
LEONARD JAMES BARBOUR

Distinguished Professor of Chemistry
Department of Chemistry and Polymer Science
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Education

- (2013) DSc, Stellenbosch University (SU),
Promotor: C. Esterhuysen
Thesis title: "*Mass transport phenomena in the crystalline solid state*"
 - (1994) PhD, University of Cape Town (UCT),
Advisors: L. R. Nassimbeni and M. R. Caira
Thesis title: "*Clathration by Diol Hosts: Thermodynamics and Structure*"
 - (1989) MSc, University of Cape Town
Advisors: A. L. Rodgers and M. A. B. Pougnet
Thesis title: "*Trace Elements in Relation to Urolithiasis*"
 - (1987) BSc (HONS), University of Cape Town
 - (1986) BSc, University of Cape Town
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Professional Experience

- 2021 – 2025 Distinguished Professor, SU
 - 2016 – 2020 Distinguished Professor, SU
 - 2017 – 2021 SA Research Chair in Nanostructured Functional Materials (2nd renewal)
 - 2012 – 2016 SA Research Chair in Nanostructured Functional Materials (1st renewal)
 - 2007 – 2011 SA Research Chair in Nanostructured Functional Materials
 - September 2005 – present Professor, SU
 - July 2003 – August 2005 Associate Professor, SU
 - June 1997- June 2003 Research Assistant Professor, University of Missouri – Columbia (UMC)
 - June 1994 – May 1997 Postdoctoral Fellow, UMC
 - 1993 - March 1994 Research Officer, UCT
 - 1992 Lecturer, UCT
 - 1987 to 1991 Teaching Assistant, UCT
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Awards & Honours

- John Herschel Medal of the Royal Society of South Africa, 2020
 - Chancellor's Award for Research, Stellenbosch University, 2017
 - Distinguished Professor, Stellenbosch University, 2016-2020 and 2021-2025
 - South African Chemical Institute Gold Medal, 2014
 - Invited Visiting Professor, University of Strasbourg, May 2014
 - Victor Pretorius Lectures, University of Pretoria, February 2014
 - SASOL Innovator of the Year Award, 2013
 - Fellow of the Royal Society of Chemistry (FRSC) (2013-)
 - Fellow of the Royal Society of South Africa (FRSSAf) (2008-)
 - NRF A2 Rating 2005-2009, 2010-2015 and 2016-2021
 - NRF A1 Rating 2022-2027
 - National Science and Technology Forum Award for "Research and its Outputs Over the Past 5 Years or Less" (2007/2008)
 - Rector's Award for Outstanding Research (2007, Stellenbosch University)
 - American Institute of Chemists Foundation & the St. Louis Institute of Chemists Postdoctoral Award (1997)
 - Foundation for Research Development Studentship (1990 & 1991)
 - Foundation for Research Development Scholarship (1988 & 1989)
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Postdoctoral Fellow Supervision

- Xeuting Wei 2023
- Alexios Vicatos 2023 – current
- Annelies de Cuyper 2021 – 2022
- Phumile Sikiti 2019 – 2021
- Somananda Sanyal 2018 – 2020
- Dominic Castell 2017 – 2018
- Leigh Loots 2017 – 2021
- Arpan Hazra 2016 – 2020
- Himanshu Aggarwal 2016
- Varvara Nikolayenko 2016 – 2018
- Banele Vatsa 2015 – 2017
- Prem Lama 2013 – 2017, Claude Leon Foundation Fellowship
- Agnieszka Janiak 2012 – 2014, NRF Innovation Postdoctoral Fellowship
- Raj Kumar Das 2012 – 2015
- Simon Herbert 2012 – 2013
- Matteo Lusi 2009 – 2012, Claude Leon Foundation Fellowship
- Vincent Smith 2009 – 2013
- Tia Jacobs 2009 – 2010, 2012 – 2013
- Prashant Bhatt 2009 – 2012, Claude Leon Foundation Fellowship
- Subhadip Neogi 2008 – 2009
- Dinabandhu Das 2007 – 2010
- Charlotte Willans 2006 – 2008, Leverhulme Trust
(shared with Profs J. W. Steed and P. C. Junk)
- Greta Heydenrych 2006, NRF Postdoctoral Fellowship
- Clive Oliver 2005 – 2007, Claude Leon Foundation Fellowship
- Elise de Vries 2005 – 2006, NRF Innovation Postdoctoral Fellowship
- Liliana Dobrzańska 2004 – 2006, Claude Leon Foundation Fellowship

PhD Student Supervision

• Rolivhuwa Mahwasane	2021 – current
• Leena Patel	2021 – current
• Shane de Beer	2021 – current
• Banele Motlounge	2020 – current
• Xeuting Wei	2020 – 2022
• Alan Eaby	2020 – 2022
• Jan Costandius	2019 – 2021
• Lisa van Wyk	2019 – 2021
• Isabella Claassens	2018 – 2019
• Mpho Ledwaba	2016 – 2021
• Wesley Feldmann	2016 – 2020
• Dewald van Heerden	2015 – 2020
• Lukman Alimi	2013 – 2018
• Phumile Sikiti	2013 – 2018
• Emile Engel	2013 – 2016
• Himanshu Aggarwal	2012 – 2015
• Varvara Nikolayenko	2012 – 2015
• Marike du Plessis	2012 – 2019
• Charl Bezuidenhout	2011 – 2017
• IIne Grobler, Upgraded to PhD	2010 – 2013
• Anneli Kleyn, Upgraded to PhD	2011 – 2012
• James Odendal	2010 – 2014
• Eustina Batisai	2010 – 2013
• Storm Potts	2009 – 2011
• Leigh Loots	2009 – 2012
• Tia Jacobs, Upgraded to PhD	2007 – 2009

MSc Student Supervision

• Raymond van Rijn	2022 – current
• Aluwani Kutama	2022 – current
• Gundo Mathada	2022 – current
• Nonhlanhla Dhlamini	2021 – 2022
• Jiajia Ye	2020 – 2021, Graduated with Distinction
• Xeuting Wei	2018 – 2019
• Alan Eaby	2018 – 2019, Graduated with Distinction
• Lisa van Wyk	2017 – 2018, Upgraded to PhD
• Jan Costandius	2017 – 2018, Upgraded to PhD
• Jeanice Basson	2016 – 2017, Graduated with Distinction
• Natasha Visser	2016 – 2017
• Dirkie Myburgh	2016 – 2017
• Isabella Claassens	2016 – 2017, Upgraded to PhD
• Kerry White	2016 – 2017, Graduated with Distinction
• Dawie de Villiers	2013 – 2014, Graduated with Distinction
• Dewald van Heerden	2012 – 2014, Graduated with Distinction
• Marike Du Plessis	2010 – 2011, Graduated with Distinction
• IIne Grobler	2010 – 2011, Upgraded to PhD
• Charl Bezuidenhout	2009 – 2010, Graduated with Distinction
• Guillaume Greyling	2009 – 2010, Graduated with Distinction
• Anneli Kleyn	2009 – 2010, Upgraded to PhD
• Eustina Batisai	2008 – 2009, Graduated with Distinction
• Storm Potts	2007 – 2008, Graduated with Distinction
• Leigh Loots	2007 – 2008, Graduated with Distinction
• Charl Marais	2007 – 2008, Graduated with Distinction
• Tia Jacobs	2005 – 2006, Upgraded to PhD
• Gareth Lloyd	2004 – 2006, Graduated with Distinction

Honours Project Supervision

- Raymond van Rijn 2021
- Anthea Farmer 2020
- Ashleigh Ye 2019
- Xeuting Wei 2017
- Lisa van Wyk 2016
- Jeanice Basson 2015
- Elaine Barnard 2013
- Dawie de Villiers 2012
- Dewald van Heerden 2011
- Marike Du Plessis 2009
- Ilne Grobler 2009
- Emile Engel 2008
- Anneli Kleyn 2008
- Leigh Loots 2006
- Storm Potts 2006
- Pieter Murray 2006
- Ilse Rootman 2005
- Tia Jacobs 2004
- Bertie Barnard 2004

Active Collaborations

- Prof. Dinabandhu Das, Jawaharlal Nehru University, New Delhi, India
- Prof. Agnieszka Janiak, Adam Mickiewicz University, Poznań, Poland
- Prof. Michael Zaworotko, University of Limerick, Ireland
- Prof. Catharine Esterhuysen, Department of Chemistry, Stellenbosch University
- Prof. Delia Haynes, Department of Chemistry, Stellenbosch University

Professional Activities

Editorial activities

- Associate Editor, *Crystal Growth and Design* (an American Chemical Society journal), 2020–
- Associate Editor, *New Journal of Chemistry* (a Royal Society of Chemistry journal), 2016 – 2019
- Associate Editor (with Jerry Atwood and George Gokel), *Comprehensive Supramolecular Chemistry*, 2nd Edition, 2017, Elsevier (a 9 volume major reference work)
- Volume Editor (*Supramolecular Chemistry – From Molecules to Nanomaterials*, Wiley VCH)
- Editorial Advisory Board, *Chemistry of Materials* (an American Chemical Society journal), 2021–
- Editorial Advisory Board, *ACS Sustainable Chemistry & Engineering* (American Chemical Society), 2018–
- Editorial Advisory Board, *Crystal Growth and Design* (American Chemical Society), 2014 – 2018
- Editorial Advisory Board, *CrystEngComm* (Royal Society of Chemistry), 2008–
- Editorial Board, *New Journal of Chemistry* (Royal Society of Chemistry), 2012 – 2015
- Guest Editor (with Jonathan Steed, Len MacGillivray and Agnieszka Szumna), 2017, *Supramolecular Chemistry* special issue.
- Guest Editor (with Mohamed Eddaoudi), 2015, *Chemical Communications*, CO₂ separation, capture and reuse: a web themed issue.
- Guest Editor (with Kari Rissanen and Len MacGillivray), 2014, *CrystEngComm*, Web-themed special issue on macrocyclic chemistry
- Co-editor: *Acta Crystallographica, Section C* (2008 – 2009)
- Co-editor: *Acta Crystallographica, Section E* (2005 – 2007)

Memberships of professional societies

- Fellow of the Royal Society of South Africa
- Fellow of the Royal Society of Chemistry
- Member of the American Chemical Society
- Member of the American Crystallographic Association
- Member of the South African Chemical Institute

International Committees

- Advisory Committee: 2014 Collaborative Conference on Crystal Growth
- International Scientific Committee (European Crystallographic School Workshop Series)
- International Advisory Board (ICCOSS Conference Series)
- International Advisory Board (ISIC Conference Series)

Local Committees

- Member of Subcommittee B, Stellenbosch University
- Central Analytical Facility, Stellenbosch University (2004 – 2012).
- Treasurer: South African Chemical Institute - Western Cape Region (2005 – 2009).
- Special Interest Group: Molecular Recognition and Inclusion, European Crystallographic Association (2004 – current).
- South African Crystallographic Association (2005 – 2011).

Reviewing

- Have reviewed numerous manuscripts for:
 - American Chemical Society: *Chemical Reviews*, *Journal of the American Chemical Society*; *Inorganic Chemistry*; *Journal of Organic Chemistry*; *Journal of Physical Chemistry*; *Crystal Growth & Design*; *Chemistry of Materials*; *Organometallics*; *Organic Letters*;
 - Royal Society of Chemistry: *Chemical Communications*; *Analytical Methods*; *CrystEngComm*; *Dalton Transactions*; *New Journal of Chemistry*, *RSC Advances*, *Chemical Science*;
 - Wiley: *Angewandte Chemie*; *Chemistry, a European Journal*; *European Journal of Inorganic Chemistry*; *European Journal of Organic Chemistry*; *ChemPlusChem*; *Advanced Materials*; *Journal of Pharmaceutical Sciences*
 - Nature Publishing Group: *Nature*; *Nature Chemistry*; *Nature Communications*; *Nature Protocols*, *Nature Reviews Materials*.
 - International Union of Crystallography: *Acta Crystallographica Section B*; *Acta Crystallographica Section C*; *Acta Crystallographica Section E*;
 - Other publishers: *Science*, *Science Advances*, *Supramolecular Chemistry*; *Catalysis Today*; *Journal of Chemical Crystallography*; *Journal of Molecular Structure*; *Solid State Sciences*; *Structural Chemistry*; *Journal of Organometallic Chemistry*; *Coordination Chemistry Reviews*; *Inorganic Chemistry Communications*; *Journal of Coordination Chemistry*; *Journal of Supramolecular Chemistry*; *Proceedings of the National Academy of Sciences, USA*; *Australian Journal of Chemistry*; *South African Journal of Science*;
- Reviewed grant proposals for: National Research Foundation (RSA), Leverhulme Trust (UK), Engineering and Physical Sciences Research Council (UK), Royal Society (UK), American Chemical Society Petroleum Research Fund, Israel Science Foundation, National Science Foundation (USA), Royal Society of Edinburgh / Scottish Government Personal Research Fellowships co-funded by Marie Curie Actions, Croatian Science Foundation
- Reviews of numerous NRF rating applications
- Regular panel member: NRF National Equipment Programme and National Nanotechnology Equipment Programme
- Reviews of Royal Society of Chemistry Travel Grant applications
- Reviews of Postdoctoral Fellowship applications for the Claude Leon Foundation
- Examination of PhD and Masters theses: University of Cape Town, Indian Institute of Technology Kanpur, National University of Singapore, Stellenbosch University, Monash University (Australia), King Abdullah University of Science and Technology (Saudi Arabia), McGill University, University of Western Australia, University of Limerick, Pondicherry University
- External Examiner: Physical Chemistry, University of Namibia (2005 – 2009)
- Review of tenure applications: University of South Florida, McGill University, University of the Witwatersrand, University of Cincinnati, University of Iceland, Jawaharlal Nehru University

Conference Organisation

- Chair: Scientific Committee, 2nd Meeting on Porous Molecular Solids, Vietri sul Mare (Italy), 6-8 June, 2018.
- Chair: Organising Committee of ICCOSS-23, Stellenbosch, South Africa, 3-7 April, 2017.
- Chair: Scientific Committee, 1st Meeting on Porous Molecular Solids, Stellenbosch, 7-9 April, 2015.
- Chair: Organising Committee of INDABA 7, Skukuza, Kruger National Park, South Africa, 2-7 September, 2012.
- Chair: Organizing Committee of the 12th International Seminar on Inclusion Compounds, Stellenbosch, South Africa, 4-9 April, 2009.
- Chair: Organizing Committee of the 39th National Convention of the South African Chemical Society, Stellenbosch, South Africa, 30 November – 5 December, 2008.
- Steering Committee: 37th International Conference on Coordination Chemistry (2005/2006).
- Co-Chair: Organizing Committee of the Third International Workshop on Advanced Materials, Stellenbosch, South Africa, 5–8 September, 2005.

