

IUCr MONOGRAPHS ON CRYSTALLOGRAPHY · 14

# Polymorphism in Molecular Crystals

JOEL BERNSTEIN

INTERNATIONAL UNION OF CRYSTALLOGRAPHY  
OXFORD SCIENCE PUBLICATIONS



Gilead 2007

INTERNATIONAL UNION OF CRYSTALLOGRAPHY  
BOOK SERIES

---

IUCr BOOK SERIES COMMITTEE

E. N. Baker, *New Zealand*  
J. Bernstein, *Israel*  
G. R. Desiraju, *India*  
A. M. Glazer, *UK*  
J. R. Helliwell, *UK*  
P. Paufler, *Germany*  
H. Schenk, (*Chairman*), *The Netherlands*

## IUCr Monographs on Crystallography

- 1 *Accurate molecular structures*  
A. Domenicano, I. Hargittai, editors
- 2 *P. P. Ewald and his dynamical theory of X-ray diffraction*  
D. W. J. Cruickshank, H. J. Juretschke, N. Kato, editors
- 3 *Electron diffraction techniques, Vol. 1*  
J. M. Cowley, editor
- 4 *Electron diffraction techniques, Vol. 2*  
J. M. Cowley, editor
- 5 *The Rietveld method*  
R. A. Young, editor
- 6 *Introduction to crystallographic statistics*  
U. Shmueli, G. H. Weiss
- 7 *Crystallographic instrumentation*  
L. A. Aslanov, G. V. Fetisov, G. A. K. Howard
- 8 *Direct phasing in crystallography*  
C. Giacovazzo
- 9 *The weak hydrogen bond*  
G. R. Desiraju, T. Steiner
- 10 *Defect and microstructure analysis by diffraction*  
R. L. Snyder, J. Fiala and H. J. Bunge
- 11 *Dynamical theory of X-ray diffraction*  
A. Authier
- 12 *The chemical bond in inorganic chemistry*  
I. D. Brown
- 13 *Structure determination from power diffraction data*  
W. I. F. David, K. Shankland, L. B. McCusker, and Ch. Baerlocher, editors
- 14 *Polymorphism in molecular crystals*  
J. Bernstein
- 15 *Crystallography of modular materials*  
G. Ferraris, E. Makovicky, S. Merlino
- 16 *Diffuse x-ray scattering and models of disorder*  
T. R. Welberry
- 17 *Crystallography of the polymethylene chain: an inquiry into the structure of waxes*  
D. L. Dorset
- 18 *Crystalline molecular complexes and compounds: structure and principles*  
F. H. Herbstein
- 19 *Molecular aggregation: structure analysis and molecular simulation of crystals and liquids*  
A. Gavezzotti
- 20 *Aperiodic crystals: from modulated phases to quasicrystals*  
T. Janssen, G. Chapuis, M. de Boissieu
- 21 *Incommensurate crystallography*  
S. van Smaalen

## IUCr Texts on Crystallography

- 1 *The solid state*  
A. Guinier, R. Julien
- 4 *X-Ray charges densities and chemical bonding*  
P. Coppens
- 5 *The basics of crystallography and diffraction, second edition*  
C. Hammond
- 6 *Crystal structure analysis: principles and practice*  
W. Clegg, editor
- 7 *Fundamentals of crystallography, second edition*  
C. Giacovazzo, editor
- 8 *Crystal structure refinement: a crystallographer's guide to SHELXL*  
P. Müller, editor
- 9 *Theories and techniques of crystal structure determination*  
U. Shmueli
- 10 *Advanced structural inorganic chemistry*  
Wai-Kee Li, Gong-Du Zhou, Thomas Mak

# Polymorphism in Molecular Crystals

JOEL BERNSTEIN

*Department of Chemistry  
Ben-Gurion University of the Negev*

CLARENDON PRESS • OXFORD  
2002

Page 4 of 81

**OXFORD**  
UNIVERSITY PRESS

Great Clarendon Street, Oxford OX2 6DP

Oxford University Press is a department of the University of Oxford.  
It furthers the University's objective of excellence in research, scholarship,  
and education by publishing worldwide in

Oxford New York

Auckland Cape Town Dar es Salaam Hong Kong Karachi  
Kuala Lumpur Madrid Melbourne Mexico City Nairobi  
New Delhi Shanghai Taipei Toronto

With offices in

Argentina Austria Brazil Chile Czech Republic France Greece  
Guatemala Hungary Italy Japan Poland Portugal Singapore  
South Korea Switzerland Thailand Turkey Ukraine Vietnam

Oxford is a registered trade mark of Oxford University Press  
in the UK and in certain other countries

Published in the United States  
by Oxford University Press Inc., New York

© Oxford University Press, 2002

The moral rights of the author have been asserted  
Database right Oxford University Press (maker)

First published 2002  
First published in paperback 2008

All rights reserved. No part of this publication may be reproduced,  
stored in a retrieval system, or transmitted, in any form or by any means,  
without the prior permission in writing of Oxford University Press,  
or as expressly permitted by law, or under terms agreed with the appropriate  
reprographics rights organization. Enquiries concerning reproduction  
outside the scope of the above should be sent to the Rights Department,  
Oxford University Press, at the address above

You must not circulate this book in any other binding or cover  
and you must impose this same condition on any acquirer

British Library Cataloguing in Publication Data  
Data available

Library of Congress Cataloging in Publication Data  
Bernstein, Joel.

Polymorphism in molecular crystals / Joel Bernstein.  
(IUCr monographs on crystallography; 14)  
Includes index.

1. Polymorphism (Crystallography) 2. Molecular crystals. I. Title. II. International  
Union of Crystallography monographs on crystallography; 14.

QD951 .B57 2002 548'.3—dc21 2001047556

Typeset by  
Newgen Imaging Systems (P) Ltd., Chennai, India  
Printed in Great Britain  
on acid-free paper by  
Biddles Ltd., King's Lynn, Norfolk

ISBN 978-0-19-850605-8 (Hbk.)  
ISBN 978-0-19-923656-5 (Pbk.)

10 9 8 7 6 5 4 3 2 1

# Explore Litigation Insights

Docket Alarm provides insights to develop a more informed litigation strategy and the peace of mind of knowing you're on top of things.

## Real-Time Litigation Alerts



Keep your litigation team up-to-date with **real-time alerts** and advanced team management tools built for the enterprise, all while greatly reducing PACER spend.

Our comprehensive service means we can handle Federal, State, and Administrative courts across the country.

## Advanced Docket Research



With over 230 million records, Docket Alarm's cloud-native docket research platform finds what other services can't. Coverage includes Federal, State, plus PTAB, TTAB, ITC and NLRB decisions, all in one place.

Identify arguments that have been successful in the past with full text, pinpoint searching. Link to case law cited within any court document via Fastcase.

## Analytics At Your Fingertips



Learn what happened the last time a particular judge, opposing counsel or company faced cases similar to yours.

Advanced out-of-the-box PTAB and TTAB analytics are always at your fingertips.

## API

Docket Alarm offers a powerful API (application programming interface) to developers that want to integrate case filings into their apps.

## LAW FIRMS

Build custom dashboards for your attorneys and clients with live data direct from the court.

Automate many repetitive legal tasks like conflict checks, document management, and marketing.

## FINANCIAL INSTITUTIONS

Litigation and bankruptcy checks for companies and debtors.

## E-DISCOVERY AND LEGAL VENDORS

Sync your system to PACER to automate legal marketing.