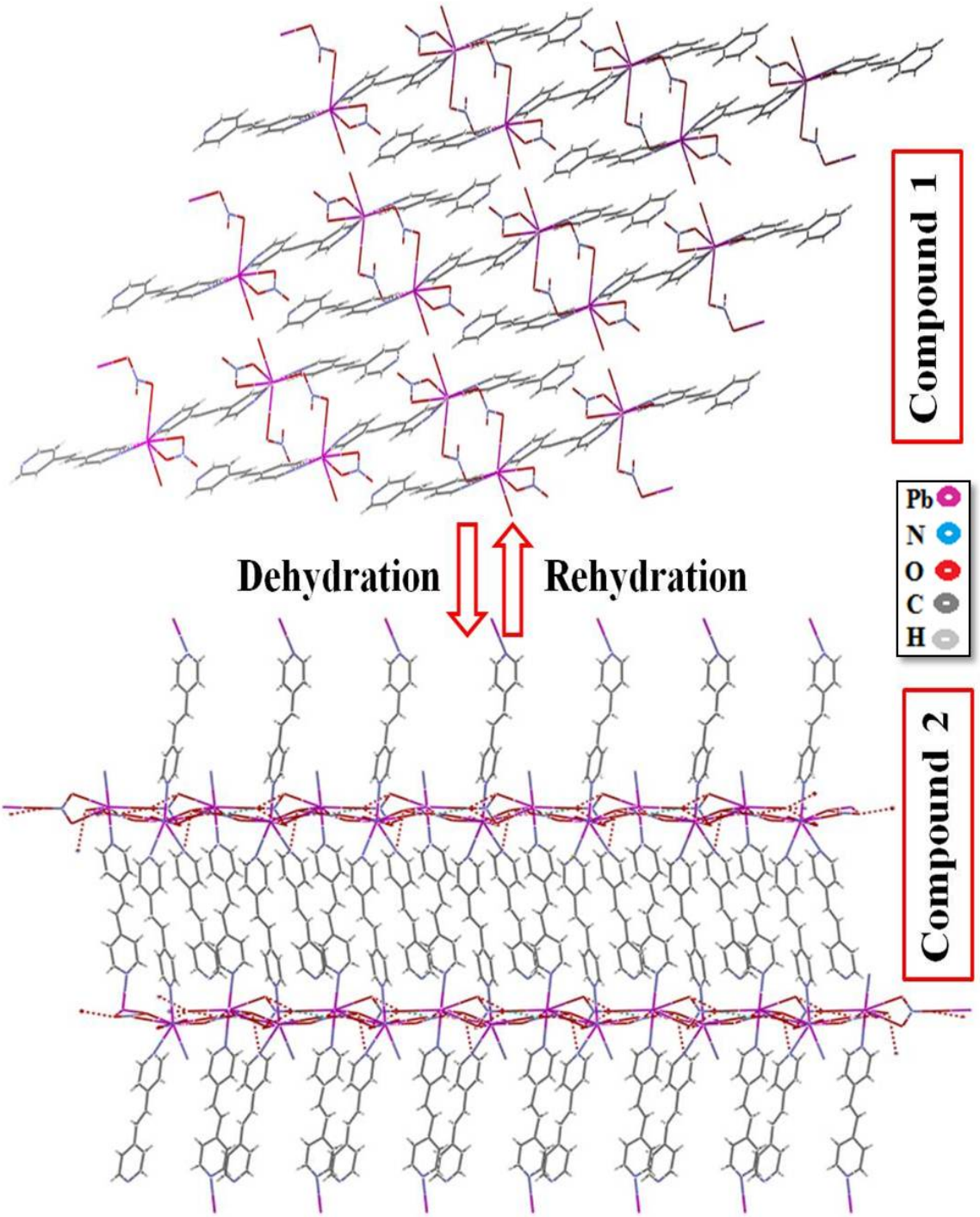


Figure S2. A schematic diagram illustrating the interactions in polymeric chains of (a) compound **1** and (b) compound **2**, H atoms have been omitted for clarity. (Pb= violet, O = red, C = gray and N= blue)

