Atmospheric chemistry in cold environments

Burlington House, London, UK and online 17–19 February 2025



FARADAY DISCUSSIONS Volume 258, 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 Claire Hedgecott and Evie Karkera

Editorial Assistant Daphne Houston

Publishing Assistants David Bishop and Lee Colwill

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 258 ISBN 978-1-83767-838-9

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 258

Chair Thorsten Bartels-Rausch, Paul Scherrer Institute, Switzerland Committee

Dwayne Heard, University of Leeds, UK Natasha Garner, Paul Scherrer Institute, Switzerland Bill Simpson, University of Alaska Fairbanks, USA Jennie L. Thomas, Université Grenoble Alpes, CNRS, France

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 Timothy Easun, Cardiff University, UK Zhong-Qun Tian, Xiamen University, 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 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





Atmospheric chemistry in cold environments

Faraday Discussions

www.rsc.org/faraday_d

A General Discussion on Atmospheric chemistry in cold environments was held in London, UK and online on the 17th, 18th and 19th of February 2025.

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 978-1-83767-838-9



Cover

See Toubin *et al., Faraday Discuss.,* 2025, **258**, 396–418.

Unveiling the influence of molecular arrangement on early-stage heterogeneous ice nucleation in organic aerosols.

Image reproduced with permission of Céline Toubin from *Faraday Discuss.*, 2025, **258**, 396–418.

INTRODUCTORY LECTURE

10 Ten crucial unknowns in atmospheric chemistry in the cold Thorsten Bartels-Rausch, Jessie Creamean, Jennie L. Thomas, Megan Willis and Paul Zieger

PAPERS AND DISCUSSIONS

- 23 In situ measurements of gas-particle partitioning of organic compounds in Fairbanks Amna Ijaz, Brice Temime-Roussel, Julien Kammer, Jingqiu Mao, William Simpson, Kathy S. Law and Barbara D'Anna
- 40 Biotic and abiotic factors controlling isoprene, DMS, and oxygenated volatile organic compounds (VOCs) at the Southern Ocean in the Austral fall Saewung Kim, Roger Seco, Daun Jeong, Alex Guenther, Kitae Kim, Ahra Mo, Jung-Ok Choi, Jisoo Park and Keyhong Park





surface ocean Solas lower atmosphere study

POSTER SPONSORSHIP



Environmental Science Atmospheres



Environmental Science Processes & Impacts



Environmental Science Advances

50 Direct high-altitude observations of 2-methyltetrols in the gas- and particle phase in air masses from Amazonia

Claudia Mohr, Joel A. Thornton, Manish Shrivastava, Anouck Chassaing, Ilona Riipinen, Federico Bianchi, Marcos Andrade and Cheng Wu

76 The impact of the Himalayan aerosol factory: results from high resolution numerical modelling of pure biogenic nucleation over the Himalayan valleys Giancarlo Ciarelli, Arineh Cholakian, Manuel Bettineschi, Bruno Vitali, Bertrand Bessagnet, Victoria A. Sinclair, Johannes Mikkola, Imad el Haddad, Dino Zardi,

Angela Marinoni, Alessandro Bigi, Paolo Tuccella, Jaana Bäck, Hamish Gordon, Tuomo Nieminen, Markku Kulmala, Douglas Worsnop and Federico Bianchi

- **Terrestrial and marine sources of ice nucleating particles in the Eurasian Arctic** Guangyu Li, André Welti, Arianna Rocchi, Germán Pérez Fogwill, Manuel Dall'Osto and Zamin A. Kanji
- 120 A comprehensive characterisation of natural aerosol sources in the high Arctic during the onset of sea ice melt

Gabriel Pereira Freitas, Julia Kojoj, Camille Mavis, Jessie Creamean, Fredrik Mattsson, Lovisa Nilsson, Jennie Spicker Schmidt, Kouji Adachi, Tina Šantl-Temkiv, Erik Ahlberg, Claudia Mohr, Ilona Riipinen and Paul Zieger

- **147** Transport of continental particulate over the Labrador Sea and entrainment are important pathways for glaciation of remote marine clouds Hugh Coe, Huihui Wu, Nicholas Marsden, Michael Biggart, Keith N. Bower, Tom Choularton, Michael Flynn, Martin W. Gallagher, Kezhen Hu, Gary Lloyd, Graeme J. Nott, Paul F. Field and Benjamin J. Murray
- 171 Aerosol, clouds and particles: general discussion
- **201 Processes regulating the sources and sinks of ammonia in the Canadian Arctic** Jennifer G. Murphy, Gregory R. Wentworth, Alexander Moravek, Douglas B. Collins and Sangeeta Sharma
- 216 Ongoing large ozone depletion in the polar lower stratospheres: the role of increased water vapour Martyn P. Chipperfield, Saffron G. Heddell, Sandip S. Dhomse, Wuhu Feng,

