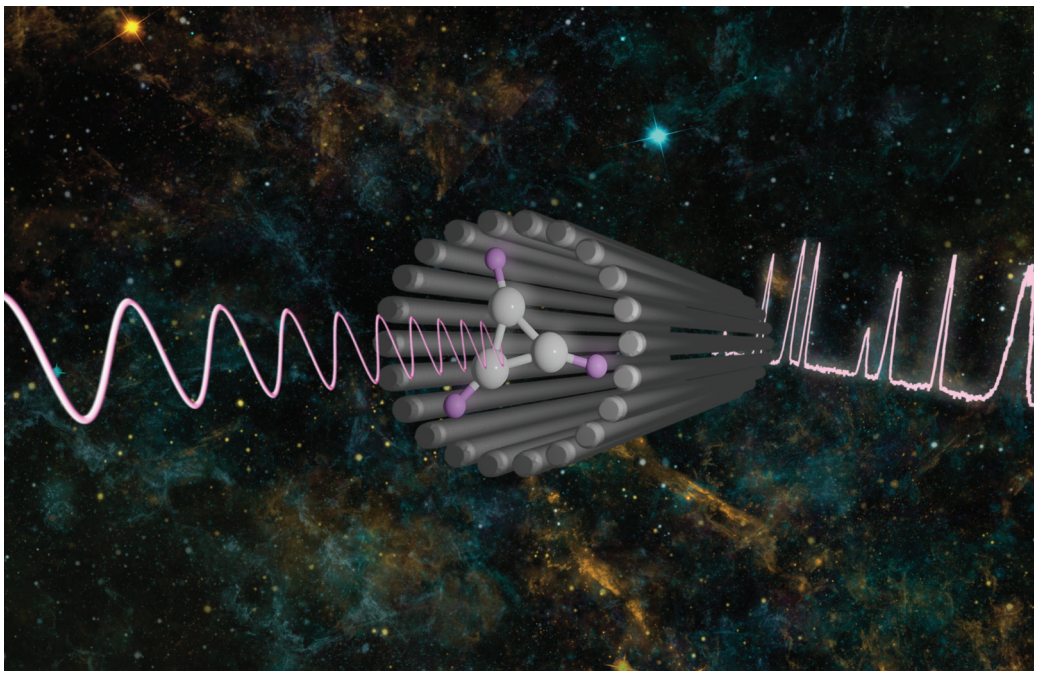
Astrochemistry at high resolution

Space Telescope Science Institute,
Baltimore, USA and online
31 May - 2 June 2023



FARADAY DISCUSSIONS

Volume 245, 2023

ROYAL SOCIETY OF CHEMISTRY

Open Access Article. Published on 25 September 2023. Downloaded on 10/21/2025 6:23:49 AM.
This article is licensed under a Creative Commons Attribution 3.0 Unported Licence.

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
Vikki Pritchard

Development Editors
Bee Hockin, Andrea Carolina Ojeda Porras

Editorial Production Manager
Gisela Scott

Senior Publishing Editor
Robin Brabham

Publishing Editors
Samuel Howell and Sam Oldknow

Editorial Assistant
Daphne Houston

Publishing Assistants
Natalie Ford and Huw Hedges

Publisher
Jeanne Andres

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 245 ISBN 978-1-83767-092-5

2023 annual subscription price: print+electronic £1223 US $2154; electronic only £1165, US $2051.
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

MIX
Paper from responsible sources
FSC® C013604
FSC www.fsc.org

ROYAL SOCIETY OF CHEMISTRY

Faraday Discussions

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

Scientific Committee volume 245

Chair
Martin R. S. McCoustra, Heriot-Watt University, UK

Ian R. Sims, University of Rennes, France
Paola Caselli, Max Planck Institute for Extra-terrestrial Physics, Germany
Susanna Widicus Weaver, University of Wisconsin-Madison, United States
Anthony J. H. M. Meijer, University of Sheffield, UK
Nick Walker, University of Newcastle, UK
Neill Reid, Space Telescope Science Institute, United States

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
David Fermin, University of Bristol, UK
Dwayne Heard, University of Leeds, UK
David Lennon, University of Glasgow, UK
Angelos Michaelides, University College London, UK
Julia Weinstein, University of Sheffield, UK

Advisory Board

Vic Arcus, The University of Waikato, New Zealand
Timothy Easun, Cardiff University, UK
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
Zhong-Qun Tian, Xiamen University, China
Siva Umapathy, Indian Institute of Science, Bangalore, India
Bert Weckhuysen, Utrecht University, The Netherlands
Julia Weinstein, University of Sheffield, UK
Sihai Yang, University of Manchester, UK

Information for Authors

This journal is © the Royal Society of Chemistry 2023 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

Open Access Article. Published on 25 September 2023. Downloaded on 10/21/2025 6:23:49 AM.
This article is licensed under a Creative Commons Attribution 3.0 Unported Licence.