Teaching Experience

- Practical Crystallography for Graduate Students (2004, US)
- Chemistry Honours (Introduction to Crystallography, Supramolecular Chemistry 2003-current, US)
- Chemistry 244/242 (Inorganic Chemistry, 2003-2006, US)
- Chemistry 402 (Introduction to Crystallography, 2002, UMC)
- Practical Crystallography for Graduate Students (2000, UMC)
- Chemistry 230 (Physical Chemistry for the Biological Sciences, 1999, UMC)
- Chemistry 402 (Introduction to Crystallography, 1997, UMC)
- Chemistry 31 (Introductory Chemistry, 1995, UMC)
- Chemistry Honours (Thermoanalytical Methods, 1993, UCT)
- Supervised Undergraduate Physical Chemistry Laboratories (1989 – 1993, UCT)

Research Interests

- Supramolecular Chemistry
- Crystal engineering
- Porous crystalline materials
- Polar order in crystals
- Anomalous thermal expansion in materials
- Nanotechnology
- Solid-gas reactions (for gas/vapor storage, sensing and separation)
- Solid state phase transitions (in particular, single-crystal to single-crystal transformations)
- Single-crystal and powder X-ray diffraction analysis
- Thermoanalytical methods
- Development of crystallographic software for structure visualization and manipulation
- Development of crystallographic software for educational purposes
- Development of novel experimental methods, including automation of data capture

Publications

A. PEER-REVIEWED JOURNAL ARTICLES

Accepted

2023

- 234 A. C. Eaby, L. Loots, J. L. Basson, C. Esterhuysen and L. J. Barbour
Programmed Pore-Shape Fixing in a Soft Porous Molecular Crystal – Navigating the Phase Interconversion Landscape.
Angew. Chem. Int. Ed. **2023**, (accepted).
DOI: 10.1002/anie.202304152

- 233 K. Koupepidou, V. I. Nikolayenko, D. Sensharma, A. A. Bezrukov, M. Vandichel, S. J. Nikkhah, D. C. Castell, K. A. Oyekan, N. Kumar, A. Subanbekova, W. G. Vandenberghe, K. Tan, L. J. Barbour and M. J. Zaworotko One Atom Can Make All the Difference: Gas-Induced Phase Transformations in Bisimidazole-Linked Diamondoid Coordination Networks. *J. Am. Chem. Soc.* **2023**, *145*, 10197. DOI: 10.1021/jacs.3c01113
- 232 D. C. Castell, V. I. Nikolayenko, D. Sensharma., K. Koupepidou, K. A. Forrest, C. J. Solanilla, B. Space, L. J. Barbour and M. J. Zaworotko Crystal Engineering of Two Light and Pressure Responsive Physisorbents. *Angew. Chem., Int. Ed.* **2023**, *62*, e2022190. DOI: 10.1002/anie.202219039
- 231 A. C. Eaby, D. C. Myburgh, A. Kosimov, M. Kwit, C. Esterhuysen, A. Janiak and L. J. Barbour Dehydration of a crystal hydrate at subglacial temperatures. *Nature* **2023**, *616*, 288. DOI: 10.1038/s41586-023-05749-7
Featured in: *Nature Africa*, 28 April 2023 (DOI: 10.1038/d44148-023-00105-3).
- 230 V. I. Nikolayenko, D. C. Castell, D. Sensharma, M. Shivanna, L. Loots, K. A. Forrest, C. J. Solanilla-Salinas, K. Otake, S. Kitagawa, L. J. Barbour, B. Space and M. J. Zaworotko Reversible transformations between the non-porous phases of a flexible coordination network enabled by transient porosity. *Nature Chem.* **2023**, *15*, 542. DOI: 10.1038/s41557-022-01128-3
- 229 V. I. Nikolayenko, D. C. Castell, D. Sensharma, M. Shivanna, L. Loots, K. Otake, S. Kitagawa, L. J. Barbour and M. J. Zaworotko Metal doping to control gate opening and increase methane working capacity in isostructural flexible diamondoid networks. *ChemSusChem.* **2023**, *16*, e202300069. DOI: 10.1002/cssc.202300069
- 228 K. Roztocki, W. Gromelska, F. Formalik, A. Giordana, L. Andreo, G. Mahmoudi, V. Bon, S. Kaskel, L. J. Barbour, A. Janiak, E. Priola Shape-memory effect triggered by π - π interactions in a flexible terpyridine metal-organic framework. *ACS Mater. Lett.* **2023**, *5*, 1256. DOI: 10.1021/acsmaterialslett.3c00068

Published

2022

- 227 J. Ye, M. du Plessis, L. Loots, L. M. van Wyk and L. J. Barbour Solid-Liquid Separation of Xylene Isomers Using a Cu-Based Metallocycle. *Cryst. Growth. Des.* **2022**, *22*, 2654. DOI: 10.1021/acs.cgd.2c00082
- 226 M. Korica, I. Balić, L. M. van Wyk, D. P. van Heerden, V. I. Nikolayenko, L. J. Barbour, T. Jednačak, I. Đilović and T. Balić Inclusion of CO₂, NH₃, SO₂, Cl₂ and H₂S in porous N₄O₄-donor macrocyclic Schiff base. *Microporous Mesoporous Mater.* **2022**, *332*, 111708. DOI: 10.1016/j.micromeso.2022.111708
- 225 N. Sun, C. Wang, B. Yu, H. Wang, L. J. Barbour and J. Jiang Stimuli-Responsive Porous Molecular Crystal with Reversible Modulation of Porosity. *ACS Appl. Mater. Interfaces.* **2022**, *14*, 1519. DOI: 10.1021/acsmi.1c18368

2021

- 224 A. Półrolniczak, S. Sobczak, V. I. Nikolayenko, L. J. Barbour and A. Katrusiak Solvent-controlled elongation and mechanochemical strain in a metal-organic framework. *Dalton Trans.* **2021**, *50*, 17478. DOI: 10.1039/D1DT01937F

- 223 N. Kumar, S. Mukherjee, N. C. Harvey-Reid, A. A. Bezrukov, K. Tan, V. Martins, M. Vandichel, T. Pham, L. M. van Wyk, K. Oyekan, A. Kumar, K. A. Forrest, K. M. Patil, L. J. Barbour, B. Space, Y. Huang, P. E. Kruger and M. J. Zaworotko
Breaking the trade-off between selectivity and adsorption capacity for gas separation.
Chem. **2021**, *7*, 3085.
DOI: 10.1016/j.chempr.2021.07.007
- 222 M. Shivanna, K. Otake, B.-Q. Song, L. M. van Wyk, Q.-Y. Yang, N. Kumar, W. K. Feldmann, T. Pham, S. Suepaul, B. Space, L. J. Barbour, S. Kitagawa and M. J. Zaworotko
Benchmark acetylene binding affinity and separation through induced fit in a flexible hybrid ultramicroporous material.
Angew. Chem. Int. Ed. **2021**, *60*, 20383.
DOI: 10.1002/anie.202106263
- 221 N. Bimbo, K. Zhang, H. Aggarwal, T. Mays, J. Jiang, L. J. Barbour and V. Ting
Hydrogen adsorption in metal-organic framework MIL-101(Cr) – Adsorbate densities and enthalpies from sorption, neutron scattering, in-situ X-ray diffraction, calorimetry, and molecular simulations.
ACS Appl. Energy Mater. **2021**, *4*, 7839.
DOI: 10.1021/acsaem.1c01196
- 220 L. M. van Wyk, L. Loots and L. J. Barbour
Tuning Extreme Anisotropic Thermal Expansion in 1D Coordination Polymers through Metal Selection and Solid Solutions.
Chem. Commun. **2021**, *57*, 7693.
DOI: 10.1039/d1cc01717a
- 219 D. P. van Heerden, V. J. Smith, H. Aggarwal and L. J. Barbour
High Pressure In Situ Single-Crystal X-Ray Diffraction Reveals Turnstile Linker Rotation Upon Room-Temperature Stepped Uptake of Alkanes.
Angew. Chem. Int. Ed. **2021**, *60*, 13430.
DOI: 10.1002/anie.202102327
- 218 L. M. van Wyk and L. J. Barbour
Colossal Trellis-Like Single-Crystal to Single Crystal Structural Transformations in Two 1D Coordination Polymers.
Cryst. Growth. Des. **2021**, *21*, 3056.
DOI: 10.1021/acs.cgd.1c00240
- 217 N. Bimbo, J. P. Smith, H. Aggarwal, A. J. Physick, A. Pugsley, L. J. Barbour, V. P. Ting and T. J. Mays
Kinetics and enthalpies of methane adsorption in microporous materials AX-21, MIL-101 (Cr) and TE7.
Chem. Eng. Res. Des. **2021**, *169*, 153.
DOI: 10.1016/j.cherd.2021.03.003
- 216 L. M. van Wyk, L. Loots and L. J. Barbour
Mechanochemical Control of Solvent Content in a 1D Coordination Polymer.
J. Coord. Chem. **2021**, *74*, 190.
DOI: 10.1080/00958972.2021.1877688
[Invited article for a special issue dedicated to Prof. Jerry Atwood](#)
- 215 D. P. van Heerden and L. J. Barbour
Guest-occupiable space in the crystalline solid state: a simple rule-of-thumb for predicting occupancy.
Chem. Soc. Rev. **2021**, *50*, 735.
DOI: 10.1039/D0CS01040E
- 2020**
- 214 W. K. Feldmann, C. Esterhuysen and L. J. Barbour
Pressure-Gradient Sorption Calorimetry of Flexible Porous Materials: Implications for Intrinsic Thermal Management.
ChemSusChem. **2020**, *13*, 5220.
DOI: 10.1002/cssc.202001469

- 213 L. J. Barbour
X-Seed 4: updates to a program for small-molecule supramolecular crystallography.
J. Appl. Cryst. **2020**, *53*, 1141.
DOI: 10.1107/S1600576720007438
- 212 S. Sobczak, A. Pórolniczak, P. Ratajczyk, W. Cai, A. Gładysiak, V. I. Nikolayenko, D. C. Castell, L. J. Barbour, A. Katrusiak
Large negative linear compressibility of a porous molecular co-crystal.
Chem. Commun. **2020**, *56*, 4324.
DOI: 10.1039/D0CC00461H
- 211 M. du Plessis, V. I. Nikolayenko and L. J. Barbour
Record-setting selectivity for p-xylene by an intrinsically porous 0D metallocycle.
J. Am. Chem. Soc. **2020**, *142*, 4529.
DOI: 10.1021/jacs.9b11314
- 210 I. Brekalo, D. Deliz, L. J. Barbour, M. D. Ward, T. Friščić, K. T. Holman
Microporosity of a Guanidinium Organodisulfonate Framework.
Angew. Chem. Int. Ed. **2020**, *59*, 1997.
DOI: 10.1002/anie.201911861
- 209 W. K. Feldmann, K.-A. White, C. X. Bezuidenhout, V. J. Smith, C. Esterhuysen and L. J. Barbour
Direct Determination of Enthalpies of Sorption Using Pressure-Gradient Differential Scanning Calorimetry: CO₂ Sorption by CuHKUST.
ChemSusChem. **2020**, *13*, 102.
DOI: 10.1002/cssc.201902990
- 2019**
- 208 A. Hazra, D. P. van Heerden, S. Sanyal, P. Lama, C. Esterhuysen and L. J. Barbour
CO₂-induced single-crystal to single-crystal transformations of an interpenetrated flexible MOF explained by *in situ* crystallographic analysis and molecular modeling.
Chem. Sci. **2019**, *10*, 10018.
DOI: 10.1039/C9SC04043A
- 207 P. Lama, A. Hazra and L. J. Barbour
Accordion and layer-sliding motion to produce anomalous thermal expansion behaviour in 2D-coordination polymers.
Chem. Commun. **2019**, *55*, 12048.
DOI: 10.1039/C9CC06634A
- 206 I. E. Claassens, L. J. Barbour and D. A. Haynes
A Multi-Stimulus Responsive Porous Coordination Polymer: Temperature-Mediated Control of Solid-state [2+2] Cycloaddition.
J. Am. Chem. Soc. **2019**, *141*, 11425.
DOI: 10.1021/jacs.9b05961
- 205 P. Sikiti, C. X. Bezuidenhout, D. P. van Heerden and L. J. Barbour
Direct *in situ* Crystallographic Visualization of a Dual Mechanism for Uptake of CO₂ Gas by a Flexible MOF.
Inorg. Chem. **2019**, *58*, 8257.
DOI: 10.1021/acs.inorgchem.9b00761
- 204 P. Sikiti, C. X. Bezuidenhout, D. P. van Heerden and L. J. Barbour
A new dynamic framework with direct *in situ* visualisation of breathing under CO₂ gas pressure.
CrystEngComm **2019**, *21*, 3415.
DOI: 10.1039/C9CE00418A
- 2018**
- 203 L. J. Barbour
EwaldSphere – an interactive approach to teaching the Ewald sphere construction.
J. Appl. Cryst. **2018**, *51*, 1734.
DOI: 10.1107/S1600576718012876

