INFLUENCE OF POWDER DIFFRACTOMETER GEOMETRY ON THE RESULTS OF STRUCTURE DETERMINATION PROCESS OF NEW POLYMORPH OF *p*-METHYL-KETOPROFEN DERIVATIVE

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Two polymorphs of *p*-methyl-ketoprofen derivative were prepared. The crystal structure of polymorph A was solved from single crystal data. No suitable single crystals were available from polymorph B and it was not possible to determine even the unit cell parameters from single crystal data. Unit cell parameters were determined from powder data and than used to index the data collected from single crystal. Direct methods applied to the single crystal data proposed the same structural model as the "molecule location" method applied to the powder data. The structure was subsequently refined and used as a model for the investigation of the relation between powder diffractometer geometry and results of each step of the structure solving process. The following four configurations of a Philips X'PertPRO diffractometer were used to collect the data from the same sample:
-Standard Bragg-Brentano geometry with proportional detector
-Focusing geometry with X'Celerator detector
-Focusing geometry with primary beam monochromator and X'Celerator detector
-Capillary transmission configuration with primary beam Hybrid monochromator and X'Celerator detector
Results of each step of structure solving process will be discussed (indexing, space group determination, structural model determination and refinement). Conformational data will be also compared with similar structures deposited in CSD.