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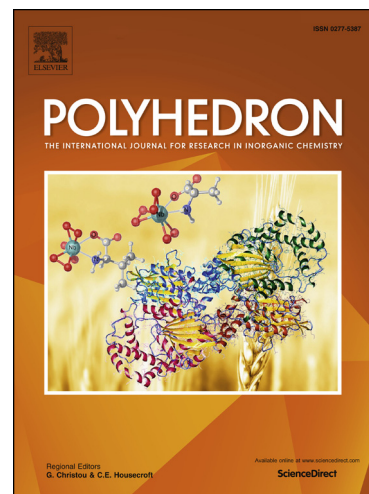
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Two Polymorphs and a Sulfate of Buprofezin: Crystal Structure and Hirshfeld Surface Analysis

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ABSTRACT :

Two different polymorphic forms and a sulfate of buprofezin were obtained by slow evaporation technique. Among them, compound **1** was formed in acetone solvent, while compounds **2-3** were gained with phosphoric acid and sulfuric acid in acetone solvent, respectively. The crystal structures of three compounds were characterized by the single-crystal X-ray diffraction, X-ray powder diffraction (XRD), Hirshfeld surface analysis, differential scanning calorimetry (DSC), thermo gravimetric analysis (TGA), Raman spectroscopy and Fourier-transform infrared spectra (FT-IR). The results revealed that the different forms had a significant effect on the crystal structures, melting points and the types of intermolecular interactions. Wherein, the melting points of the three compounds were all higher than the starting materials and follow the order of compound **1** < compound **2** < compound **3**. The structure determination showed that the main intermolecular interactions experienced by buprofezin in compounds **1-3** were H-H, C-H, O-H and S-H intermolecular interactions. In addition, the experimental results of compounds **1-2** suggested that the nature of the polymorph of buprofezin that crystallizes from solution depends on the soluble additives.

Keywords: Crystal Structure; Polymorph; Salt; Hirshfeld Surface

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