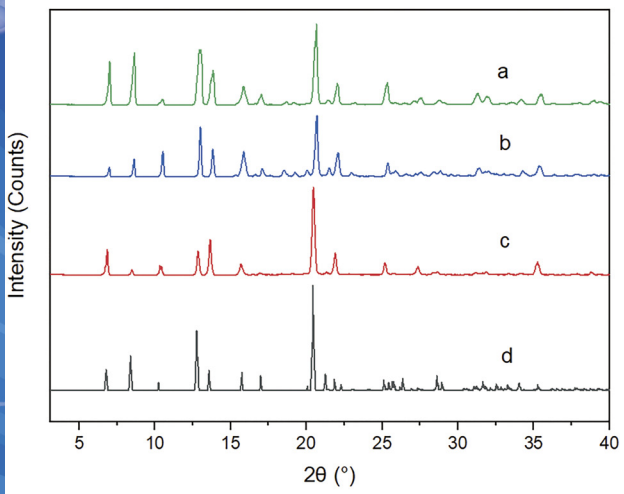
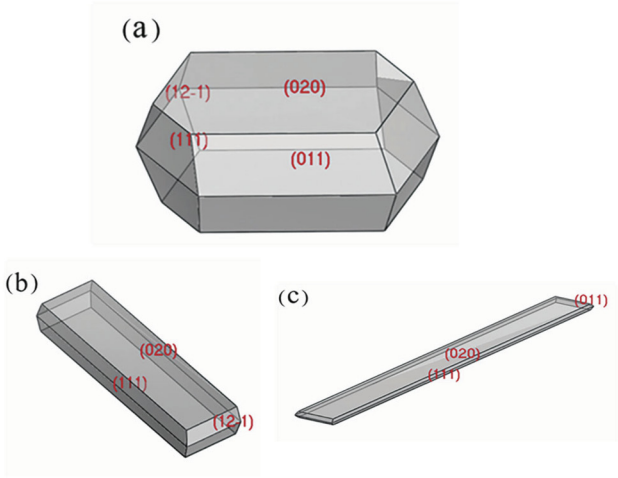
Powder Diffraction PDJ

Journal of Materials Characterization

Predicting Crystal Morphology of Venlafaxine Hydrochloride



PXRD patterns of precipitates from three solvents (a)–(c) and the calculated pattern (d) that is without preferred orientation.



Predicted crystal morphologies for each of the three precipitates

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Aims & Scope
ICDD's quarterly, and special topical issue, international journal, *Powder Diffraction*, focuses on materials characterization employing X-ray powder diffraction and related techniques. With feature articles covering a wide range of applications, from mineral analysis to epitactic growth of thin films to advances in application software and hardware, this journal offers a wide range of practical applications. ICDD, in collaboration with the Denver X-ray Conference Organizing Committee, has increased services for the subscribers of Powder Diffraction and authors of Advances in X-ray Analysis. Beginning in 2006, ICDD offered a copy of the previous year's edition of AXA to Powder Diffraction institutional subscribers who receive both print and on-line versions. This effectively doubles the number of articles annually available to Powder Diffraction subscribers and significantly increases the circulation for the authors in Advances in X-ray Analysis.

Subject coverage includes:
- Techniques and procedures in X-ray powder diffractometry
- Advances in instrumentation
- Study of materials including organic materials, minerals, metals and thin film superconductors
- Publication of powder data on new materials

International Centre for Diffraction Data
The International Centre for Diffraction Data (ICDD®) is a non-profit scientific organization dedicated to collecting, editing, publishing, and distributing powder diffraction data for the identification of materials. The membership of the ICDD consists of worldwide representation from academe, government, and industry.

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EDITORIAL

TECHNICAL ARTICLES

NEW DIFFRACTION DATA

INTERNATIONAL REPORT

CALENDARS OF MEETINGS, SHORT COURSES AND WORKSHOPS

On the Cover: In the manuscript "Crystal Morphology Prediction and Experimental Verification of Venlafaxine Hydrochloride" by C. Liang, *et al*, it was shown that modeling can be successfully used to predict the influence of solvent effects on crystal habit of venlafaxine hydrochloride. Modeling of habit of the precipitates was based on the modified attachment energy model using molecular dynamics simulation and was supported by showing the differences in the X-ray powder diffraction patterns of the three precipitates compared with the calculated pattern. Further, physical properties of the precipitates from the three solvents were shown to be related with the morphologies of the crystals.

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Please email sample patterns to:

Denise DelCasale
ICDD Grant-in-Aid Coordinator
Delcasale@icdd.com

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