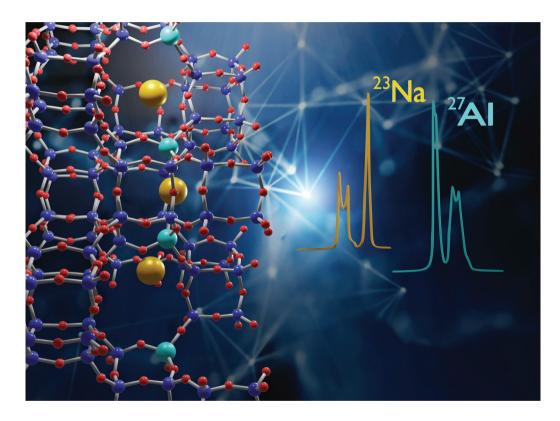
NMR Crystallography

Alan Walters Building, Birmingham, United Kingdom and online

4-6 September 2024



FARADAY DISCUSSIONS Volume 255, 2025



The Faraday Community for Physical Chemistry of the Royal Society of Chemistry, previously the Faraday Society, was founded in 1903 to promote the study of sciences lying between chemistry, physics and biology.

Editorial Staff

Executive Editor Michael A. Rowan

Deputy Editor Edward Gardner

Development Editors Bee Hockin, Andrea Carolina Ojeda-Porras

Editorial Manager Gisela Scott

Associate Editorial Manager Chris Goodall

Publishing Coordinator Konoya Das

Publishing Editors Sam Mansell and Kate Tustain

Editorial Assistant Daphne Houston

Publishing Assistants Natalie Ford and Julie-Ann Roszkowski

Publisher Sam Keltie

Faraday Discussions (Print ISSN 1359-6640, Electronic ISSN 1364-5498) is published 8 times a year by the Royal Society of Chemistry, Thomas Graham House, Science Park, Milton Road, Cambridge, UK CB4 0WF.

Volume 255 ISBN 978-1-83767-441-1

2025 annual subscription price: print+electronic £1342 US \$2363; electronic only £1279, US \$2250. Customers in Canada will be subject to a surcharge to cover GST. Customers in the EU subscribing to the electronic version only will be charged VAT.

All orders, with cheques made payable to the Royal Society of Chemistry, should be sent to the Royal Society of Chemistry Order Department, Royal Society of Chemistry, Thomas Graham House, Science Park, Milton Road, Cambridge, CB4 0WF, UK Tel +44 (0)1223 432398; E-mail orders@rsc.org

If you take an institutional subscription to any Royal Society of Chemistry journal you are entitled to free, site-wide web access to that journal. You can arrange access via Internet Protocol (IP) address at www.rsc.org/ip

Customers should make payments by cheque in sterling payable on a UK clearing bank or in US dollars payable on a US clearing bank.

Whilst this material has been produced with all due care, the Royal Society of Chemistry cannot be held responsible or liable for its accuracy and completeness, nor for any consequences arising from any errors or the use of the information contained in this publication. The publication of advertisements does not constitute any endorsement by the Royal Society of Chemistry or Authors of any products advertised. The views and opinions advanced by contributors do not necessarily reflect those of the Royal Society of Chemistry which shall not be liable for any resulting loss or damage arising as a result of reliance upon this material. The Royal Society of Chemistry is a charity, registered in England and Wales, Number 207890, and a company incorporated in England by Royal Charter (Registered No. RC000524), registered office: Burlington House, Piccadilly, London W1J 0BA, UK, Telephone: +44 (0) 207 4378 6556.

Printed in the UK

Faraday Discussions

Faradav Discussions are unique international discussion meetings that focus on rapidly developing areas of chemistry and its interfaces with other scientific disciplines.

Scientific Committee volume 255

Co-Chairs

John Griffin, Lancaster University, UK David Bryce, University of Ottawa, Andrew Morris, University of Birmingham, UK

Committee Canada Martin Dracinsky, Czech Academy of Sciences, Czech Republic Danielle Laurencin, Institut Charles

Gerhardt Montpellier, France

Sally Price, University College

London, UK

Faraday Standing Committee on Conferences

Chair

Susan Perkin, University of Oxford, UK

Secretary

Susan Weatherby, Royal Society of Chemistry, UK

George Booth, King's College London, UK Rachel Evans, University of Cambridge, UK

UK Julia Lehman, University of Birmingham, UK David Lennon, University of Glasgow, UK Andrew Mount, University of Edinburgh, UK Julia Weinstein, University of Sheffield, UK