- 202 I. E. Claassens, V. I. Nikolayenko, D. A. Haynes and L. J. Barbour
Solvent-mediated synthesis of cyclobutane isomers in a photoactive cadmium(II) porous coordination polymer.
Angew. Chem. Int. Ed. **2018**, *57*, 15563.
DOI: 10.1002/anie.201809050
- 201 H. Yang, F. Guo, P. Lama, W.-Y. Gao, H. Wu, L. J. Barbour, W. Zhou, J. Zhang, B. Aguilá and S. Ma
Visualizing Structural Transformation and Guest Binding in a Flexible Metal–Organic Framework under High Pressure and Room Temperature.
ACS Cent. Sci. **2018**, *4*, 1194.
DOI: 10.1021/acscentsci.8b00378
- 200 M. du Plessis, V. I. Nikolayenko and L. J. Barbour
Single-crystal to single-crystal uptake of volatile solids and associated chromatic response in a porous metallocycle.
Inorg. Chem. **2018**, *57*, 12331.
DOI: 10.1021/acs.inorgchem.8b02028
- 199 D. Das and L. J. Barbour
Uniaxial negative thermal expansion induced by moiety twisting in an organic crystal.
CrystEngComm **2018**, *20*, 5123.
DOI: 10.1039/C8CE01169A
- 198 V. I. Nikolayenko, D. C. Castell, D. P. van Heerden and L. J. Barbour
Guest-induced structural transformations in a porous halogen bonded framework.
Angew. Chem. Int. Ed. **2018**, *57*, 12086.
DOI: 10.1002/anie.201806399
- 197 V. I. Nikolayenko, L. M. van Wyk, O. Q. Munro and L. J. Barbour
Supramolecular Solvatochromism: Mechanistic Insight from Crystallography, Spectroscopy and Theory.
Chem. Commun. **2018**, *54*, 6975.
[Cover article](#)
DOI: 10.1039/C8CC02197J
- 196 L. O. Alimi, D. P. van Heerden, P. Lama, V. J. Smith and L. J. Barbour
Reversible Thermosaliency of 4-Aminobenzonitrile.
Chem. Commun. **2018**, *54*, 6208.
DOI: 10.1039/C8CC03636E
- 195 M. Petryk, A. Janiak, L. J. Barbour and M. Kwit
Awkwardly-shaped dimers, capsules and tetramers: molecular and supramolecular motifs in C5-arylated chiral calixsalens.
Eur. J. Org. Chem. **2018**, 1916.
DOI: 10.1002/ejoc.201800314
- 194 Q.-Y. Yang, P. Lama, S. Sen, M. Lusi, K.-J. Chen, W.-Y. Gao, M. Shivanna, T. Pham, N. Hosono, S. Kusaka, J. J. Perry, S. Ma, B. Space, L. J. Barbour, S. Kitagawa and M. J. Zaworotko
Reversible switching between highly porous and non-porous phases of an interpenetrated diamondoid coordination network that exhibits gate-opening at methane storage pressures.
Angew. Chem. Int. Ed. **2018**, *57*, 5684.
DOI: 10.1002/anie.201800820
- 193 A. Janiak, C. Esterhuysen and L. J. Barbour
A thermo-responsive structural switch and colossal anisotropic thermal expansion in a chiral organic solid.
Chem. Commun. **2018**, *54*, 3727.
DOI: 10.1039/C8CC00952J
- 192 L. Alimi, P. Lama, V. J. Smith and L. J. Barbour
Hand-twistable Plastically Deformable Crystals of a Rigid Small Organic Molecule.
Chem. Commun. **2018**, *54*, 2994.
DOI: 10.1039/C8CC00775F

- 191 A. Janiak, M. Kwit and L. J. Barbour
An unexpected relationship between solvent inclusion and gas sorption properties of chiral calixsalen solids.
Supramol. Chem. **2018**, *30*, 479.
DOI: 10.1080/10610278.2018.1427865
[Invited article for a special issue dedicated to Jerry Atwood in honour of his 75th birthday](#)
- 190 P. Lama and L. J. Barbour
Distinctive Three-Step Hysteretic Sorption of Ethane with In-situ Crystallographic Visualization of the Pore Forms in a Soft Porous Crystal.
J. Am. Chem. Soc. **2018**, *140*, 2145.
[Cover article; ACS Editors' Choice; Featured as a Spotlight article: *J. Am. Chem. Soc.* **2018**, *140*, 1977.](#)
DOI: 10.1021/jacs.7b10352
- 189 L. O. Alimi, P. Lama, V. J. Smith and L. J. Barbour
Large volumetric thermal expansion of a novel organic cocrystal over a wide temperature range.
CrystEngComm **2018**, *20*, 631.
DOI: 10.1039/C7CE01848G
- 2017**
- 188 V. I. Nikolayenko, L. J. Barbour, A. Arauzo, J. Campo, J. M. Rawson and D. A. Haynes
Inclusion of a dithiadiazolyl radical in a seemingly non-porous solid.
Chem. Commun. **2017**, *53*, 11310.
- 187 V. I. Nikolayenko, A. Heyns and L. J. Barbour
Threading the needle: guest transport in a versatile 0D porous molecular crystal.
Chem. Commun. **2017**, *53*, 11306.
- 186 V. I. Nikolayenko, S. A. Herbert and L. J. Barbour
Reversible structural switching of a metal-organic framework by photoirradiation.
Chem. Commun. **2017**, *53*, 11142.
- 185 E. Macedi, A. Meli, F. De Riccardis, P. Rossi, V. J. Smith, L. J. Barbour, I. Izzo and C. Tedesco
Molecular recognition and solvatomorphism in a cyclic peptoid. Formation of a stable 1D porous framework.
CrystEngComm **2017**, *19*, 4704.
- 184 R. AbdulHalim, P. Bhatt, Y. Belmabkhout, A. Shkurenko, L. J. Barbour and M. Eddaoudi
A fine-tuned Metal-Organic Framework for Autonomous Indoor Moisture Control.
J. Am. Chem. Soc. **2017**, *139*, 10715.
- 183 E. R. Engel, A. Jouaiti, C. X. Bezuidenhout, M. W. Hosseini and L. J. Barbour
Activation-dependent breathing in a flexible metal-organic framework and the effects of repeated sorption/desorption cycling.
Angew. Chem. Int. Ed. **2017**, *56*, 8874.
- 182 C. X. Bezuidenhout, C. Esterhuysen and L. J. Barbour
Solvatochromism as a probe to observe the solvent exchange process in a 1-D porous coordination polymer with 1-D solvent accessible channels.
Chem. Commun. **2017**, *53*, 5618.
- 181 C. X. Bezuidenhout, V. J. Smith, C. Esterhuysen and L. J. Barbour
Solvent and pressure-induced phase changes in two 3D copper glutarate-based MOFs via glutarate (+gauche \rightleftharpoons -gauche) conformational isomerism.
J. Am. Chem. Soc. **2017**, *139*, 5923.
[Featured as a Spotlight article: *J. Am. Chem. Soc.* **2017**, *139*, 6017.](#)
- 180 H. Aggarwal, R. K. Das, E. R. Engel and L. J. Barbour
A five-fold interpenetrated metal-organic framework showing large variation in thermal expansion behaviour owing to dramatic structural transformation upon dehydration-rehydration.
Chem. Commun. **2017**, *53*, 861.

2016

- 179 C. Tedesco, A. Meli, E. Macedi, V. Iuliano, A. G. Ricciardulli, F. De Riccardis, G. Vaughan, V. J. Smith, L. J. Barbour and I. Izzo
Ring size effect on the solid state assembly and inclusion properties of propargyl substituted hexa- and octacyclic peptoids.
CrystEngComm **2016**, *18*, 8838.
- 178 P. Lama, H. Aggarwal, C. X. Bezuidenhout and L. J. Barbour
Giant Hysteretic Sorption of CO₂: *In situ* Crystallographic Visualization of Guest Binding within a Breathing Framework at 298 K.
Angew. Chem. Int. Ed. **2016**, *55*, 13271.
- 177 P. M. Bhatt, E. Batisai, V. J. Smith and L. J. Barbour
Creation of new guest accessible space under gas pressure in a flexible MOF: Multidimensional insight through combination of in situ techniques.
Chem. Commun. **2016**, *52*, 11374.
- 176 P. M. Bhatt, Y. Belmabkhout, A. Cadiou, K. Adil, O. Shekhah, Shkurenko, L. J. Barbour and M. Eddaoudi
A fine-tuned fluorinated MOF addresses the needs for trace CO₂ removal and air capture using physisorption.
J. Am. Chem. Soc. **2016**, *138*, 9301.
- 175 E. R. Engel, V. J. Smith, C. X. Bezuidenhout and L. J. Barbour
Thermoresponsive organic inclusion compounds: modifying thermal expansion and thermosolvent behavior by simple guest replacement.
Chem. Mater. **2016**, *28*, 5073.
- 174 C. M. Kane, A. Banisafar, T. P. Dougherty, L. J. Barbour and K. T. Holman
Enclathration and Confinement of Small Gases by the Intrinsically 0D Porous Molecular Solid, MeHSiMe₂.
J. Am. Chem. Soc. **2016**, *138*, 4377.
- 173 A. Meli, E. Macedi, F. De Riccardis, V. J. Smith, L. J. Barbour, I. Izzo and C. Tedesco
Solid state conformational flexibility at work: zipping and unzipping a cyclic peptoid single crystal.
Angew. Chem. Int. Ed. **2016**, *55*, 4679.
- 172 D. P. van Heerden, C. Esterhuysen and L. J. Barbour
Elucidating the mechanism responsible for anomalous thermal expansion in a Metal-Organic Framework.
Dalton Trans. **2016**, *45*, 4141.
- 171 A. Janiak, M. Petryk, L. J. Barbour and M. Kwit
Readily Prepared Inclusion Forming Chiral Calixsalens.
Org. Biomol. Chem. **2016**, *14*, 669.
- 170 P. Lama, L. O. Alimi, R. K. Das and L. J. Barbour
Hydration-Dependent Anomalous Thermal Expansion Behaviour in a Polar Coordination Polymer.
Chem. Commun. **2016**, *52*, 3231.

2015

- 169 C. Kane, O. Ugono, L. J. Barbour and K. T. Holman
Many Simple Molecular Cavitands are Intrinsically Porous (Zero-dimensional Pore) Materials.
Chem. Mater. **2015**, *27*, 7337.
- 168 R. K. Das, H. Aggarwal and L. J. Barbour
Anomalous Anisotropic Thermal Expansion in a One Dimensional Coordination Polymer Driven by Conformational Flexibility.
Inorg. Chem. **2015**, *54*, 8171.
- 167 W. Cai, A. Gładysiak, M. Anioła, V. J. Smith, L. J. Barbour and A. Katrusiak
Giant negative area compressibility tunable in a soft porous framework material.
J. Am. Chem. Soc. **2015**, *137*, 9296.
[Cover article; ACS Editors' Choice; Featured as a Spotlight article: *J. Am. Chem. Soc.* **2015**, *137*, 9197.](#)
- 166 H. Aggarwal, R. K. Das, P. M. Bhatt and L. J. Barbour
Isolation of a Structural Intermediate During Switching of Degree of Interpenetration in a Metal-Organic Framework.
Chem. Sci. **2015**, *6*, 4986.

