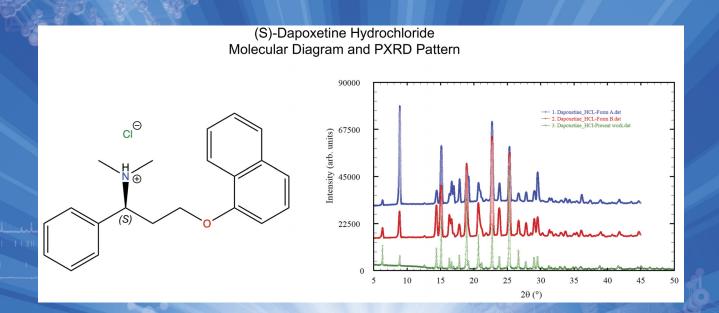
# Powder Diffraction PDJ Journal of Materials Characterization



Volume 37 / Number 04 / December 2022





### **Powder Diffraction**

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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**

Camden R. Hubbard Advancing X-ray powder data compilation and crystal structures of pharmaceutical 189

compounds

doi:10.1017/S0885715622000537

### TECHNICAL ARTICLE

Kezhou Yan, Yaru Guo,
Yuanyuan Zhang,
Yanxia Guo and
Fangqin Cheng

Comparative study of the isothermal solid-state reaction systems of kaolinite—Na<sub>2</sub>CO<sub>3</sub>
and kaolinite—quartz—Na<sub>2</sub>CO<sub>3</sub> for coal gangue activation
doi:10.1017/S0885715622000434

### **NEW DIFFRACTION DATA**

James A. Kaduk, Amy M. Gindhart, Stacy Gates-Rector and Thomas N. Blanton	Crystal structure of aminopentamide hydrogen sulfate, (C $_{19}\rm{H}_{25}N_2O)(HSO_4)$ doi:10.1017/S0885715622000343	200
James A. Kaduk, Amy M. Gindhart, Stacy Gates-Rector and Thomas N. Blanton	Crystal structure of imepitoin, C <sub>13</sub> H <sub>14</sub> ClN <sub>3</sub> O <sub>2</sub> doi:10.1017/S0885715622000392	206
James A. Kaduk, Amy M. Gindhart, Stacy Gates-Rector and Thomas N. Blanton	Crystal structure of nequinate, C <sub>22</sub> H <sub>23</sub> NO <sub>4</sub> doi:10.1017/S0885715622000379	211
Analio J. Dugarte-Dugarte, Robert A. Toro, Jacco van de Streek, José Antonio Henao, Graciela Díaz de Delgado and José Miguel Delgado	Crystal structure from laboratory X-ray powder diffraction data, DFT-D calculations, and Hirshfeld surface analysis of ( <i>S</i> )-dapoxetine hydrochloride doi:10.1017/S0885715622000380	216
James A. Kaduk, Stacy Gates-Rector and Thomas N. Blanton	Crystal structure of ponazuril, C <sub>18</sub> H <sub>14</sub> F <sub>3</sub> N <sub>3</sub> O <sub>6</sub> S doi:10.1017/S0885715622000409	225
James A. Kaduk, Stacy Gates-Rector and Thomas N. Blanton	Crystal structure of diclazuril, $C_{17}H_9Cl_3N_4O_2$ doi:10.1017/S0885715622000410	230

Crystal structure of haloxon, C<sub>14</sub>H<sub>14</sub>C<sub>13</sub>O<sub>6</sub>P

doi:10.1017/S0885715622000422

James A. Kaduk,

Thomas N. Blanton

Stacy Gates-Rector and

### **DATA REPORT**

James A. Kaduk,
Amy M. Gindhart,
Stacy Gates-Rector and
Thomas N. Blanton

Powder X-ray diffraction of altrenogest, C<sub>21</sub>H<sub>26</sub>O<sub>2</sub>
doi:10.1017/S0885715622000331

### INTERNATIONAL REPORT

Stephanie Jennings 71st Annual Denver X-ray Conference Report doi:10.1017/S0885715622000458

### CALENDARS OF MEETINGS, SHORT COURSES AND WORKSHOPS

Gang Wang Calendar of short courses and workshops doi:10.1017/S0885715622000483

Gang Wang Calendar of forthcoming meetings 249 doi:10.1017/S0885715622000471

On the Cover: In the manuscript "Crystal structure from laboratory X-ray powder diffraction data, DFT-D calculations, and Hirshfeld surface analysis of (S)-Dapoxetine Hydrochloride by Analio J. Dugarte-Dugarte, Robert A. Toro, Jacco van de Streek, Jose Antonio Henao, Graciela Diaz de Delgado, Jose Miguel Delgado the authors presented a thorough analysis of the structure of this active pharmaceutical ingredient and compared it to patterns reported in patents (Form A and Form B).