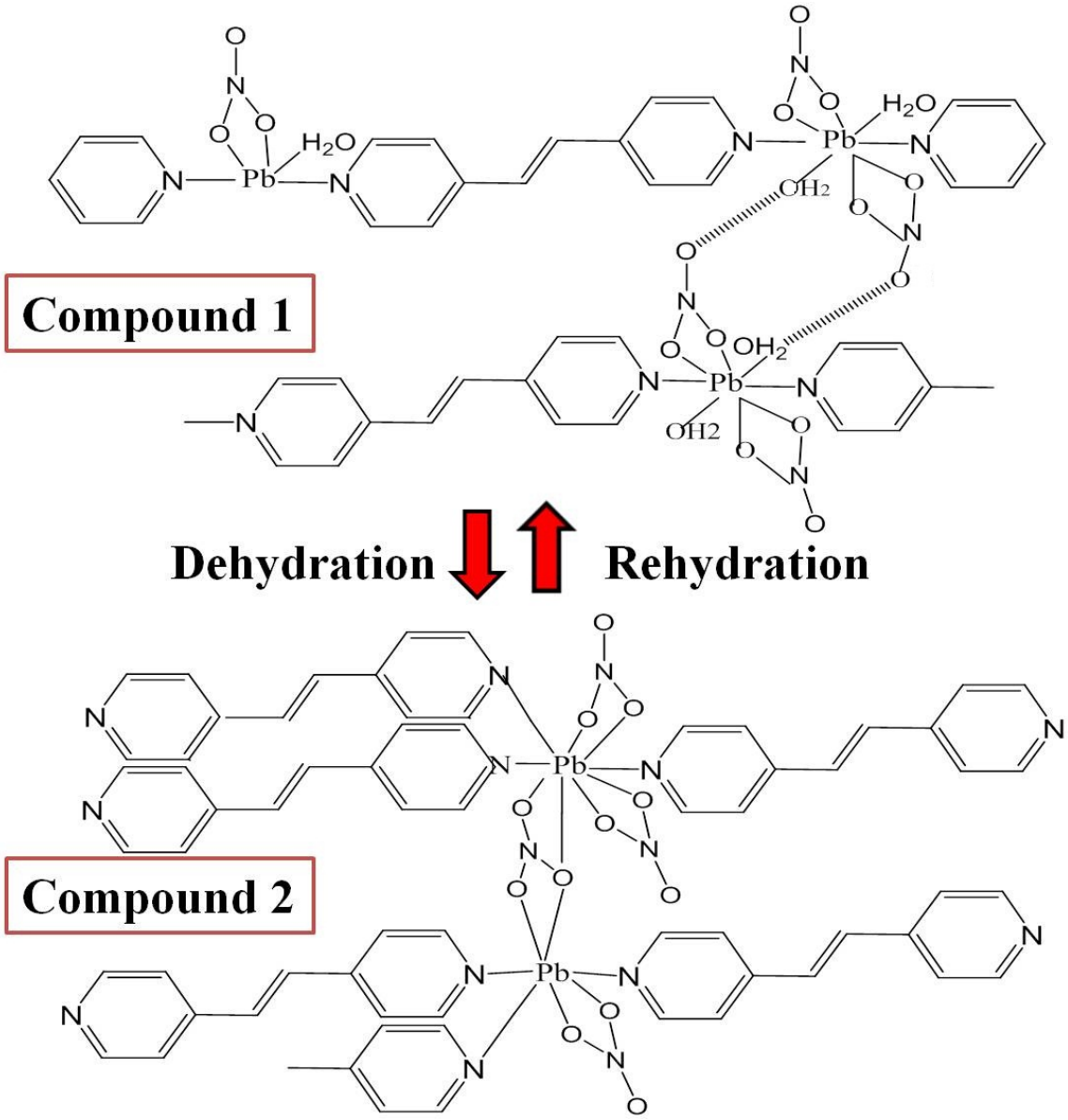


Figure S3. Schematic representation and mechanism for con-version of compound 1 to compound 2 by hydration and dehydration.