- 165 V. J. Smith, C. G. Marais, K. Suwinska, J. Lipkowski, A. Szumna, C. Esterhuysen and L. J. Barbour
Concomitant Polymorphs of *p*-iso-Propylcalix[4]arene.
CrystEngComm **2015**, *17*, 5129.
- 164 C. X. Bezuidenhout, V. J. Smith, P. M. Bhatt, C. Esterhuysen and L. J. Barbour
Extreme CO₂ Sorption Hysteresis in Open-Channel Rigid Metal-Organic Frameworks.
Angew. Chem. Int. Ed. **2015**, *54*, 2079.
- 2014**
- 163 S. A. Herbert, A. Janiak, P. K. Thallapally, J. L. Atwood and L. J. Barbour
Diffusion of guests into a seemingly non-porous organic crystal.
Chem. Commun. **2014**, *50*, 15509.
- 162 H. Aggarwal, P. Lama and L. J. Barbour
Transformation from non- to double-interpenetration in robust Cd(II) doubly-pillared-layered metal-organic frameworks.
Chem. Commun. **2014**, *50*, 14543.
- 161 P. Lama, R. K. Das, V. J. Smith and L. J. Barbour
A combined stretching-tilting mechanism produces negative, zero and positive linear thermal expansion in a semi-flexible Cd(II)-MOF.
Chem. Commun. **2014**, *50*, 6464.
- 160 H. Aggarwal, P. M. Bhatt, C. X. Bezuidenhout, and L. J. Barbour
Direct Evidence for Single-Crystal to Single-Crystal Switching of Degree of Interpenetration in a Metal–Organic Framework.
J. Am. Chem. Soc. **2014**, *136*, 3776.
- 159 M. du Plessis, V. J. Smith and L. J. Barbour
Single-crystal to single-crystal guest exchange and phase transformations in a porous metallocycle.
CrystEngComm **2014**, *16*, 4126.
- 158 E. R. Engel, V. J. Smith, C. X. Bezuidenhout and L. J. Barbour
Uniaxial negative thermal expansion facilitated by weak host-guest interactions.
Chem. Commun. **2014**, *50*, 4238.
- 157 O. Shekhah, R. Swaidan, Y. Belmabkhout, M. du Plessis, T. Jacobs, L. J. Barbour, I. Pinnau and M. Eddaoudi
The liquid phase epitaxy approach for the successful construction of ultra-thin and defect-free ZIF-8 membranes: Pure and mixed gas transport study.
Chem. Commun. **2014**, *50*, 2089.
- 156 T. Jacobs, V. J. Smith, L. H. Thomas and L. J. Barbour
Carbon dioxide entrapment in an organic molecular host.
Chem. Commun. **2014**, *50*, 85.
- 155 M. Lusi and L. J. Barbour
Temperature-dependent guest reorientation: a reversible order-disorder transformation in a single crystal.
CrystEngComm **2014**, *16*, 36.
- 2013**
- 154 H. Kumari, A. Good, V. J. Smith, C. A. Deakayne, L. J. Barbour and J. L. Atwood
18-Crown-6 templates offset-linked pyrogallol[4]arene dimers.
Supramol. Chem. **2013**, *25*, 591.
- 153 H. Kumari, L. Erra, A. C. Webb, P. M. Bhatt, C. L. Barnes, C. A. Deakayne, J. E. Adams, L. J. Barbour and J. L. Atwood
Pyrogallol[4]arenes as frustrated organic solids.
J. Am. Chem. Soc. **2013**, *135*, 16963.
- 152 H. Kumari, J. Zhang, L. Erra, L. J. Barbour, C. A. Deakayne and J. L. Atwood
Cocrystals of gabapentin with C-alkylresorcin[4]arenes.
CrystEngComm **2013**, *15*, 4045.

- 151 I. Grobler, V. J. Smith, P. M. Bhatt, S. A. Herbert and L. J. Barbour
Tunable Anisotropic Thermal Expansion of a Porous Zinc(II) Metal-Organic Framework.
J. Am. Chem. Soc. **2013**, *135*, 6411.
- 150 M. Lusi and L. J. Barbour
Solid–vapour reactions as a post-synthetic modification tool for molecular crystals: the enclathration of benzene and toluene by Werner complexes.
Chem. Commun. **2013**, *49*, 2634.
- 149 J. Bera, M. Sarkar, N. Sadhukhan, T. Ghatak, L. J. Barbour and S. M. W. Rahaman
Reactions of Acids with Naphthyridine-Functionalized Ferrocenes: Protonation and Metal Extrusion.
Inorg. Chem. **2013**, *52*, 1432.
- 148 T. Jacobs and L. J. Barbour
Solvent diffusion and binding in a ‘nonporous’ molecular crystal.
CrystEngComm **2013**, *15*, 1512.
- 147 L. Loots and L. J. Barbour
An infinite catenane self-assembled by $\pi\cdots\pi$ interactions.
Chem. Commun. **2013**, *49*, 671.
- 146 T. Jacobs and L. J. Barbour
Single-crystal to single-crystal transformations in discrete solvated metallocycles: the role of the metal ion.
New J. Chem. **2013**, *37*, 71.
- 2012**
- 145 E. Batisai, M. Lusi, T. Jacobs and L. J. Barbour
A mechanochemically synthesised solid solution enables engineering of the sorption properties of a Werner clathrate.
Chem. Commun. **2012**, *48*, 12171.
- 144 T. Jacobs, G. O. Lloyd, J.-A. Gertenbach, K. K. Müller-Nedebock, C. Esterhuysen and L. J. Barbour
In situ X-ray structural studies of a flexible host responding to incremental gas loading.
Angew. Chem. Int. Ed. **2012**, *51*, 4913.
- 143 S. Das, K. Bhar, S. Chattopadhyay, P. Mitra, V. J. Smith, L. J. Barbour and B. K. Ghosh
Syntheses, structures and luminescence behaviours of Group 12 metal(II) thiocyanate complexes with a tetradentate Schiff base: Variation in molecular and crystalline architectures with the change of congeneric metal ions.
Polyhedron **2012**, *38*, 26.
- 142 M. Lusi and L. J. Barbour
Solid-vapor sorption of xylenes: prioritized selectivity as a means of separating all three isomers using a single substrate.
Angew. Chem. Int. Ed. **2012**, *51*, 3928.
[Featured in Chemistry World.](#)
[Featured in Chemical and Engineering News.](#)
- 141 M. du Plessis and L. J. Barbour
Supramolecular isomerism and solvatomorphism in a novel coordination compound.
Dalton Trans. **2012**, *41*, 3895.
[Invited article; Featured on the journal's web site as a “Hot Article”.](#)
- 140 L. Loots and L. J. Barbour
A simple and robust method for the identification of pi-pi packing motifs of aromatic compounds.
CrystEngComm. **2012**, *14*, 300.
- 2011**
- 139 M. Lusi and L. J. Barbour
Determining hydrogen atom positions for hydrogen bonded interactions: A distance-dependent neutron-normalized method.
Cryst. Growth Des. **2011**, *11*, 5515.
- 138 S. V. Potts, L. J. Barbour, D. A. Haynes, J. M. Rawson and G. O. Lloyd
Inclusion of thiazyl radicals in porous crystalline materials.
J. Am. Chem. Soc. **2011**, *133*, 12948.

- 137 K. Fucke, K. M. Anderson, Maria H. Filby, J. A. K. Howard, J. W. Steed, M. Henry, Matthias J. Gutmann, J. Wright, S. A. Mason, L. J. Barbour, C. L. Oliver and A. W. Coleman
The structure of water: Behaviour in p-sulfonatocalix[4]arene, a highly hydrated clay mimic.
Chem. Eur. J. **2011**, *17*, 10259.
- 136 M. Lusi, L. R. MacGillivray, J. L. Atwood and L. J. Barbour
Isostructural coordination polymers: epitaxis vs. solid solution.
CrystEngComm. **2011**, *13*, 4311.
[Invited article](#)
- 135 D. Das, T. Jacobs, A. Pietraszko and L. J. Barbour
Anomalous thermal expansion of an organic crystal – implications for elucidating the mechanism of an enantiotropic phase transformation.
Chem. Commun. **2011**, *47*, 6009.
[Invited article](#); [Featured on the journal's web site as a "Hot Article"](#).
- 134 A. Kleyn, T. Jacobs and L. J. Barbour
Solid-state structural studies of oxacalix[2]arene[2]naphthalene as a molecular tweezer.
CrystEngComm. **2011**, *13*, 3175.
[Invited article](#)
- 133 C. E. Willans, S. French, K. M. Anderson, L. J. Barbour, J-A. Gertenbach, G. O. Lloyd, R. J. Dyer, P. C. Junk and J. W. Steed
Tripodal imidazole frameworks: Reversible vapour sorption both with and without significant structural changes.
Dalton Trans. **2011**, *40*, 573.
- 2010**
- 132 J. M. Bakker, L. J. Barbour, G. B. Deacon, P. C. Junk, G. O. Lloyd and J. W. Steed
Successful extrapolation of an f-element synthetic method to the pseudo light lanthanoid, aluminium.
J. Organomet. Chem. **2010**, *695*, 2720.
- 131 S. Potts and L. J. Barbour
Solvent-mediated conformational similarities within a series of 1D coordination polymers constructed from a new flexible ditopic bis-imidazole ligand.
New. J. Chem. **2010**, *34*, 2451.
[Invited article](#)
- 130 P. Lama, A. Aijaz, S. Neogi, L. J. Barbour and P. K. Bharadwaj
Microporous La(III) metal-organic framework using a semi-rigid tricarboxylic ligand: synthesis, single-crystal to single-crystal sorption properties and gas adsorption studies.
Cryst. Growth Des. **2010**, *10*, 3410.
- 129 T. Jacobs, M. W. Bredenkamp, P. H. Neethling, E. G. Rohwer and L. J. Barbour
Templated polar order of a guest in a quasiracemic organic host.
Chem. Commun. **2010**, *46*, 8341.
- 128 T. Jacobs, J.-A. Gertenbach, D. Das and L. J. Barbour
Single-crystal to single-crystal transformations – guest removal and substitution in a robust solvent-templated metallocyclic compound.
Aust. J. Chem. **2010**, *63*, 573.
[Invited article for *Research Front on Crystal Engineering*](#)
- 127 D. Das, E. Engel and L. J. Barbour
Reversible single-crystal to single-crystal polymorphic phase transformation of an organic crystal.
Chem. Commun. **2010**, *46*, 1676.
- 126 D. Das, T. Jacobs and L. J. Barbour
Exceptionally Large Positive and Negative Anisotropic Thermal Expansion of an Organic Crystalline Material.
Nature Mater. **2010**, *9*, 36.
[Featured in: *News and Views, Nature Mater.* **2010**, *9*, 7.](#)
[Research Highlights, *Nature Chem.* **2010**, *2*, 72.](#)

2009

- 125 U. E. I. Horvath, J. M. McKenzie, S. Cronje, H. G. Raubenheimer and L. J. Barbour
Intermolecular aurophilic interactions facilitate assembly of a complex rotaxane in solution.
Chem. Commun. **2009**, 6598.
- 124 J. W. Steed, L. J. Barbour, S. French, J. -A. Gertenbach, P. C. Junk, G. O. Lloyd and C. E. Willans
A catenated imidazole-based coordination polymer exhibiting significant CO₂ sorption at low pressure.
Dalton Trans. **2009**, 6480.
- 123 T. Jacobs, G. O. Lloyd, M. W. Bredenkamp and L. J. Barbour
Breaking the trigonal host packing motif of Dianin's compound.
CrystEngComm **2009**, 11, 1545.
- 122 C. E. Willans, K. M. Anderson, M. J. Paterson, P. C. Junk, L. J. Barbour and J. W. Steed
Bis(N-heterocyclic carbene) dipalladium complexes: synthesis, solid-state conformational studies and solution behavior.
Eur. J. Inorg. Chem. **2009**, 2835.
- 121 T. Jacobs, G. O. Lloyd, M. W. Bredenkamp and L. J. Barbour
Co-crystallization of ionic and neutral supramolecular motifs derived from identical components.
Cryst. Growth Des. **2009**, 9, 1284.
- 120 D. Das and L. J. Barbour
Unusual conformations of a hexa-host molecule in solvate inclusion compounds.
Cryst. Growth Des. **2009**, 9, 1599.

2008

- 119 D. Das and L. J. Barbour
Concomitant formation of two different solvates of a hexa-host from a binary mixture of solvents.
Chem. Commun. **2008**, 5110.
- 118 D. Das and L. J. Barbour
Polymorphism of a hexa-host: isolation of four different single-crystal phases by melt crystallization.
J. Am. Chem. Soc. **2008**, 130, 14033.
- 117 L. Dobrzańska, D. J. Kleinmans and L. J. Barbour
Influence of the metal-to-ligand ratio on the formation of metal organic complexes.
New J. Chem. **2008**, 32, 813.
[Invited article](#)
- 116 E. S. Meadows, B. D. Levin, E. K. Elliott, L. J. Barbour and G. W. Gokel
The solid-state structure of a 4,13-diaza-18-crown-6 NaI complex: A unique chain-link assembly.
J. Chem. Cryst. **2008**, 38, 425.

2007

- 115 P. K. Lee, R. P. Chapman, L. Zhang, J. Hu, L. J. Barbour, E. K. Elliott, G. W. Gokel and D. L. Bryce
K-39 quadrupolar and chemical shift tensors for organic potassium complexes and diatomic molecules.
J. Phys. Chem. A, **2007**, 111, 12859.
- 114 C. E. Willans, K. M. Anderson, P. C. Junk, L. J. Barbour and J. W. Steed
A small tris(imidazolium) cage forms an N-heterocyclic carbene complex with silver(I).
Chem. Commun. **2007**, 3634.
- 113 L. Dobrzańska, G. O. Lloyd and L. J. Barbour
The solvent-templating effect as the driving factor that influences the formation of crystalline materials based on the stacking of metallocycles.
New J. Chem. **2007**, 31, 669.
[Invited article](#)
- 112 S. J. Dalgarno, P. K. Thallapally, L. J. Barbour and J. L. Atwood
Engineering void space in organic van der Waals crystals: calixarenes lead the way.
Chem. Soc. Rev. **2007**, 36, 236.