Astrochemistry at High Resolution

Faraday Discussions

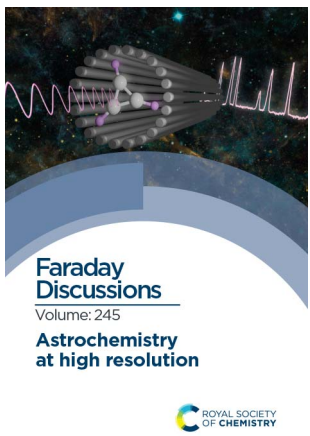
www.rsc.org/faraday_d

A General Discussion on Astrochemistry at High Resolution was held in Baltimore, USA and online on the 31st May, 1st June and 2nd June 2023.

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 978-1-83767-092-5



Cover
See Asvany *et al.*, *Faraday Discuss.*, 2023, **245**, 298–308.

Spectrum of a cyclic hydrocarbon ion measured using an ion trap is shown in the context of space.

Image reproduced with permission of Divita Gupta from Asvany *et al.*, *Faraday Discuss.*, 2023, **245**, 298–308.

PREFACE

9 **Astrochemistry at high resolution: preface**
Martin R. S. McCoustra

INTRODUCTORY LECTURE

11 **Spiers Memorial Lecture: Astrochemistry at high resolution**
Cecilia Ceccarelli

PAPERS AND DISCUSSIONS

52 **The diverse chemistry of protoplanetary disks as revealed by JWST**
Sedigheh Alavinia, Ramin Ghorbani-Vaghei, Ramin Ghiai and Alireza Gharekhani

ROYAL SOCIETY OF CHEMISTRY | FARADAY COMMUNITY FOR PHYSICAL CHEMISTRY

Open Access Article. Published on 25 September 2023. Downloaded on 10/21/2025 6:23:49 AM.
This article is licensed under a Creative Commons Attribution 3.0 Unported Licence.

Open Access Article. Published on 25 September 2023. Downloaded on 10/21/2025 6:23:49 AM.
This article is licensed under a Creative Commons Attribution 3.0 Unported Licence.

80 **Chemical conditions on Hycean worlds**
Nikku Madhusudhan, Julianne I. Moses, Frances Rigby and Edouard Barrier

112 **The chemical inventory of the inner regions of planet-forming disks – the JWST/MINDS program**
I. Kamp *et al.*

138 **New interstellar laboratories in the molecular ring**
Olivia H. Wilkins and Geoffrey A. Blake

164 **Streamers feeding the SVS13-A protobinary system: astrochemistry reveals accretion shocks?**
Eleonora Bianchi, Ana López-Sepulcre, Cecilia Ceccarelli, Claudio Codella, Linda Podio, Mathilde Bouvier, Joan Enrique-Romero, Rafael Bachiller and Bertrand Lefloch

181 **Tracing the chemical footprint of shocks in AGN-host and starburst galaxies with ALMA multi-line molecular studies**
Ko-Yun Huang and Serena Viti

199 **Observational astrochemistry in the age of ALMA, NOEMA, JWST and beyond!: general discussion**

221 **Fingerprinting fragments of fragile interstellar molecules: dissociation chemistry of pyridine and benzonitrile revealed by infrared spectroscopy and theory**
Daniël B. Rap, Aude Simon, Kim Steenbakkers, Johanna G. M. Schrauwen, Britta Redlich and Sandra Brünken

245 **Kinetics of CN ($v = 1$) reactions with butadiene isomers at low temperature by cw-cavity ring-down in a pulsed Laval flow with theoretical modelling of rates and entrance channel branching**
Shameemah Thawoos, Gregory E. Hall, Carlo Cavallotti and Arthur G. Suits

261 **Experimental, theoretical, and astrochemical modelling investigation of the gas-phase reaction between the amidogen radical (NH_2) and acetaldehyde (CH_3CHO) at low temperatures**
Kevin M. Douglas, Lok Hin Desmond Li, Catherine Walsh, Julia H. Lehman, Mark A. Blitz and Dwayne E. Heard

