

ACCURATE POWDER STRUCTURAL STUDY OF PHARMACEUTICALS USING MAXIMUM ENTROPY METHOD

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We have determined the structure of prednisolone succinate by a newly developed analytical method for ab-initio structure determination and refinements from X-ray powder data. It consists of Genetic Algorithm (GA) part for structure determination process and Maximum Entropy Method (MEM) including its variations for structure refinements process. The MEM is a powerful tool for charge-density determination from a limited number of structure factors. In the structure refinements process, the various kinds of MEM analyses, such as the difference MEM, and the omit MEM analyses play crucial roles to have a better structure model in addition to the ordinary MEM. The reliability factors, R_{wp} and R_I , of the final structure analysis by the Rietveld refinement reach less than 1.3 % and 4.8 %, respectively.