2006

- 111 P. K. Thallapally, L. Dobrzańska, T. R. Gingrich, T. B. Wirsig, L. J. Barbour and J. L. Atwood
Acetylene absorption and binding in a nonporous lattice.
Angew. Chem. Int. Ed. **2006**, *45*, 6506.
- 110 L. Dobrzańska, G. O. Lloyd, T. Jacobs, I. Rootman, C. L. Oliver, M. W. Bredenkamp and L. J. Barbour
Construction of one and two dimensional coordination polymers using ditopic imidazole ligands.
J. Mol. Struct. **2006**, *796*, 107.
[Invited article for special issue on coordination polymers](#)
- 109 L. Dobrzańska, G. O. Lloyd, C. Esterhuysen and L. J. Barbour
Guest-induced conformational switching in a single crystal.
Angew. Chem. Int. Ed. **2006**, *45*, 5856.
- 108 G. O. Lloyd, J. Alen, M. W. Bredenkamp, E. J. C. de Vries, C. Esterhuysen and L. J. Barbour
Solid-state self-inclusion: the missing link.
Angew. Chem. Int. Ed. **2006**, *45*, 5354.
- 107 C. R. Smith, L. J. Barbour, M. Makha, C. L. Raston and A. N. Sobolev
Unlocking the elusive binding cavity in *p*-sulfonatocalix[8]arene.
New. J. Chem. **2006**, 991.
[Featured on the cover](#)
- 106 M. Makha, C. L. Raston, A. N. Sobolev, L. J. Barbour and P. Turner
Endo- versus *exo*-cavity interplay of *p*-benzylcalix[4]arene with spheroidal molecules.
CrystEngComm. **2006**, *8*, 306.
- 105 L. J. Barbour
Crystal porosity and the burden of proof.
Chem. Commun. **2006**, 1163.
[Invited 40th Anniversary Focus Article](#)
- 104 C. B. Smith, L. J. Barbour, M. Makha, C. L. Raston and A. N. Sobolev
Lanthanide-induced helical arrays of $\{[Co(III) \text{ sepulchrate}] \cap \{p\text{-sulfonatocalix[4]arene}\}\}$ supermolecules.
Chem. Commun. **2006**, 950.
[Featured on the cover.](#)
- 103 L. Dobrzańska, G. O. Lloyd, H. G. Raubenheimer and L. J. Barbour
Permeability of a seemingly nonporous crystal formed by a discrete metallocyclic complex.
J. Am. Chem. Soc. **2006**, *128*, 698.

2005

- 102 P. K. Thallapally, G. O. Lloyd, T. B. Wirsig, M. W. Bredenkamp, J. L. Atwood and L. J. Barbour
Organic crystals absorb hydrogen gas under mild conditions.
Chem. Commun. **2005**, 5272.
- 101 L. Dobrzańska, H. G. Raubenheimer and L. J. Barbour
Borromean sheets assembled by self-supporting argentophilic interactions.
Chem. Commun. **2005**, 5050.
- 100 L. Dobrzańska, G. O. Lloyd, H. G. Raubenheimer and L. J. Barbour
A discrete metallocyclic complex that retains its solvent-templated channel structure on guest removal to yield a porous, gas sorbing material.
J. Am. Chem. Soc. **2005**, *127*, 13134.
- 99 P. K. Thallapally, T. B. Wirsig, L. J. Barbour and J. L. Atwood
Crystal engineering of nonporous organic solids for methane sorption.
Chem. Commun. **2005**, 4420.
- 98 G. O. Lloyd, M. W. Bredenkamp and L. J. Barbour
Enclathration of morpholinium cations by Dianin's compound: salt formation by partial host-to-guest proton transfer.
Chem. Commun. **2005**, 4053.

- 97 P. K. Thallapally, G. O. Lloyd, J. L. Atwood and L. J. Barbour
Diffusion of water through a nonporous, hydrophobic crystal.
Angew. Chem. Int. Ed. **2005**, *44*, 3848.
[Featured in Editors' Choice: Highlights of the recent literature, *Science* **2005**, *308*, 1521.](#)
- 96 G. O. Lloyd, J. L. Atwood and L. J. Barbour
Water-assisted self-assembly of harmonic single and triple helices in a polymeric coordination complex.
Chem. Commun. **2005**, 1845.
- 95 J. L. Atwood, L. J. Barbour, P. K. Thallapally and T. B. Wirsig
A crystalline organic substrate absorbs methane under STP conditions.
Chem. Commun. **2005**, 51.
[Featured on the journal's web site as a "Hot Paper".](#)

2004

- 94 U. E. I. Horvath, S. Cronje, J. M. McKenzie, L. J. Barbour and H. G. Raubenheimer
Mono- and binuclear gold(I) amido compounds of purine derivatives.
Z. Naturforsch. **2004**, *59b*, 1605.
- 93 J. L. Atwood, L. J. Barbour, S. J. Dalgarno, M. J. Hardie, C. L. Raston and H. R. Webb
Towards mimicking viral geometry with metal-organic systems.
J. Am. Chem. Soc. **2004**, *126*, 13170.
- 92 G. W. V. Cave, J. Antesberger, L. J. Barbour, R. M. McKinlay and J. L. Atwood
Inner core composition and structure responds to communication between nanocapsule walls.
Angew. Chem. Int. Ed. **2004**, *43*, 5263.
[Featured on the cover.](#)
- 91 J. Hu, L. J. Barbour and G. W. Gokel
Ferrocene derivatives as receptors to explore ammonium cation- π interaction.
New J. Chem. **2004**, *28*, 907.
- 90 J. Hu, L. J. Barbour, R. Ferdani and G. W. Gokel
Cation- π interactions between alkali metal cations and neutral double bonds.
Coll. Czech. Chem. Commun. **2004**, *69*, 1050.
- 89 J. L. Atwood, L. J. Barbour and A. Jerga
A new type of material for the recovery of hydrogen from gas mixtures.
Angew. Chem. Int. Ed. **2004**, *43*, 2948.
[Featured in: *News of the Week, C&E News* **2004**, *82*, 7.
Process **2004**, Issue 6, p8.
Science News, **2004**, *165*, 380.](#)
- 88 J. L. Atwood, L. J. Barbour, G. O. Lloyd and P. K. Thallapally
Polymorphism of pure *p*-*tert*-butylcalix[4]arene: subtle thermally-induced modifications.
Chem. Commun. **2004**, 922.
[Featured on the journal's web site as a "Hot Paper".](#)

2003

- 87 J. L. Atwood, L. J. Barbour, M. W. Heaven and C. L. Raston
Association and orientation of C₇₀ on complexation with calix[5]arene.
Chem. Commun. **2003**, 2270.
- 86 J. L. Atwood, L. J. Barbour, M. W. Heaven and C. L. Raston
Controlling van der Waals contact in complexes of fullerene C₆₀.
Angew. Chem. Int. Ed. **2003**, *42*, 3254.
- 85 R. Kannan, K. K. Katti, L. J. Barbour, C. L. Barnes and K. V. Katti
Aminoacid-water interactions *via* a two-dimensional primary water layer.
J. Am. Chem. Soc. **2003**, *125*, 6955.
- 84 J. L. Atwood, L. J. Barbour, M. W. Heaven and C. L. Raston
Synthesis of 2-imino-5-phenylimidazolidin-4-one and the structure of its trifluoroacetate salt.
J. Chem. Cryst. **2003**, *33*, 175.

- 83 J. L. Atwood and L. J. Barbour
Molecular graphics: from science to art.
Cryst. Growth Des. **2003**, 3, 3.
[Perspective and Cover article \(Cover design used for all 2003 issues\)](#)
- 2002**
- 82 R. Ferdani, L. J. Barbour and G. W. Gokel
Cation- π interactions in the crystal structures of alkali metal calixarene complexes.
J. Supramol. Chem. **2002**, 2, 131.
- 81 L. J. Barbour, M. R. Caira, T. le Roex and L. R. Nassimbeni
Inclusion compounds with mixed guests: controlled stoichiometries and kinetics of enclathration.
J. Chem. Soc., Perkin Trans. 2 **2002**, 1973.
- 80 J. L. Atwood, L. J. Barbour and A. Jerga
Polymorphism of pure *p*-*tert*-butylcalix[4]arene: conclusive identification of the phase obtained by desolvation.
Chem. Commun. **2002**, 2952.
- 79 J. L. Atwood, L. J. Barbour, S. Dalgarno, C. L. Raston and H. R. Webb
Supramolecular assemblies of *p*-sulfonatocalix[4]arene with aquated trivalent lanthanide ions.
J. Chem. Soc., Dalton Trans. **2002**, 4351.
- 78 J. L. Atwood, L. J. Barbour, A. Jerga and B. L. Schottel
Guest transport in a non-porous organic solid *via* dynamic van der Waals cooperativity.
Science **2002**, 298, 1000.
[Featured in:](#) [News of the Week, C&E News 2002, 80\(44\), 8.](#)
[J. W. Steed, Perspectives in Science 2002, 298, 976.](#)
[Chemistry Highlights 2002, C&E News 2002, 80\(50\), 44.](#)
- 77 G. W. Gokel, L. J. Barbour, R. Ferdani and J. Hu
Lariat ether receptor systems show experimental evidence for alkali metal cation- π interactions.
Acc. Chem. Res. **2002**, 35, 878.
- 76 J. Hu, L. J. Barbour and G. W. Gokel
The indole sidechain of tryptophan as a versatile π -donor.
J. Am. Chem. Soc. **2002**, 124, 10940.
- 75 J. Hu, L. J. Barbour, R. Ferdani and G. W. Gokel
Calcium cation complexation by lariat ether receptors having arene-terminated sidearms.
Chem. Commun. **2002**, 1806.
- 74 J. Hu, L. J. Barbour and G. W. Gokel
 σ -Donor, π -donor, and anion competition in π -complexation of alkali metal cations.
Chem. Commun. **2002**, 1808.
- 73 J. Hu, L. J. Barbour, R. Ferdani and G. W. Gokel
Sodium cation complexation behavior of the heteroaromatic sidechains of histidine and tryptophan.
Chem. Commun. **2002**, 1810.
- 72 J. L. Atwood, L. J. Barbour and A. Jerga
Storage of methane and freon by interstitial van der Waals confinement.
Science **2002**, 296, 2367.
[Featured in:](#) [Science & Technology Concentrates, C&E News 2002, 80\(27\), 27.](#)
[B.C. Gibb, Highlights in Angew. Chem. Int. Ed. 2003, 42, 1686.](#)
[Chemistry Highlights 2002, C&E News 2002, 80\(50\), 44.](#)
- 71 J. L. Atwood, L. J. Barbour and A. Jerga
Supramolecular control of the interior of large spherical molecular capsules.
Proc. Natl Acad. Sci. USA **2002**, 99, 4837.
[Featured in:](#) [J. Alper, Science 2002, 295, 2395.](#)
- 70 J. Hu, L. J. Barbour and G. W. Gokel
Lariat ether complexes used as experimental probes of cation- π interactions.
Proc. Natl Acad. Sci. USA **2002**, 99, 5121.

- 69 J. L. Atwood, L. J. Barbour and A. Jerga
Supramolecular stabilization of $N_2H_7^+$.
J. Am. Chem. Soc. **2002**, *124*, 2122.
- 68 R. G. Harrison, O. D. Fox, M. O. Meng, N. K. Dalley and L. J. Barbour
Cation control of pore and channel size in cage-based metal-organic porous materials.
Inorg. Chem. **2002**, *41*, 838.
- 67 J. L. Atwood, L. J. Barbour and C. L. Raston
Supramolecular organization of C_{60} into linear columns of five-fold, Z-shaped strands.
Cryst. Growth Des. **2002**, *2*, 3.
- 2001**
- 66 R. Ferdani, L. J. Barbour, J. Hu, N. K. Djedovic and G. W. Gokel
Solid state structures of N-2-(3-indolethyl)-9-crown-3, N,N'-bis(2-(3-indolethyl)-18-crown-6), and their protonated forms.
J. Supramol. Chem. **2001**, *1*, 305.
- 65 L. J. Barbour
X-Seed – A software tool for supramolecular crystallography.
J. Supramol. Chem. **2001**, *1*, 189.
- 64 J. Hu, L. J. Barbour, R. Ferdani and G. W. Gokel
Solid state network formation in arene-sidearmed lariat ether complexes: contrasting behavior of sodium, potassium, and calcium cation complexes.
J. Supramol. Chem. **2001**, *1*, 157.
- 63 J. L. Atwood, L. J. Barbour and A. Jerga
On the synthesis and structure of the very large spherical capsules derived from hexamers of pyrogallol[4]arenes.
J. Supramol. Chem. **2001**, *1*, 131.
[Cover article](#)
- 62 E. S. Meadows, L. J. Barbour, R. Ferdani and G. W. Gokel
Dimer formation in alkali metal complexes of 15- and 18-membered indole-containing lariat ether amides.
J. Supramol. Chem. **2001**, *1*, 111.
- 61 R. Ferdani, J. Hu, W. M. Leevy, J. Pajewska, R. Pajewski, V. Villalobos, L. J. Barbour and G. W. Gokel
Solid-state evidence for alkali metal to arene pi-complexation.
J. Incl. Phenom. Macro. **2001**, *41*, 7.
- 60 J. L. Atwood, L. J. Barbour and A. Jerga
Hydrogen bonded molecular capsules are stable in polar media.
Chem. Commun. **2001**, 2376.
- 59 J. Hu, L. J. Barbour and G. W. Gokel
Solid state evidence for π -complexation of sodium cation by carbon-carbon double bonds.
Chem. Commun. **2001**, 1858.
- 58 J. Hu, L. J. Barbour and G. W. Gokel
Solid state evidence for π -complexation of potassium cation by a carbon-carbon triple bond.
J. Am. Chem. Soc. **2001**, *123*, 9486.
- 57 L. J. Barbour and J. L. Atwood
Non-covalent interactions exert extraordinary influence over conformation and properties of a well-known supramolecular building block.
Chem. Commun. **2001**, 2020.
- 56 J. L. Atwood, L. J. Barbour, T. J. Ness, P. L. Raston and C. L. Raston
A well-resolved ice-like $(H_2O)_8$ cluster in an organic supramolecular complex.
J. Am. Chem. Soc. **2001**, *123*, 7192.
- 55 G. W. Gokel, L. J. Barbour, S. L. De Wall and E. S. Meadows
Macrocyclic polyethers as probes to assess and understand alkali metal cation- π interactions.
Coord. Chem. Rev. **2001**, *222*, 127.