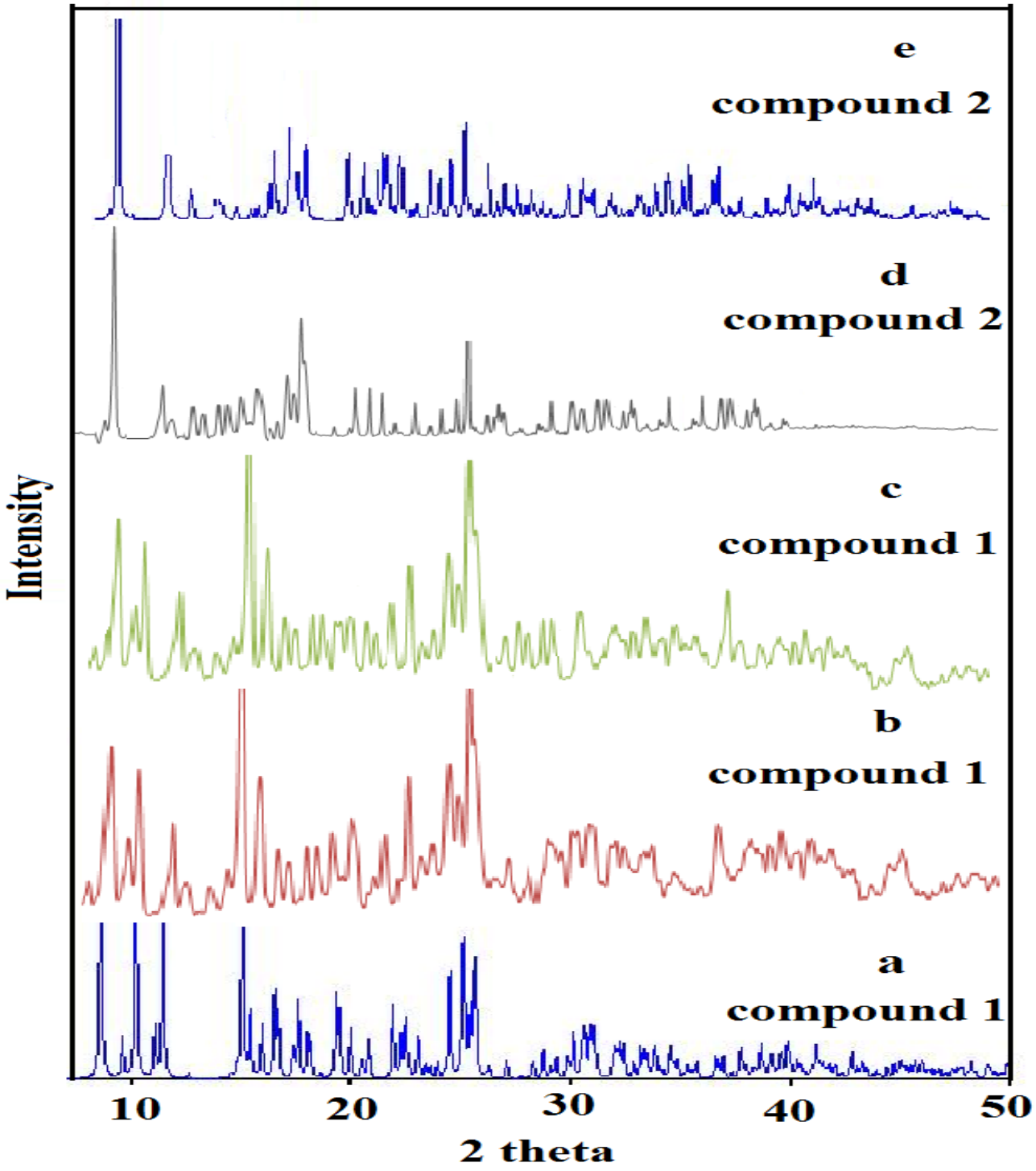


Figure S4. The XRD patterns of (**a**) simulated from single crystal X-ray data of compound (**1**), (**b**) bulk materials as synthesized of $[Pb_2(\mu\text{-bpe})_3(\mu\text{-}NO_3)_2(NO_3)_2(H_2O)_2]_n$ (**1**), (**c**) bulk materials of (**1**) obtained by rehydration of compound (**2**), (**d**) compound (**2**) obtained by dehydration of compound (**1**), and (**e**) simulated from single crystal X-ray data of compound $[Pb_2(\mu\text{-bpe})_3(\mu\text{-}NO_3)_2(NO_3)_2]_n$ (**2**).