Martyn P. Chipperfield, Saffron G. Heddell, Sandip S. Dhomse, Wuhu Feng Shujie Chang, Graham Mann, Xin Zhou and Hugh C. Pumphrey

- 234 Modeling attainment in Fairbanks, Alaska, for the wintertime PM_{2.5} 24-hour nonattainment area using the CMAQ (community multi-scale air quality) model Deanna Huff, Tom Carlson, Lakshmi Pradeepa Vennam, Chao-Jung Chien, Kathleen Fahey, Robert Gilliam and Nick Czarnecki
- 265 Arctic tropospheric ozone seasonality, depletion, and oil field influence Evelyn M. Widmaier, Andrew R. Jensen and Kerri A. Pratt
- 293 Impacts of Arctic oil field NO_x emissions on downwind bromine chemistry: insights from 5 years of MAX-DOAS observations Peter K. Peterson, Kerri A. Pratt, Paul B. Shepson and William R. Simpson
- 307 Low-cost electrochemical gas sensing of vertical differences in wintertime air composition (CO, NO, NO₂, O₃) in Fairbanks, Alaska Tjarda J. Roberts, Meeta Cesler-Maloney and William R. Simpson
- 328 Transport and chemistry: general discussion

Amna Ijaz, Brice Temime-Roussel, Barbara D'Anna, Damien Ketcherside, James H. Flynn, Jason M. St. Clair, Athanasios Nenes and Rodney J. Weber component films at 21 °C and 3 °C Ben Woden, Yizhou Su, Maximilian W. A. Skoda, Adam Milsom and Christian Pfrang 396 Unraveling aqueous alcohol freezing: new theoretical tools from graph theory to extract molecular processes in MD simulations Rawan AbouHaidar, Sana Bouqueroua, Denis Duflot, Marie-Pierre Gaigeot, Barbara Wyslouzil and Céline Toubin 419 Multiphase chemistry: general discussion 441 lodine speciation in snow during the MOSAiC expedition and its implications for Arctic iodine emissions Hans-Werner Jacobi, Markus M. Frey, Stephen D. Archer, Stefanie Arndt, Johannes G. M. Barten, Byron W. Blomquist, Ruzica Dadic, Laurens N. Ganzeveld, Henna-Reetta Hannula, Detlev Helmig, Matthias Jaggi, Daniela Krampe, Amy R. Macfarlane, Shaun Miller, Martin Schneebeli and Lucy J. Carpenter 473 Sönke Maus The interplay between snow and polluted air masses in cold urban environments Jonas Kuhn, Jochen Stutz, Thorsten Bartels-Rausch, Jennie L. Thomas, Meeta Cesler-Maloney, William R. Simpson, Jack E. Dibb, Laura M. D. Heinlein and Cort Anastasio Elucidating how trace gases interact with ice surfaces utilizing sum frequency generation spectroscopy Gurivi Reddy Yettapu, Luca B. Manning and Jenée D. Cyran

Uptake of ammonia by ice surfaces at atmospheric temperatures Clemens Richter, Shirin Gholami, Yanisha Manoharan, Tillmann Buttersack, Luca Longetti, Luca Artiglia, Markus Ammann, Thorsten Bartels-Rausch and Hendrik Bluhm

Trapping intermediates of the NO₂ hydrolysis reaction on ice Josée Maurais, Clément Wespiser, Raphaël Robidas, Claude Y. Legault and Patrick Avotte

Snow and ice: general discussion

CONCLUDING REMARKS

Concluding remarks: Atmospheric chemistry in cold environments Markus Ammann

ADDITIONAL INFORMATION

- 614 Poster titles
- List of participants

Multiphase sulfur chemistry facilitates particle growth in a cold and dark urban environment

Jingqiu Mao, Kunal Bali, James R. Campbell, Ellis S. Robinson, Peter F. DeCarlo, Robert J. Yokelson, Lu Hu, Meeta Cesler-Maloney, William R. Simpson, Fangzhou Guo,

Oxidation by ozone of linoleic acid monolayers at the air-water interface in multi-

Lucy V. Brown, Ryan J. Pound, Matthew R. Jones, Matthew J. Rowlinson, Rosie Chance,

Growth rate dependence of the permeability and percolation threshold of young sea ice