284 **Searches for bridged bicyclic molecules in space—norbornadiene and its cyano derivatives**
Marie-Aline Martin-Drumel, Jean-Thibaut Spaniol, Helen Hölzel, Marcelino Agúndez, Jose Cernicharo, Kasper Moth-Poulsen and Ugo Jacovella

298 **High-resolution rovibrational and rotational spectroscopy of the singly deuterated cyclopropenyl cation, c-$C_3H_2D^+$**
Divita Gupta, Weslley G. D. P. Silva, José L. Doménech, Eline Plaar, Sven Thorwirth, Stephan Schlemmer and Oskar Asvany

309 **Hunting for interstellar molecules: rotational spectra of reactive species**
Cristina Puzzarini, Silvia Alessandrini, Luca Bizzocchi and Mattia Melosso

327 **An experimental and theoretical investigation of the $N(^2D) + C_6H_6$ (benzene) reaction with implications for the photochemical models of Titan**
Nadia Balucani, Adriana Caracciolo, Gianmarco Vanuzzo, Dimitrios Skouteris, Marzio Rosi, Leonardo Pacifici, Piergiorgio Casavecchia, Kevin M. Hickson, Jean-Christophe Loison and Michel Dobrijevic

Open Access Article. Published on 25 September 2023. Downloaded on 10/21/2025 6:23:49 AM.
This article is licensed under a Creative Commons Attribution 3.0 Unported Licence.

352 **Experimental radiative cooling rates of a polycyclic aromatic hydrocarbon cation**
José E. Navarro Navarrete, James N. Bull, Henrik Cederquist, Suvasthika Indrajith, MingChao Ji, Henning T. Schmidt, Henning Zettergren, Boxing Zhu and Mark H. Stockett

368 **Direct frequency comb spectroscopy of HCN to evaluate line lists**
D. Michelle Bailey, Eric M. Crump, Joseph T. Hodges and Adam J. Fleisher

380 **Size distribution of polycyclic aromatic hydrocarbons in space: an old new light on the 11.2/3.3 μm intensity ratio**
Alexander K. Lemmens, Cameron J. Mackie, Alessandra Candian, Timothy M. J. Lee, Alexander G. G. M. Tielens, Anouk M. Rijs and Wybren Jan Buma

391 **Laboratory astrochemistry of the gas phase: general discussion**

446 **Infrared photodesorption of CO from astrophysically relevant ices studied with a free-electron laser**
Emily R. Ingman, Domantas Laurinavicius, Jin Zhang, Johanna G. M. Schrauwen, Britta Redlich, Jennifer A. Noble, Sergio Ioppolo, Martin R. S. McCoustra and Wendy A. Brown

467 **Thermal behavior of astrophysical amorphous molecular ices**
Murthy S. Gudipati, Benjamin Fleury, Robert Wagner, Bryana L. Henderson, Kathrin Altwegg and Martin Rubin

488 **Vacuum UV photodesorption of organics in the interstellar medium: an experimental study of formic acid HCOOH and methyl formate $HCOOCH_3$-containing ices**
Mathieu Bertin, Romain Basalgète, Antonio J. Ocaña, Géraldine Féraud, Claire Romanzin, Laurent Philippe, Xavier Michaut and Jean-Hugues Fillion

508 **A systematic mechanistic survey on the reactions between OH radical and CH_3OH on ice**
W. M. C. Sameera, Avon P. Jayaweera, Atsuki Ishibashi, Hiroshi Hidaka, Yasuhiro Oba and Naoki Watanabe

519 **Laboratory astrochemistry of and on dust and ices: general discussion**

541 **Preferential destruction of NH_2-bearing complex interstellar molecules *via* gas-phase proton-transfer reactions**
Robin T. Garrod and Eric Herbst

569 **A statistical and machine learning approach to the study of astrochemistry**
Johannes Heyl, Serena Viti and Gijs Vermariën

586 **Disentangling physics and chemistry in AGB outflows: revealing degeneracies when adding complexity**
Marie Van de Sande, Catherine Walsh and Tom J. Millar

609 **Predicting observable infrared signatures of nanosilicates in the diffuse interstellar medium**
Sascha T. Zeegers, Joan Mariñoso Guiu, Francisca Kemper, Jonathan P. Marshall and Stefan T. Bromley

620 **Computational astrochemistry: general discussion**

CONCLUDING REMARKS

638 **Concluding remarks: *Faraday Discussion* on astrochemistry at high resolution**
T. J. Millar

ADDITIONAL INFORMATION

651 **Poster titles**

653 **List of participants**

 This journal is © The Royal Society of Chemistry 2023