- 54 J. L. Atwood, L. J. Barbour, M. J. Hardie, E. Lygris, C. L. Raston and H. R. Webb
Inclusion complexes of 18-crown-6 and (Na⁺[2,2,2]-cryptand) in [C-methylcalix[4]resorcinarene-H_n], n = 0, 1.
Cryst. Eng. Comm. **2001**, 10.
- 53 J. L. Atwood, L. J. Barbour, M. J. Hardie, and C. L. Raston
Metal sulfonatocalixarene complexes: bi-layers, capsules, spheres, tubular arrays and beyond.
Coord. Chem. Rev. **2001**, 222, 3.
- 52 J. L. Atwood, L. J. Barbour, M. J. Hardie, C. L. Raston, M. N. Statton and H. R. Webb
Heterobimetallic cage molecules: solvated. Na₂M₂(p-sulfonatocalix[4]arene)₂, M = Y, Eu.
Cryst. Eng. Comm. **2001**, 4.
- 51 L. J. Barbour, S. L. De Wall, R. Ferdani, F. R. Fronczek and G. W. Gokel
Intermolecular axial solvation of bound cations by sidearm donor groups in lariat ethers: formation of a supramolecular network.
Inorg. Chim. Acta. **2001**, 316, 121.
- 50 S. L. De Wall, L. J. Barbour and G. W. Gokel
Experimental evidence for alkali metal cation- π interactions obtained by using a lariat ether model system.
J. Phys. Org. Chem. **2001**, 14, 383.
- 49 E. S. Meadows, S. L. De Wall, L. J. Barbour and G. W. Gokel
Alkali metal cation- π interactions observed by using a lariat ether model system.
J. Am. Chem. Soc. **2001**, 123, 3092.
- 2000**
- 48 S. L. De Wall, L. J. Barbour, O. F. Schall and G. W. Gokel
Sodium cation complexation in a macrocycle containing thymines as sidearm donor groups.
J. Chem. Cryst. **2000**, 30, 227.
- 47 E. Elisabeth, L. J. Barbour, G. W. Orr, K.T. Holman and J. L. Atwood
Synthesis of a one dimensional coordination polymer based upon a calix[4]arene in the cone conformation.
Supramol. Chem. **2000**, 12, 317.
- 46 L. J. Barbour, G. W. Orr and J. L. Atwood
Characterization of a well-resolved supramolecular ice-like (H₂O)₁₀ cluster in the solid state.
Chem. Commun. **2000**, 859.
- 45 S. L. De Wall, E. S. Meadows, L. J. Barbour, and G. W. Gokel
Synthetic receptors as models for alkali metal cation- π binding sites in proteins.
Proc. Natl Acad. Sci. USA **2000**, 97, 6271.
- 44 E. S. Meadows, S. L. De Wall, L. J. Barbour, F. R. Fronczek, M.-S. Kim and G. W. Gokel
Structural and dynamic evidence for C-H...O hydrogen bonding in lariat ethers: implications for protein structure.
J. Am. Chem. Soc. **2000**, 122, 3325.
- 43 L. J. Barbour, S. L. De Wall, E. S. Meadows and G. W. Gokel
Experimental evidence for alkali metal ion cation- π interactions using bibracchial lariat ether complexes.
Ind. Eng. Chem. Res. **2000**, 39, 3436-3441.
- 42 E. S. Meadows, L. J. Barbour, F. R. Fronczek, C. M. Evans, S. F. Watkins and G. W. Gokel
Channel-like structures formed from extended networks of 4,13-diaza-18-crown-6 complexes.
Inorg. Chim. Acta. **2000**, 300-302, 333-338.
- 1999**
- 41 L. J. Barbour
LAYER – A computer program for the graphic display of intensity data as simulated precession photographs.
J. Appl. Cryst. **1999**, 32, 351.
- 40 L. J. Barbour
SECTION – A computer program for the graphic display of cross-sections through a unit cell.
J. Appl. Cryst. **1999**, 32, 353.

- 39 E. S. Meadows, S. L. De Wall, L. J. Barbour and G. W. Gokel
Cation- π complexation of potassium cation with the phenolic sidechain of tyrosine.
J. Am. Chem. Soc. **1999**, *121*, 8405.
- 38 P. C. Andrews, J. L. Atwood, L. J. Barbour, P. D. Croucher, P. J. Nichols, N. O. Smith, B. W. Skelton, A. H. White, C. L. Raston
Supramolecular confinement of C₆₀, S₈, P₄Se₃ and toluene by metal(II) macrocyclic complexes.
J. Chem. Soc., Dalton Trans. **1999**, 2927.
- 37 J. J. Tanner, S.-C. Tu, L. J. Barbour, C. L. Barnes and K. L. Krause
Unusual folded conformation of nicotinamide adenine dinucleotide bound to flavin reductase P.
Protein Science, **1999**, *8*, 1725.
- 36 G. W. Orr, L. J. Barbour and J. L. Atwood
Controlling molecular self-organization: formation of nanometer-scale spheres and tubules.
Science, **1999**, *285*, 1049.
[Cover article](#)
Featured in: [News of the Week, C&E News 1999, 77\(33\), 5.](#)
- 35 E. S. Meadows, S. L. De Wall, L. J. Barbour and G. W. Gokel
1- and 2-Naphthylmethyl sidearms of isomeric bibracchial lariat ethers significantly affect alkali metal cation complexation.
Chem. Commun. **1999**, 1555.
- 34 S. L. De Wall, E. S. Meadows, L. J. Barbour and G. W. Gokel
Intramolecular C-H...O hydrogen bonding reduces cation complexation strength in a fluorescent crown ether.
Chem. Commun. **1999**, 1553.
- 33 S. L. De Wall, E. S. Meadows, L. J. Barbour and G. W. Gokel
Solution- and solid state evidence for alkali metal, cation- π interactions with indole, the side chain of tryptophan.
J. Am. Chem. Soc., **1999**, *121*, 5613.
- 32 J. L. Atwood, L. J. Barbour, P. J. Nichols, C. L. Raston and C. A. Sandoval
Symmetry-aligned supramolecular encapsulation of C₆₀: [C₆₀(L)₂], L = *p*-benzylcalix[5]arene or *p*-benzylhexahomooxalix[3]arene.
Chem. Eur. J. **1999**, *5*, 990.
- 1998**
- 31 E. Abel, R. Castro, I. M. McRobbie, L. J. Barbour, J. L. Atwood, A. E. Kaifer and G. W. Gokel
A redox-switchable molecular receptor based on anthraquinone.
Supramol. Chem. **1998**, *9*, 199.
- 30 L. J. Barbour, G. W. Orr and J. L. Atwood
Supramolecular assembly of well-separated, linear columns of closely-spaced C₆₀ molecules facilitated by dipole induction.
Chem. Commun. **1998**, 1901.
Featured in: [Science/Technology Concentrates, C&E News 1998, 76\(37\), 28.](#)
- 29 L. J. Barbour and J. L. Atwood
RES2INS - A graphical interface for the SHELX program suite.
J. Appl. Cryst. **1998**, *31*, 963.
- 28 L. J. Barbour, G. W. Orr and J. L. Atwood
An intermolecular (H₂O)₁₀ cluster in a solid-state supramolecular complex.
Nature **1998**, *393*, 671.
- 27 P. C. Andrews, J. L. Atwood, L. J. Barbour, P. J. Nichols and C. L. Raston
Rigid concave surfaces: an entry to confinement of globular molecules.
Chem. Eur. J. **1998**, *4*, 1384.
- 26 L. J. Barbour, S. J. Belfield, P. C. Junk and M. K. Smith
Bidentate nitrogen base adducts of bismuth(III) nitrate.
Aust. J. Chem. **1998**, *51*, 337.

- 25 J. L. Atwood, L. J. Barbour, C. L. Raston and I. B. N. Sudria
C₆₀ and C₇₀ compounds in the pincerlike jaws of calix[6]arene.
Angew. Chem. Int. Ed. Engl. **1998**, *37*, 981.
- 24 K. N. Rose, L. J. Barbour, G. W. Orr and J. L. Atwood
Self-assembly of carcerand-like dimers of calix[4]resorcinarene facilitated by hydrogen bonded solvent bridges.
Chem. Commun. **1998**, 407.
- 23 D. E. Berning, K. V. Katti, L. J. Barbour and W. A. Volkert
Multifaceted reactions of P(CH₂OH)₃ with rhenium(V) precursors. Synthesis, characterization and X-ray structural studies of trans-[ReO₂{P(CH₂OH)₃}₂(py)₂]Cl, cis-[ReO₂{P(CH₂OH)₃}₂(py)₂]Cl and a novel alkoxide [Re(O)(m-O){P(CH₂OH)₃}(μ-η²-P{CH₂OH}₂CH₂O)]₄.
Inorg. Chem. **1998**, *37*, 334.
- 1997**
- 22 C. J. Smith, V. S. Reddy, S. R. Karra, K. V. Katti and L. J. Barbour
Synthesis and coordination chemistry of the first water-soluble dithio-bis(phosphine) ligands [(HOH₂C)₂P(CH₂)₂S-X-S(CH₂)₂P(CH₂OH)₂] (X = (CH₂)₃ or C₆H₄). X-ray Crystal Structure of [Pd(HOH₂C)₂P(CH₂)₂S(CH₂)₃S(CH₂)₂P(CH₂OH)₂] (Cl)₂.
Inorg. Chem. **1997**, *36*, 1786.
- 21 L. J. Barbour, G. W. Orr and J. L. Atwood
Supramolecular intercalation of C₆₀ into a calixarene bilayer - a well-ordered solid-state structure dominated by van der Waals contacts.
Chem. Commun. **1997**, 1439.
- 20 C. J. Smith, K. V. Katti, W. A. Volkert, A. R. Ketring and L. J. Barbour
The synthesis and characterization of chemically flexible water-soluble dithiobisphosphines: A systematic investigation of the effect of chain length on the coordination chemistry of rhenium(V). X-ray crystal structures of [ReO₂(HOH₂C)₂P(CH₂)₂S(CH₂)₃S(CH₂)₂P(CH₂OH)₂](Cl)₂, [ReO₂(HOH₂C)₂P(CH₂)₂S(CH₂)₄S(CH₂)₂P(CH₂OH)₂](ReO₄⁻)₂ and [ReO₂(HOH₂C)₂P(CH₂)₃S(CH₂)₃S(CH₂)₃P(CH₂OH)₂](Cl).
Inorg. Chem. **1997**, *36*, 1786.
- 1996**
- 19 J. L. Atwood, L. J. Barbour, E. S. Dawson, P. C. Junk and J Kienzle
X-ray structure of the water soluble [adeninium][p-sulfonatocalix[4]arene] which displays cationic and anionic bilayers.
Supramol. Chem. **1996**, *7*, 271.
- 18 L. J. Barbour, A. K. Damon, G. W. Orr and J. L. Atwood
Inclusion of organic cations by p-sulfonatocalix[4]arene. Crystal and molecular structure of the supramolecular complexes Na₂(pyridinium)₂[Cu(H₂O)₄(NC₅H₅)₂][Cu(H₂O)₄(p-sulfonatocalix[4]arene)₂·10H₂O and Na₄(morpholinium)(p-sulfonatocalix[4]arene)·8H₂O.
Supramol. Chem. **1996**, *7*, 167.
- 17 L. J. Barbour, L. R. MacGillivray and J. L. Atwood
Structural consequences of M-Cl...H-N hydrogen bonds in substituted pyridinium salts of the Cobalt(II) tetrachloride anion isolated from a liquid clathrate medium.
Supramol. Chem. **1996**, *7*, 209.
- 16 L. J. Barbour, L. R. MacGillivray and J. L. Atwood
Crystal and molecular structure of [H₂O·18-crown-6]₂[ReCl₆] isolated from a liquid clathrate medium.
J. Chem. Cryst. **1996**, *26*, 59.
- 1995**
- 15 J. L. Atwood, L. J. Barbour, P. C. Junk and G. W. Orr
Structure of the p-sulfonatocalix[4]arene complex with tetramethylammonium ions, [NMe₄]₅[p-sulfonatocalix[4]arene]·4H₂O.
Supramol. Chem. **1995**, *5*, 105.