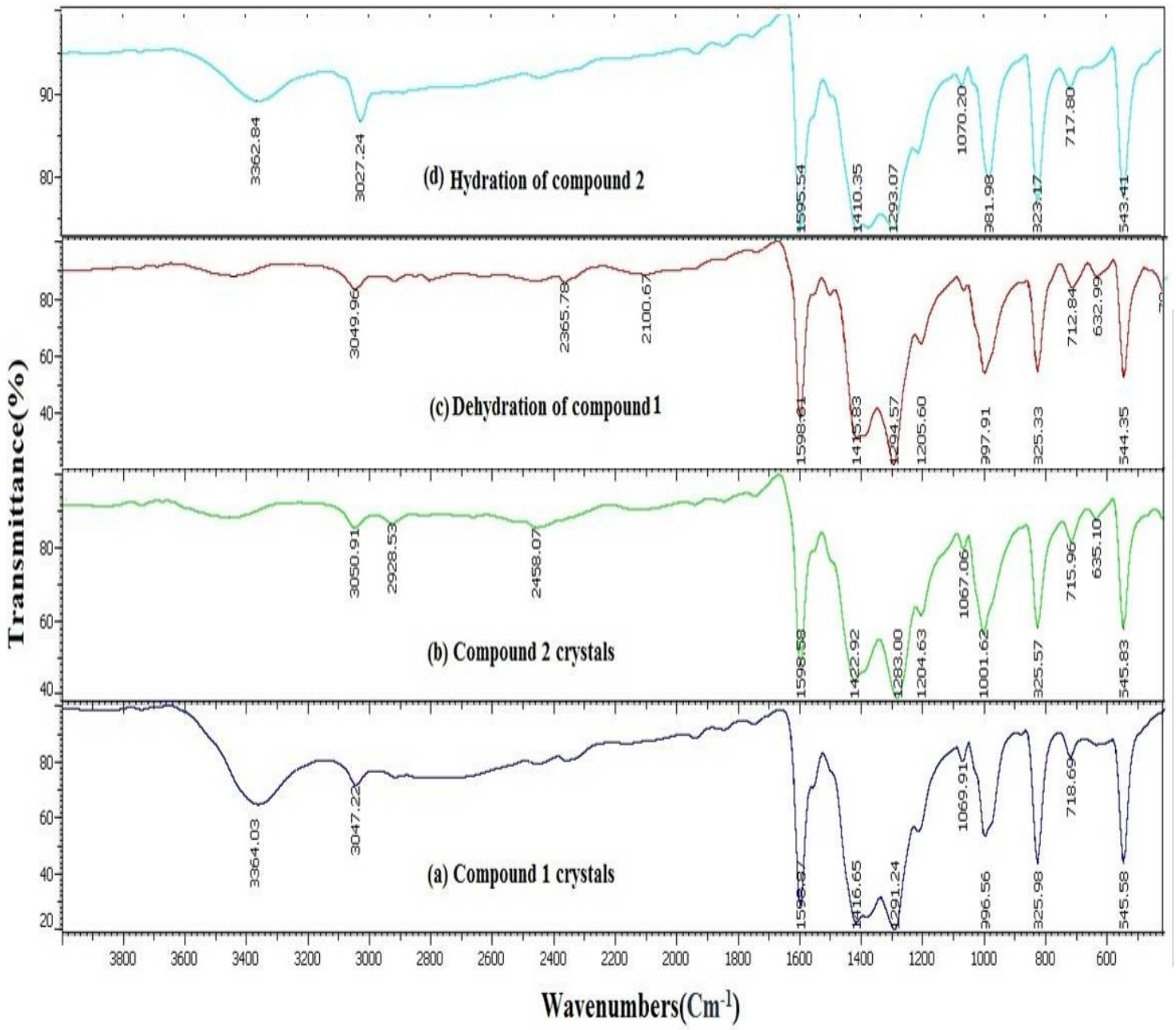
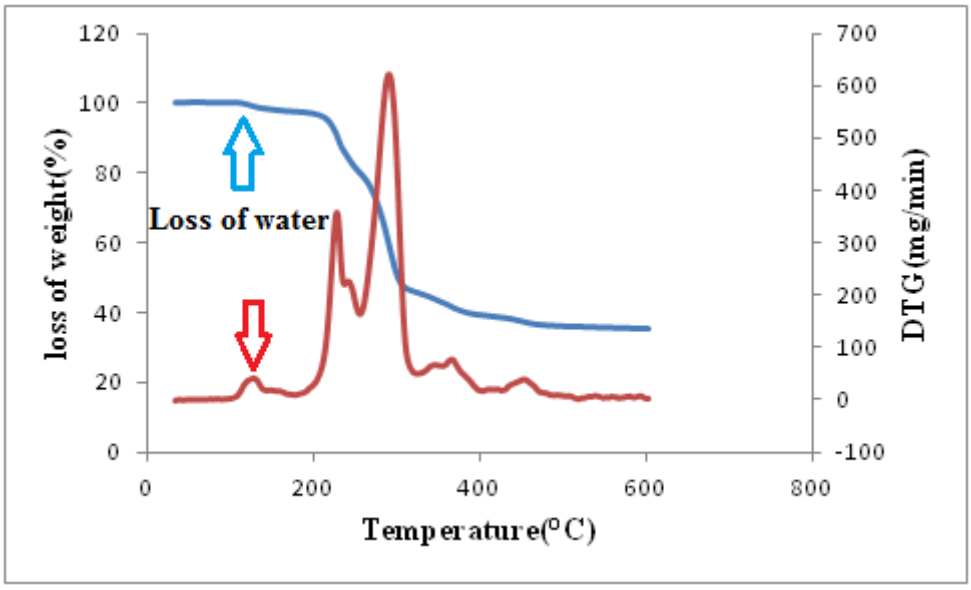


