Study on Existence of the H-bond Interaction between Polymers and ZnO in the XRD

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In order to determine the structure of the polymers (**P1-P4**) and surface modified nanoparticle ZnO (**Scheme 1**) were studied by powder X-Ray diffraction (PXRD) measurements.

Based on the theoretical geometries estimated by CS ChemOffice, the molecular lengths of H-bonded polymer complexes **P1/ZnO,P3/ZnO** are 16 Å, which are calculated from the molecular projection lengths of the fully extended molecular lengths along the rigid cores. The values presented are only rough estimates. As shown in Figure 1and 2, **P1, P3** are compared with **P1/ZnO, P3/ZnO**, which are H-bond interaction, and *d*-spacing values are shorted from 16 Å **(P1,P3)** shift to 12Å(**P1/ZnO ,P3/ZnO)**. The XRD data demonstrate existence of the H-bond interaction between **P1, P3** and **ZnO**.The structure of ZnO matches the wurtzite of JCPDS card.（JCPDS 36-1451）Peaks of polymers are broad in powder X-Ray diffraction spectra. It is demonstrated existence of characteristic of polymer.

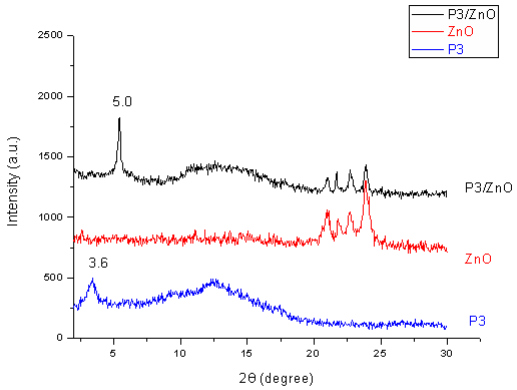

Figure1. Powder X-ray diffraction spectra of hydrogen bonded complex of pyridyl-modified ZnO nanopartcles and **P3** with 1:1 mol %.

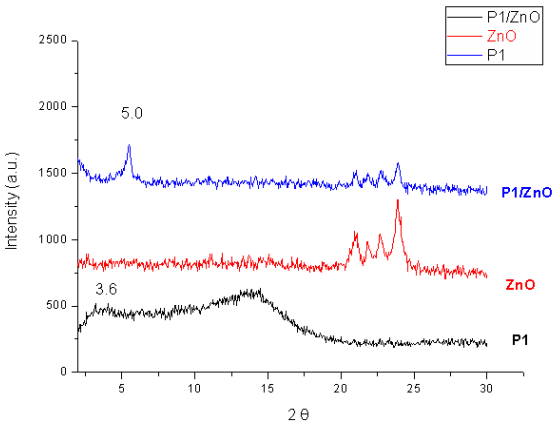

Figure2. Powder X-ray diffraction spectra of hydrogen bonded complex of pyridyl-modified ZnO nanopartcles and **P1** with 1:1 mol %.