- 14 L. J. Barbour, J. W. Steed and J. L. Atwood
Inclusion properties of cyclotetracatechylene.
J. Chem. Soc., Perkin Trans. 2 **1995**, 857.
- 13 L. J. Barbour, M. R. Caira and L. R. Nassimbeni
Complexation with diol host compounds. Part 18. Structures and thermal analysis of *trans*-9,10-dihydroxy-9,10-di-p-tolyl-9,10-dihydroanthracene and its inclusion complexes of acetone, diethyl ether and pyridine.
Supramol. Chem. **1995**, 5, 167.
- 12 L. J. Barbour, M. R. Caira, A. Coetzee and L. R. Nassimbeni
Kinetics of desolvation of inclusion compounds of 9,10-derivatives of *trans*-9,10-dihydroxy-9,10-dihydroanthracene with benzene.
J. Chem. Soc., Perkin Trans. 2 **1995**, 1345.
- 11 L. J. Barbour, M. R. Caira, L. R. Nassimbeni and E. Weber
Complexation with diol host compounds. Part 17. Structures and thermal analysis of 9,9'-dihydroxy-9,9'-bifluorene with ethanol, 1-butanol and pyridine.
Supramol. Chem. **1995**, 5, 153.
- 10 A. L. Rodgers, L. J. Barbour, M. A. B. Pougnet, C. J. Lombard and R. L. Ryall
Re-evaluation of the "week-end effect" data: possible role of urinary copper and phosphorus in the pathogenesis of renal calculi.
J. Trace Elem. Med. Biol. **1995**, 9, 150.
- 1994**
- 9 L. J. Barbour, M. R. Caira and L. R. Nassimbeni
Complexation with diol host compounds. Part 19. Structures and thermal analyses of inclusion compounds of *trans*-9,10-dihydroxy-9,10-diphenyl-9,10-dihydroanthracene with dimethylsulfoxide diethylketone, and (\pm)-2-butanol.
J. Chem. Cryst. 1994, **24**, 539.
- 8 L. J. Barbour, M. A. B. Pougnet, A. L. Rodgers, C. J. Lombard and R. L. Ryall
Urinary element concentrations in kidney stone formers and normal controls: the week-end effect.
J. Trace Elem. Electrolytes in Health and Dis. **1994**, 8, 87.
- 1993**
- 7 L. J. Barbour, M. R. Caira and L. R. Nassimbeni
Kinetics of inclusion.
J. Chem. Soc., Perkin Trans. 2 **1993**, 2321.
- 6 L. J. Barbour, M. R. Caira and L. R. Nassimbeni
Enclathration of diethyl ether.
J. Chem. Soc., Perkin Trans. 2 **1993**, 1413.
- 5 L. J. Barbour, S. A. Bourne, M. R. Caira, L. R. Nassimbeni, E. Weber, K. Skobridis and A. Wierig
Complexation with diol host compounds. Part 14. Inclusion compounds of 2,2'-bis(9-hydroxy-9-fluorenyl)biphenyl with acetonitrile, cyclohexanone, di-n-propylamine and dimethylformamide.
Supramol. Chem. **1993**, 1, 331.
- 4 E. Weber, K. Skobridis and A. Wierig, L. J. Barbour, M. R. Caira and L. R. Nassimbeni
Synthesis and solid-state inclusion properties of bis(diarylhydroxymethyl)-substituted 1,1'-binaphthyls. Crystal structures of a host and its pyridine clathrate.
Chem. Ber. **1993**, 126, 1141.
- 3 A. L. Rodgers, L. J. Barbour, M. A. B. Pougnet, C. Lombard and R. Ryall
Role of urinary copper and phosphorus in kidney-stone formation.
Kidney Int. **1993**, 43, 1182.
- 1992**
- 2 L. J. Barbour, K. Achleitner and J. R. Greene
A system for studying gas-solid reaction kinetics in controlled atmospheres.
Thermochim. Acta **1992**, 205, 171.

1989

- 1 L. J. Barbour, M. A. B. Pougnet and M. Peisach
Determination of urinary bromine by PIXE.
J. Radioanal. Chem. Lett. **1989**, 137, 327.

B. EDITORIAL ARTICLES

- 7 L. J. Barbour, L. R. MacGillivray, J. W. Steed and A. Szumna
Jerry Lee Atwood
Supramol. Chem. **2017**, 30, 351.
[Short biographical sketch of Prof. J. L. Atwood as the foreword to a special issue of *Supramolecular Chemistry* in honour of his 75th birthday](#)
- 6 M. Eddaoudi and L. J. Barbour
CO₂ separation, capture and reuse: a web themed issue.
Chem. Commun. **2015**, 51, 5554.
- 5 L. J. Barbour
Supramolecular joinery.
Nature Chem. **2015**, 7, 97.
[News & Views editorial article](#)
- 4 L. J. Barbour
Crystallographic studies of gas sorption in metal-organic frameworks.
Acta Cryst. Section B **2014**, B70, 403.
[Scientific Commentary on the review article *Acta Cryst. Section B*, 2014 B70, 404.](#)
- 3 L. J. Barbour
An introduction to the virtual issue on coordination polymers.
Acta Cryst. Section C **2014**, C70, 638.
[Editorial: special virtual issue on coordination polymers](#)
- 2 K. Rissanen, L. J. Barbour and L. R. MacGillivray
Structural macrocyclic supramolecular chemistry.
CrystEngComm **2014**, 16, 3644.
[Editorial for a web-themed special issue on macrocyclic chemistry](#)
- 1 L. J. Barbour
Single crystal to single crystal transformations.
Aust. J. Chem. **2006**, 59, 595.
[Invited lead essay for *Research Front* on single crystal to single crystal transformations](#)

C. BOOK CHAPTERS

- 6 L. J. Barbour, Single-crystal X-ray diffraction in *Comprehensive Supramolecular Chemistry II*. J. L. Atwood, G. W. Gokel and L. J. Barbour, Eds. Elsevier, **2017**.
- 5 L. Loots and L. J. Barbour, A Rudimentary Method for Classification of $\pi\cdots\pi$ Packing Motifs for Aromatic Molecules in *Frontiers in Crystal Engineering - III: The Importance of pi-interactions in Crystal Engineering*. E. R. T. Tiekink & J. Zukerman-Schpector, Eds. John Wiley & Sons, **2011**.
- 4 L. J. Barbour, D. Das, T. Jacobs, G. O. Lloyd and V. J. Smith, Concepts and nomenclature in chemical crystallography. Volume 5: *Supramolecular Materials Chemistry*, *Supramolecular Chemistry: From Molecules to Nanomaterials*, Wiley, **2011**.
- 3 J. L. Atwood, L. J. Barbour and A. Jerga, Very large supramolecular capsules based on hydrogen bonding. Perspectives in *Supramolecular Chemistry*, Vol 7. G. R. Desiraju, Ed., Wiley, **2003**.
[Cover design](#)
- 2 J. L. Atwood, L. R. MacGillivray, K. N. Rose, L. J. Barbour, K. T. Holman and G. W. Orr, Large molecular assemblies held together by non-covalent bonds, *NATO Sci. Ser., Ser. C* **1999**, 519 (Current Challenges on Large Supramolecular Assemblies), 7-16.

- 1 A. L. Rodgers, L. J. Barbour, M. A. B. Pougnet, C. J. Lombard and R. L. Ryall, *The Weekend Effect*. In R. L. Ryall, R. Bais, V. Marshall, A. Rofe, L. Smith, V. Walker, (Eds), *Urolithiasis II*, New York, Plenum, **1994**.

D. PATENTS

- 5 M. Lusi, L. J. Barbour, Separating xylene isomers. International Patent Application (2013), WO 2013/118011 A1
- 4 J. L. Atwood, L. J. Barbour, A. Jerga, Method of separating and storing volatile gases. U.S. Patent (2012), US 8,172,924 B2
- 3 J. L. Atwood, L. J. Barbour, A. Jerga, Calixarene-based guest-host assemblies for guest storage and transfer. U.S. Patent (2007), US 7,217.846 B2
- 2 J. L. Atwood, L. J. Barbour, A. Jerga, Self-assembled calixarene-based guest-host assemblies for guest storage by van der Waals confinement. U.S. Patent (2003), US 7,132,571 B2
- 1 J. L. Atwood, G. W. Orr, L. J. Barbour, Formation of nanometer-scale structures, U.S. Patent (2002), US 6,495,669 B1

Invited Lectures

- 65 Visualizing the Invisible: Exploring the World of Molecular Crystal Structures
April 20, **2023**, Chalmers University, Gothenburg, Sweden
- 65 Thermal stability of molecular inclusion compounds – from one extreme to another
April 5, **2023**, University of Jyväskylä, Finland
- 64 Thermal stability of molecular inclusion compounds – from one extreme to another
April 3, **2023**, Stockholm University, Sweden
- 63 Dehydration of a crystal hydrate at ultralow temperatures
March 21, **2023**, AstraZeneca, Gothenburg, Sweden
- 62 Dynamic host-guest systems
February 24, **2023**, Jawaharlal Nehru University, New Delhi, India
- 61 In defence of basic research
March 17, **2022**, Science Café, Stellenbosch, South Africa
- 60 Structural flexibility in the solid state
February 24, **2020**, McGill University, Montreal, Canada
- 59 Flexible porous materials
November 25, **2019**, Nankai University, Tianjin, China
- 58 Flexible porous materials
November 22, **2019**, University of Science and Technology Beijing, Beijing, China
- 57 Structural flexibility in the solid state
October 31, **2019**, Rhodes University, Grahamstown, South Africa
- 56 Porous materials: molecular-scale engineering – the ‘hole’ story
October 30, **2019**, Science Café, Grahamstown, South Africa
- 55 Developing complementary in situ methods for characterising porous crystalline materials
October 30, **2019**, Rhodes University, Grahamstown, South Africa
- 54 Understanding porosity in flexible metal-organic systems
April 8, **2019**, Zagreb University, Croatia
- 52 Structural flexibility in the solid state: implications for porosity
June 23, **2017**, Moscow State University, Moscow, Russia
- 51 Structural Flexibility in the Solid State
July 11, **2016**, Georgetown University, Washington DC, USA

- 50 Structural Flexibility in the Solid State
June 5, **2015**, York University Canada
- 49 Structure-Property Relationships of Solid-State Host-Guest Systems
June 3, **2015**, McGill University, Canada
- 48 Understanding Porosity in Flexible Metal-organic Systems
June 2, **2015**, University of Montreal, Canada
- 47 Flexible metal-organic frameworks - design, characterisation and properties
May 7, **2015**, University of Strasbourg, France
- 46 Porosity in flexible metal-organic frameworks
November 21, **2014**, Royal Society of Chemistry Roadshow in SA, University of Cape Town, South Africa
- 45 Structural flexibility in the solid state – implications for porous crystals
October 30, **2014**, University of Jyväskylä, Finland
- 44 Structural flexibility in the solid state – implications for porous crystals
October 29, **2014**, Helsinki University, Finland
- 43 Structural flexibility in the solid state
October 22, **2014**, Adam Mickiewicz University, Poland
- 42 Building a research career in South Africa
July 25, **2014**, Motivational Talk at the NRF Career Advancement Awards Launch, Lord Charles Hotel, Somerset West, South Africa
- 41 Why is 2014 the International Year of Crystallography?
July 3, **2014**, Motivational Talk, 16th Annual NSTF-BHP Billiton Awards Gala Dinner, Emperor's Palace, Kempton Park, Gauteng, South Africa
- 40 Structure-property relationships of solid-state host-guest systems
Jun 5, **2014**, University of Salerno, Italy
- 39 Understanding porosity in flexible metal-organic systems
May 23, **2014**, University of Lund, Sweden
- 38 Mass transport in the crystalline solid state
May 21, **2014**, KTH Stockholm, Sweden
- 37 Understanding porosity in flexible metal-organic systems
May 15, **2014**, University of Strasbourg, France
- 36 Structure-property relationships of solid-state host-guest systems
May 14, **2014**, University of Strasbourg, France
- 35 Structural flexibility in the solid state
May 6, **2014**, University of Strasbourg, France
- 34 Revealing the secret lives of crystals (Victor Pretorius Lecture)
February 28, **2014**, University of Pretoria, South Africa
- 33 Visualising structural dynamics in the crystalline solid state (Victor Pretorius Lecture)
February 27, **2014**, University of Pretoria, South Africa
- 32 Porosity in flexible metal-organic systems
August 14, **2013**, University of Bath, United Kingdom
- 31 Porosity in flexible metal-organic systems
July 18, **2013**, University of Missouri-Columbia, U.S.A.
- 30 Porosity in flexible metal-organic systems
May 30, **2013**, University of Salerno, Italy
- 29 What should chemists (and other scientists) be thinking about?
April 24, **2013**, University of Cape Town, South Africa (RSC Annual General Meeting – guest speaker)
- 28 Porosity in flexible metal-organic systems
April 27, **2012**, Chinese Academy of Science, Beijing, China