Figure S5. IR spectra of **a**) single crystal of compound **1, b**) single crystal of compound **2 c**) the species obtained by dehydration of compound **1,** and **d**) the species obtained by hydration of compound **2.**

a



b

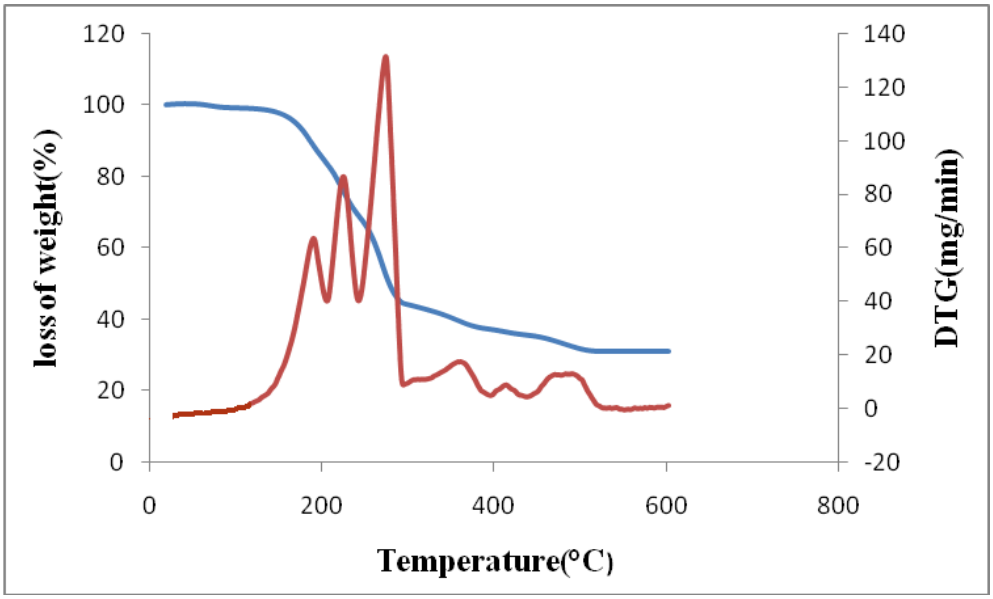


Figure S6. TGA and DTG diagrams of **a**) compound **1** and **b**) compound **2.**

