

STRUCTURE DETERMINATION OF A NEW POLYMORPH OF RACEMIC IBUPROFEN FROM LAB XRPD DATA

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Ibuprofen, 2(4-isobutylphenyl)propanoic acid, is a widely used non-steroidal anti-inflammatory drug with analgesic and antipyretic properties. Dudognon *et al* recently identified a new polymorph of ibuprofen using thermal methods although did not report the crystal structure ^[1]. The experimental conditions reported in ref 1 were used as the basis for an *in situ* variable-temperature powder diffraction experiment in which a sample of form I ibuprofen ^[2] sealed in a 0.7mm borosilicate capillary was melted at 380 K and then quench cooled to 133 K using a Cryostream 700 Series Plus device. The amorphous sample was then heated through its glass transition temperature to 258K where it was held for five hours. During this time, the powder pattern of form II ibuprofen emerged. A data set was collected at 258K in the range 3 – 70 °2θ using a variable count time collection scheme. The pattern indexed to a monoclinic space group and structure determination was attempted using the simulated annealing approach implemented in the DASH program ^[3]. The resultant disordered structure was subject to a final Rietveld refinement using the full data range in TOPAS ^[4]. Here we present the crystal structure of form II ibuprofen and contrast the solid-state structure with that of form I ibuprofen.

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[4] Coelho, A. A. (2006). Topas Academic v4.1