David Fermin, University of Bristol,

Advisory Board

Vic Arcus, The University of Waikato, New Zealand Dirk Guldi, University of Erlangen-Nuremberg, Germany Marina Kuimova, Imperial College London UK Luis Liz-Marzán, CIC biomaGUNE, Spain Andrew Mount, University of Edinburgh, UK Frank Neese Max Planck Institute for Chemical Energy Conversion, Germany

Michel Orrit, Leiden University, The Netherlands Timothy Easun, Cardiff University, UK Zhong-Qun Tian, Xiamen University, China Siva Umapathy, Indian Institute of Science, Bangalore, India Bert Weckhuysen, Utrecht University, The Netherlands Iulia Weinstein, University of Sheffield, UK Sihai Yang, University of Manchester, UK

Information for Authors

This journal is © the Royal Society of Chemistry 2025 Apart from fair dealing for the purposes of research or private study for non-commercial purposes, or criticism or review, as permitted under the Copyright, Designs and Patents Act 1988 and the Copyright and Related Rights Regulation 2003, this publication may only be reproduced, stored or transmitted, in any form or by any means, with the prior permission in writing of the Publishers or in the case of reprographic reproduction in accordance with the terms of licences issued by the Copyright Licensing Agency in the UK. US copyright law is applicable to users in the USA.

The paper used in this publication meets the requirements of ANSI/NISO Z39.48-1992 (Permanence of Paper).

Registered charity number: 207890





NMR Crystallography

Faraday Discussions

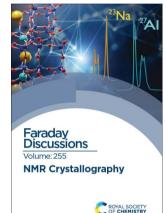
www.rsc.org/faraday_d

A General Discussion on NMR Crystallography was held in Birmingham, UK and online on 4th, 5th and 6th of September 2024.

The Royal Society of Chemistry is the world's leading chemistry community. Through our high impact journals and publications we connect the world with the chemical sciences and invest the profits back into the chemistry community.

CONTENTS

ISSN 1359-6640; ISBN 978-1-83767-441-1



Cover

See Christopher J. Heard *et al., Faraday Discuss.*, 2025, **255**, 46–71.

Zeolite structure alongside calculated NMR spectra.

Image reproduced with permission of Christopher J. Heard from Christopher J. Heard *et al., Faraday Discuss.*, 2025, **255**, 46-71.

INTRODUCTORY LECTURE

Spiers Memorial Lecture: NMR crystallography Lyndon Emsley

PAPERS AND DISCUSSIONS

- 46 A machine learning approach for dynamical modelling of Al distributions in zeolites via ²³Na/²⁷Al solid-state NMR Chen Lei, Carlos Bornes, Oscar Bengtsson, Andreas Erlebach, Ben Slater, Lukas Grajciar and Christopher J. Heard
- 72 High-throughput calculations and machine learning modeling of ¹⁷O NMR in nonmagnetic oxides Zhiyuan Li, Bo Zhao, Hongbin Zhang and Yixuan Zhang