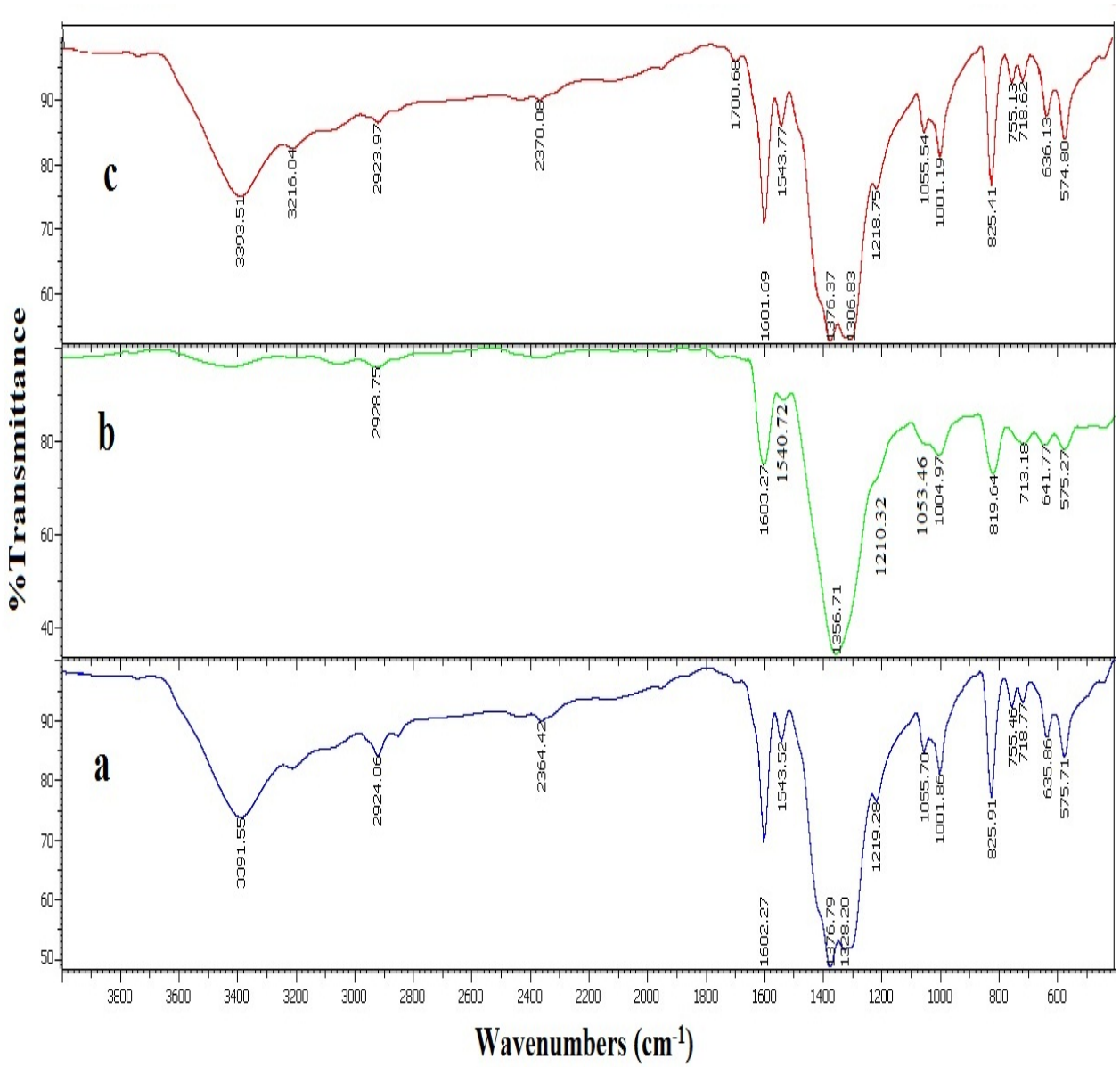


Figure S7. IR spectra of (a) nano-particles of compound **1** produced by sonochemical method**,** (b) nano-particles of compound **2** obtained by dehydration of compound **1** and (c) the reversed nano-particles obtained by rehydration of compound **2**.