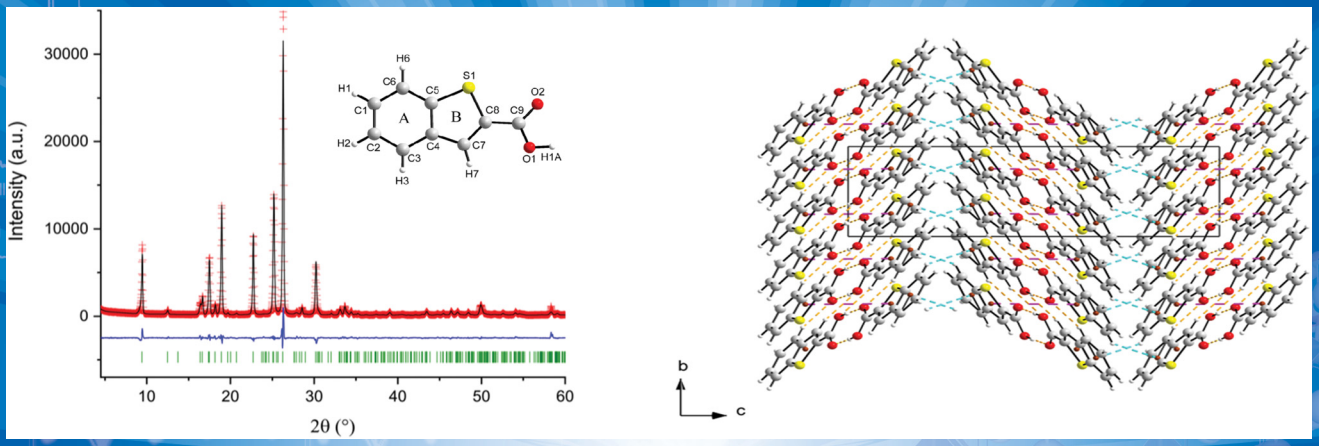
Powder Diffraction PDJ

Journal of Materials Characterization



CAMBRIDGE UNIVERSITY PRESS

Volume 36 / Number 01 / March 2021

Published online by Cambridge University Press

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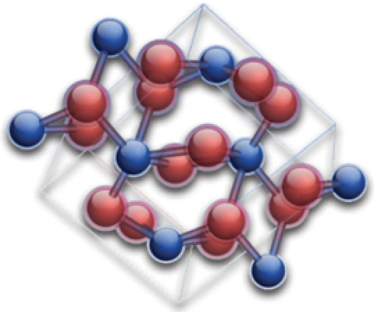

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https://doi.org/10.1017/S0885715621000142 Published online by Cambridge University Press

Powder Diffraction
An International Journal of Materials Characterization

Volume 36 Number 1 March 2021

CODEN: PODIE2
ISSN: 0885-7156

EDITORIAL

TECHNICAL ARTICLES

NEW DIFFRACTION DATA

DATA REPORTS

https://doi.org/10.1017/S0885715621000142 Published online by Cambridge University Press

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Powder Diffraction

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On the Cover: The cover figures come from the manuscript "Crystal structure from laboratory X-ray powder diffraction data, DFT+D calculations, Hirshfeld surface analysis, and energy frameworks of 1-Benzothiophene-2-carboxylic acid" (BTCA) published in this issue of Powder Diffraction by Analio J. Dugarte-Dugarte, Jacco van de Streek, Graciela Díaz de Delgado, Alicja Rafalska Lasocha, and José Miguel Delgado. This study used state-of-the-art PXRD data collection, performed both Rietveld structure solution and then applied DFT+D calculations to optimize the structure. The structure is a complex 3D arrangement involving hydrogen bonded dimers of the BTCA molecules.

The cover shows the PXRD data, Rietveld fit, atomic arrangement and molecular packing within the crystal viewed down the a-axis. The combined use of DFT optimization methods following Rietveld structure refinement is increasing in use, particularly for obtaining the best model of many solid state crystalline organic materials. These combined Rietveld and DFT optimization tools are becoming more widely used for analysis of compounds with important pharmacological activity.

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Powder Diffraction (ISSN: 0885-7156) is published quarterly (4X annually) by the JCPDS-International Centre for Diffraction Data through Cambridge University Press, One Liberty Plaza, 20th floor, New York, NY 10006. Periodicals postage rate paid at New York, NY, and at additional mailing offices. POSTMASTER: Send address changes in the USA, Canada, and Mexico to: Powder Diffraction, Cambridge University Press, Journals Fulfillment Department, One Liberty Plaza, 20th floor, New York, NY 10006. Send address changes elsewhere to Powder Diffraction, Cambridge University Press, Journals Fulfillment Department, UPH, Shaftesbury Road, Cambridge CB2 8BS, England.

https://doi.org/10.1017/S0885715621000142 Published online by Cambridge University Press

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