and Christopher J. HeardHigh-throughput calculations a

Zhiyuan Li, Bo Zhao, Hongbin Zhang and fixuan Zha



FARADAY COMMUNITY FOR PHYSICAL CHEMISTRY

POSTER SPONSOR

N R SERVICE (cc) BY PROBF

BATTERY ANALYSIS TECHNOLOGY SOLUTIONS



THE OWNER

88	Characterization of ephedrine HCl and pseudoephedrine HCl using quadrupolar NMR crystallography guided crystal structure prediction Carl H. Fleischer, III, Sean T. Holmes, Kirill Levin, Stanislav L. Veinberg and Robert W. Schurko
119	The interplay of density functional selection and crystal structure for accurate NMR chemical shift predictions Sebastian A. Ramos, Leonard J. Mueller and Gregory J. O. Beran
143	Crystal structure validation of verinurad via proton-detected ultra-fast MAS NMR and machine learning Daria Torodii, Jacob B. Holmes, Pinelopi Moutzouri, Sten O. Nilsson Lill, Manuel Cordova, Arthur C. Pinon, Kristof Grohe, Sebastian Wegner, Okky Dwichandra Putra, Stefan Norberg, Anette Welinder, Staffan Schantz and Lyndon Emsley
159	Big data and simulations in NMR crystallography: general discussion
192	Accurate predictions of chemical shifts with the rSCAN and r ² SCAN mGGA exchange–correlation functionals Jonathan R. Yates and Albert P. Bartók
203	Uniform chi-squared model probabilities in NMR crystallography Leonard J. Mueller
222	Organic NMR crystallography: enabling progress for applications to pharmaceuticals and plant cell walls Zainab Rehman, Jairah Lubay, W. Trent Franks, Albert P. Bartók, Emily K. Corlett, Bao Nguyen, Garry Scrivens, Brian M. Samas, Heather Frericks-Schmidt and Steven P. Brown
244	Combined ⁷ Li NMR, density functional theory and <i>operando</i> synchrotron X-ray powder diffraction to investigate a structural evolution of cathode material LiFeV ₂ O ₇ Taiana L. E. Pereira, Jon Serrano Sevillano, Beatriz D. Moreno, Joel W. Reid, Dany Carlier and Gillian R. Goward
266	The EFG Rosetta Stone: translating between DFT calculations and solid state NMR experiments Javier Valenzuela Reina, Federico Civaia, Angela F. Harper, Christoph Scheurer and Simone S. Köcher
288	Challenges and opportunities for NMR calculations: general discussion
311	When can we trust structural models derived from pair distribution function measurements? Phillip M. Maffettone, William J. K. Fletcher, Thomas C. Nicholas, Volker L. Deringer,

Phillip M. Maffettone, William J. K. Fletcher, Thomas C. Nicholas, Volker L. Deringer, Jane R. Allison, Lorna J. Smith and Andrew L. Goodwin

325 The essential synergy of MD simulation and NMR in understanding amorphous drug forms

Jamie L. Guest, Esther A. E. Bourne, Martin A. Screen, Mark R. Wilson, Tran N. Pham and Paul Hodgkinson

This article is licensed under a Creative Commons Attribution 3.0 Unported Licence.

ÅЗ

Open Access Article. Published on 10 January 2025. Downloaded on 8/29/2025 4:51:03 AM.

342 Atomic-level structure of the amorphous drug atuliflapon via NMR crystallography Jacob B. Holmes, Daria Torodii, Martins Balodis, Manuel Cordova, Albert Hofstetter, Federico Paruzzo, Sten O. Nilsson Lill, Emma Eriksson, Pierrick Berruver, Bruno Simones de Almeida, Mike Quayle, Stefan Norberg, Anna Svensk Ankarberg, Staffan Schantz and Lyndon Emsley Investigating the effect of particle size distribution and complex exchange dynamics on NMR spectra of ions diffusing in disordered porous carbons through a mesoscopic model El Hassane Lahrar and Céline Merlet 370 First-principles NMR of oxide glasses boosted by machine learning Thibault Charpentier 391 Generating models that describe complex disorder: general discussion 411 Tracking Li atoms in real-time with ultra-fast NMR simulations Angela F. Harper, Tabea Huss, Simone S. Köcher and Christoph Scheurer 429 Metastable layered lithium-rich niobium and tantalum oxides via nearly instantaneous cation exchange Sarah L. Ko. Jordan A. Dorrell. Andrew J. Morris and Kent J. Griffith 451 Temperature-induced mobility in octacalcium phosphate impacts crystal symmetry: water dynamics studied by NMR crystallography Adam Nelson, Wassilios Papawassiliou, Subhradip Paul, Sabine Hediger, Ivan Hung, Zhehong Gan, Amrit Venkatesh, W. Trent Trent Franks, Mark E. Smith, David Gajan, Gaël De Paëpe, Christian Bonhomme, Danielle Laurencin and Christel Gervais Exploring the crystallisation of aspirin in a confined porous material using solid-state nuclear magnetic resonance Marie Juramy, Eric Besson, Stéphane Gastaldi, Fabio Ziarelli, Stéphane Viel, Giulia Mollica and Pierre Thureau 495 Probing assembly/disassembly of ordered molecular hydrogels Susana M. Ramalhete, Karol P. Nartowski, Hayley Green, Jesús Angulo, Dinu luga, László Fábián, Gareth O. Lloyd and Yaroslav Z. Khimyak NMR crystallization: in situ NMR strategies for monitoring the evolution of crystallization processes Colan E. Hughes, Naomi V. Ratnasingam, P. Andrew Williams, Erwan Benhenou, Rhian Patterson and Kenneth D. M. Harris Understanding dynamics and mechanisms: general discussion

CONCLUDING REMARKS

Concluding remarks: Faraday Discussion on NMR crystallography Sharon E. Ashbrook

ADDITIONAL INFORMATION

- Poster titles
- 604 List of participants