### LET OUR TEAM OF EXPERTS HELP YOU TAKE YOUR SKILLS TO THE NEXT LEVEL!



### Fundamentals of X-ray Powder Diffraction Clinic:

For the novice with some XRD knowledge or for the experienced with an interest in the theory behind XRD, this clinic offers a strong base for increased lab performance.

The clinic covers instrumentation, specimen preparation, data acquisition and qualitative phase analysis through live demonstrations. It also covers hands-on use of personal computers for demonstration of the latest software including data mining with the Powder Diffraction File (PDF) and use of the powder diffractometer: optical arrangement, factors affecting instrumentation profile width, choice and function of divergence slit, calibration and alignment, detectors, and X-ray optics.

www.icdd.com/xrd



### Advanced Methods in X-ray Powder Diffraction Clinic:

For the experienced XRD scientist, this session offers enhanced analysis skills through intense problem solving, as well as an introduction to the Rietveld Method. The course emphasizes computer-based methods of data interpretation, both for qualitative and quantitative phase analysis.

The advanced course covers a wide range of topics including systematic errors, factors affecting intensities of diffraction peaks; data reduction algorithms; phase identification; advanced data mining with the PDF and its application in search/match; powder pattern indexing methods; structure solution methods; quantitative phase analysis using both reference intensity ratio (RIR) and Rietveld Method.

www.icdd.com/xrd



### Rietveld Refinement & Indexing Clinic:

Powder pattern indexing and Rietveld structural refinement techniques are complementary and are often combined to determine the structure of a material. Successful indexing of a powder pattern is considered strong evidence for phase purity. Indexing is considered a prelude to determining the crystal structure, and permits phase identification by lattice matching techniques. This clinic introduces the theory and formalisms of various indexing methods and structural refinement techniques along with quantitative analysis. One unique aspect of this clinic is the extensive use of computer laboratory problem solving and exercises that teach method development in a hands-on environment.

www.icdd.com/rietveld



### Practical X-ray Fluorescence Clinic:

From theory to hands-on exercises, this course offers techniques and skills to improve lab performance. Discover the latest in cutting-edge instruments such as TXRF, hand-held devices, energy dispersive and wavelength dispersive spectrometers through live demonstrations.

The XRF course covers the basics of X-ray spectra; instrumentation design; methods of qualitative and quantitative analysis; specimen preparation and applications for both wavelength and energy dispersive spectrometry. The course emphasizes quantitative methods, use of automated X-ray spectrometers, review of mathematical matrix correction procedures, and new developments in XRF.

www.icdd.com/xrf

### More information at www.icdd.com/icdd-education

**Please note:** A minimum of 10 registrants per course is required, otherwise the course will be cancelled and your registration fee will be refunded. You will be notified of a course cancellation no later than two weeks prior to the start of the course.







### For More Information Contact:

Eileen Jennings, Education Coordinator Tel: 610.325.9814 Fax: 610.325.9823

Email: clinics@icdd.com

### Location

ICDD Headquarters 12 Campus Boulevard Newtown Square, Pennsylvania 19073-3273 USA

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## GRANT-IN-AID FUNDS ARE AVAILABLE DO NOT DELAY!

Proposal Submission Deadlines 31 January and 31 July

Does your research project involve the preparation and characterization of new materials using powder diffraction techniques?

If the answer is YES, then ICDD's Grant Program is the perfect fit for you!

https://www.icdd.com/grant-in-aid

Please email sample patterns to:

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

ICDD for over *80 years* has been dedicated to collecting, editing, publishing, and distributing powder diffraction data for the identification of crystalline materials. To assist us in this growth, ICDD has called on researchers from around the world to contribute their experimental data. In return, ICDD supports their efforts by funds provided through our Grant-in-Aid Program.



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