

PXRD Characterization of Microporous Organophosphates that Contain Accessible Metal-centres

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Our research focused on the design and synthesis of new classes of functionality porous material that are not available in inorganic zeolites. Interesting, our microporous materials have a reasonable degree of thermal stability and rigid structure upon the guest molecule removal, as characterized by TGA and XRD. However, among them some materials undergo a reversible phase transition in the course of guest molecule removal and a concomitant change in color.

For example, a novel copper-centred ethylenediphosphate, $\text{Cu}_2(\text{ethylenediphosphate})_2(\text{phen})_2 \cdot 4\text{H}_2\text{O}$ compound **1**, possess a zigzag structure along *a*-axis. The thermo-stability and phase transition of **1** was studied by

synchrotron powder X-ray diffraction pattern (PXRD). The image of variable- temperature powder X-ray diffraction pattern revealed in real time the evolution of phase diagram, providing comprehensive insight into the porous structure changing when pore-containing water leaving. Figure 1 displays the PXRD diagram for the compound **1** and 2-theta angle from $40^\circ\text{C} \sim 350^\circ\text{C}$ shows that **1** maintain the phase angle during heating process. That means the structure crystalline of compound **1** does not change when removing water during heating process and the structure during the reflux process was same as the high temperature.

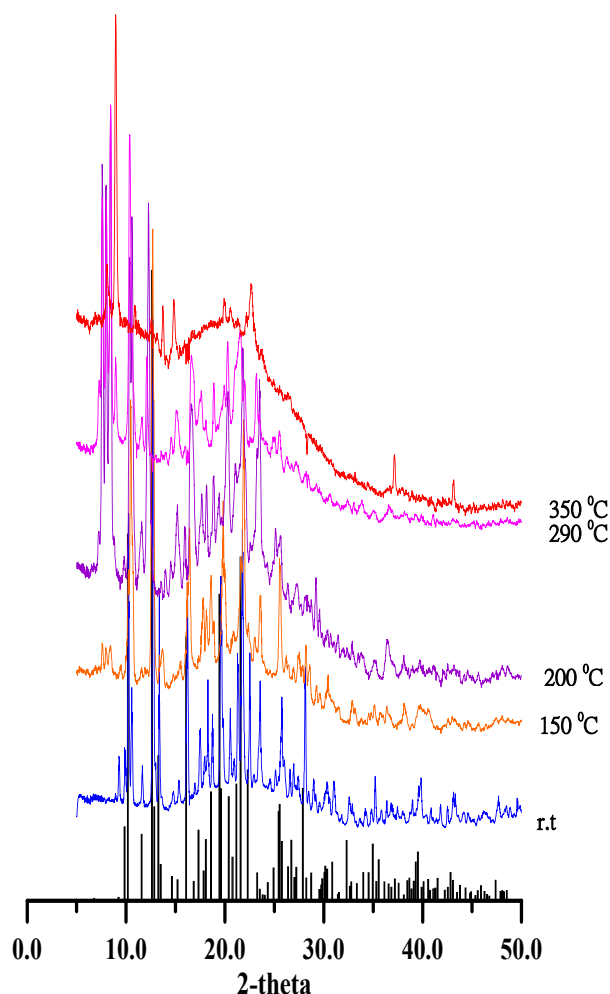


Figure 1. Powder X-ray diffraction pattern (PXRD) of $\text{Cu}_2(\text{ethylenediphosphate})_2(\text{phen})_2 \cdot 4\text{H}_2\text{O}$