- 27 Structure-property relationships of some diyne-diol compounds
April 25, **2012**, East China University of Science and Technology, Shanghai, China
- 26 Porosity in flexible metal-organic systems
April 23, **2012**, University of Hong Kong, China
- 25 The secret life of crystals
September 22, **2011**, University of Cape Town, South Africa (Distinguished Alumni Lecture)
- 24 Porous molecular crystals: Discovery and design
December 3, **2010**, Georgetown University, Washington DC, U.S.A.
- 23 Structure-property relationships of molecular crystals
September 24, **2010**, University of Liverpool, United Kingdom
- 22 Structure-property relationships of molecular crystals
September 22, **2010**, Cambridge University, United Kingdom
- 21 Porous Crystals: Discovery and Design
September 14, **2007**, Monash University, Australia
- 20 Understanding Molecular Lego: Controlling the Construction of New Materials from the Bottom Up
February 14, **2007**, Royal Society of South Africa, Cape Town
- 19 Porous Crystals: Discovery and Design
November 30, **2006**, Polish Academy of Sciences, Warsaw, Poland
- 18 Porous Crystals: Discovery and Design
November 28, **2006**, University of Toruń, Poland
- 17 Porous Crystals: Discovery and Design
November 22, **2006**, University of York, United Kingdom
- 16 Porous Crystals: Discovery and Design
October 3, **2006**, University of Cape Town, Merck Lecture.
- 15 Porous Crystals: Discovery and Design
July 19, **2006**, Bruker Users' Meeting, Farm Inn, Pretoria, South Africa.
- 14 Porous Crystals: Discovery and Design
June 22, **2006**, Stratingh Institute and MSC, Groningen University, The Netherlands
- 13 Porous Crystals: Discovery and Design
December 12, **2005**, Department of Chemistry, University of Durham, United Kingdom
- 12 Crystal Engineering of Porous Solids
June 8, **2005**, Department of Chemistry, University of the Witwatersrand, South Africa
- 11 Crystal Engineering
June 2, **2005**, Stellenbosch University, Meeting of Young Chemists of SACI.
- 10 Gas Sorption in Organic Crystals.
November 15, **2004**, University of Durham, United Kingdom
- 9 Small Molecules, Large Assemblies.
November 20, **2003**, Inaugural lecture, Stellenbosch University, South Africa
- 8 Molecular Encapsulation in Nanotechnology.
May 29, **2002**, Stellenbosch University, South Africa
- 7 Molecular Encapsulation.
May 16, **2002**, University of Cape Town, South Africa
- 6 Nanometer-Scale Supramolecular Assemblies.
June 1, **2001**, King's College London, United Kingdom
- 5 Nanometer-Scale Supramolecular Systems.
May 23, **2001**, Cardiff University, United Kingdom

- 4 Nanoscale Supramolecular Systems.
May 17, **2001**, University of Leeds, United Kingdom
- 3 Nanoscale Supramolecular Systems.
April 18, **2001**, University of Cape Town, South Africa
- 2 Nanoscale Supramolecular Assemblies.
February 15, **2000**, Monash University, Australia
- 1 Small Molecule Crystallography and Large Supramolecular Systems.
February 18, **2000**, James Cook University, Townsville, Australia

Conferences, Symposia & Workshops

- 87 Conference on Crystal Engineering and Solid State Chemistry
IISER Thiruvananthapuram, India, February 22, **2023**
Invited Lecture: "Dynamic host-guest systems"
- 86 3rd Pan-African Conference on Crystallography
BOMAS of Kenya, Nairobi, Kenya, January 17-21, **2023**
Plenary Lecture: "Dynamic processes in crystals"
- 85 3rd Middle-Eastern Materials Science Conference
NYU Abu Dhabi, Abu Dhabi, United Arab Emirates, November 21-23, **2022**
Invited Lecture: "Dynamic Host-Guest Chemistry"
- 84 25th International Conference on the Chemistry of the Organic Solid State
Ohrid, Macedonia, July 3-8, **2022**
Plenary Lecture: "Crystal Engineering – Recent Progress and Future Outlook"
- 83 International School of Crystallography, 55th Course: Molecular Crystal Engineering, Online conference
hosted at Ettore Majorana Foundation and Centre for Scientific Culture, Erice, Italy, 31 May – 4 June, **2021**
Invited lecture: "Solid-state host-guest chemistry – the iconic Dianin's compound."
- 82 International School of Crystallography, 55th Course: Molecular Crystal Engineering, Online conference
hosted at Ettore Majorana Foundation and Centre for Scientific Culture, Erice, Italy, 31 May – 4 June, **2021**
Invited lecture: "Elucidating structural dynamics of flexible porous crystals."
- 81 Crystal Engineering and Emerging Materials Workshop of Ontario and Quebec (CEMWOQ 6.5)
Online conference hosted at Concordia University, Montreal, Canada, May 30-31, **2020**
Invited lecture: "Developing complementary *in situ* methods for characterising porous crystalline materials"
- 80 2020 Bruker/MIT Symposium
Massachusetts Institute of Technology, Cambridge MA, U.S.A., February 22, **2020**
Invited lecture: "Structural flexibility in the solid state – implications for porosity"
- 79 2020 Bruker/MIT Symposium – pre-symposium workshop
Massachusetts Institute of Technology, Cambridge MA, U.S.A., February 21, **2020**
"X-Seed – a software tool for supramolecular crystallography"
- 78 The Conference of Comprehensive Chemistry
Beijing Institute of Technology, Beijing, China, November 29, **2019**
Invited lecture: "Structure-property relationships in solid-state host-guest systems"
- 77 Visionary trends in molecular science III. A one-day symposium in honour of Nobel Laureate Sir Fraser
Stoddart
Tianjin University, Tianjin, China, November 27, **2019**
Invited lecture: "Structural flexibility in the solid state"
- 76 A Nature Conference – Physical Properties of Metal-Organic Frameworks
Tianjin, China, November 19-21, **2019**
Keynote Lecture: "Developing complementary *in situ* methods for characterising porous crystalline
materials"

- 75 24th International Conference on the Chemistry of the Organic Solid State
New York City, USA, June 16-21, **2019**
Keynote Lecture: "Structural flexibility in the solid state – implications for porous materials"
- 74 14th International Symposium on Macrocyclic and Supramolecular Chemistry (ISMSC-2009)
Lecce, Italy, June 2-6, **2019**
Invited Lecture: "Structural flexibility in the solid state – implications for porous materials"
- 73 26th Croatian Meeting of Chemists & Chemical Engineers (26HSKIK)
Šibenik, Croatia, April 9-12, **2019**
Plenary Lecture: "Structural flexibility in the solid state – implications for porous materials"
- 72 Crystal Engineering Laboratory Technology & Innovation Conference (CELTIC-2019)
Killarney, Ireland, March 29-31, **2019**
Plenary Lecture: "Structural flexibility in the solid state"
- 71 6th International Conference on Metal-Organic Frameworks (MOF 2018)
Auckland, New Zealand, December 9-13, **2018**
Keynote Lecture: "Structural flexibility in the solid state"
- 70 International Workshop on Porous Materials and their Applications
Pretoria, South Africa, September 13-14, **2018**
Invited Lecture – "Structural flexibility in the solid state: implications for porosity"
- 69 Crystal Engineering Gordon Research Conference - Progress in Crystal Engineering - Design, Properties, and Function
Newry ME, USA, June 24-29, **2018**
Invited Lecture – "Complementary Methods for the Characterization of Porous Crystalline Materials"
- 68 POMOS2 - 2nd Meeting on Porous Molecular Solids
Vietri sul Mare, Italy, 6-8 June **2018**
Keynote Lecture – "Structural flexibility in the solid state"
- 67 55th European High Pressure Research Group Meeting
Poznań, Poland, September 3 – 8, **2017**.
Invited Lecture – "Tools for studying the effects of gas pressure on porous materials in the solid state"
Session chair
- 66 SILQCOM 2017, 6th Latin American Symposium on Coordination and Organometallic Chemistry
Puerto Iguazú, Misiones, Argentina, August 6 – 11, **2017**.
Plenary Lecture – "Structural flexibility in the solid state: implications for porosity"
Session chair
- 65 4th European Crystallographic School
Warsaw, Poland, July 2 – 7, **2017**.
Invited Lecture – "X-Seed – a set of utility programs"
- 64 4th European Crystallographic School
Warsaw, Poland, July 2 – 7, **2017**.
Invited Lecture – "Supramolecular Chemistry and Crystallography"
- 63 16th International Symposium on inclusion Compounds
Kazan, Russia, June 26 – 30, **2017**.
Invited Lecture – "Structural flexibility in the solid state: implications for porosity"
Session chair
- 62 Workshop on CO₂ capture
University of the Western Cape, South Africa, June 5 – 7, **2017**.
Invited Lecture – "Structural flexibility in the solid state"
- 61 67th Annual Meeting of the American Crystallographic Association
New Orleans LA, USA, May 26 – 30, **2017**.
Invited Lecture – "Research and teaching tools: A SHELX/POV-Ray interface (X-Seed) and simulation of a diffractometer (SMART1k)."

- 60 67th Annual Meeting of the American Crystallographic Association
New Orleans LA, USA, May 26 – 30, **2017**.
Invited Lecture – “Structural flexibility in the solid state”
- 59 Telluride Science Center Workshop on Energy and Movement in Coherent Chemical Systems
Telluride CO, USA, July 4 – 8, **2016**.
Invited Lecture – “Structural flexibility in the solid state”
- 58 99th Canadian Chemistry Conference and Exhibition
Halifax, Canada, June 5 – 9, **2016**.
Invited Lecture – “Structural flexibility in the solid state”
- 57 MASC2015, Annual Meeting of the RSC Macrocyclic and Supramolecular Chemistry Group
Durham, United Kingdom, December 21-22, **2015**.
Invited Lecture – “Structural flexibility in the solid state”
- 56 42nd National Convention of the South African Chemical Institute
Durban, South Africa, November 29 to December 4, **2015**.
SACI Gold Medal Lecture – “Structural flexibility in the solid state”
- 55 2nd ICSU/IUPAC Workshop on Crystal Engineering
Como, Italy, August 30 to September 1, **2015**.
Invited lecture – “Structural flexibility in the solid state”
- 54 29th European Crystallographic Association Meeting
Rovinj, Croatia, August 23-28, **2015**.
Invited lecture – “Dynamics of porous metal-organic frameworks”
- 53 Smarter Materials for a Sustainable Future - ordered and semi-ordered materials for application in sustainable chemical technologies
South Africa - UK Scientific Seminar, Stellenbosch University, South Africa, January 21-23, **2015**.
Plenary lecture – “New approaches to understanding gas-solid interactions”
- 52 Midwest Regional Meeting of the American Chemical Society
Columbia MO, USA, November 12-15, **2014**.
Invited lecture – “Guest-induced single-crystal transformations”
- 51 Particle Technology Workshop (Jointly organized by SASOL and PORETECH)
Cape Town, South Africa, November 4, **2014**.
Plenary lecture – “Porosity in Flexible Metal-Organic Frameworks”
- 50 5th IUPAC International Conference on Green Chemistry
Durban, South Africa, August 17-21, **2014**.
Plenary lecture – “Understanding porosity in flexible metal-organic systems”
- 49 XXIII Congress of the International Union of Crystallography
Montreal, Canada, August 5-12, **2014**.
Invited lecture – “In-situ analysis of gas-loaded porous materials”
- 48 Particle Technology Workshop (Jointly organized by SASOL and PORETECH)
Pretoria, South Africa, November 12-13, **2013**.
Plenary lecture – “Porosity in Flexible Metal-Organic Systems”
- 47 XIV International Seminar on Inclusion Compounds
Edinburgh, U.K., August 18-24, **2013**.
Plenary lecture – “Porosity in Flexible Metal-Organic Systems”
- 46 2013 Meeting of the American Crystallographic Association
Honolulu, Hawaii, USA., July 20-24, **2013**.
Keynote lecture – “Porosity in Flexible Metal-Organic Systems”
- 45 South African Chemical Institute Conference on Inorganic Chemistry (INORG2013)
Durban, South Africa, July 1-4, **2013**.
Plenary Lecture – “Porosity in Flexible Metal-Organic Systems”

- 45 Past, Present, and Future of Crystallography - From Small Molecules to Macromolecules and Supramolecular Structures (An event to celebrate the 150th anniversary of the founding of the Politecnico di Milano and the 50th anniversary of the award of a Nobel Prize to Giulio Natta). Politecnico di Milano, Milan, Italy June 6-7, **2013**.
Plenary Lecture – “Porosity in Flexible Metal-Organic Systems”
- 44 22nd Midwest Organic Solid-State Chemistry Symposium; MOSSCS-XXII Missouri State University, Springfield, MO, USA June 1-2, **2012**.
Keynote Lecture – “Structural Flexibility in the Solid State”
- 43 243rd American Chemical Society National Meeting San Diego, California, U.S.A., March 25-29, **2012**.
Keynote lecture – “Porosity in Flexible Metal-Organic Systems”
- 42 Inauguration of the Centre for Advanced Membranes and Porous Materials King Abdullah University of Science and Technology, Saudi Arabia, March 6-7, **2012**.
Invited lecture – “Porosity in Flexible Metal-Organic Systems”
- 41 3rd Asian Conference on Coordination Chemistry New Delhi, India, October, 17-20, **2011**.
Keynote lecture – “Porosity in Flexible Metal-Organic Systems”
- 40 XIII International Seminar on Inclusion Compounds Gierloz, Poland, September 11-16, **2011**.
Invited lecture – “Structure-property relationships of inclusion compounds”
- 39 XXII Congress of the International Union of Crystallography Madrid, Spain, August 22-30, **2011**.
Keynote lecture – “Structure-property relationships of inclusion compounds”
- 38 40th South African Chemical Institute National Convention Johannesburg, South Africa, January 17-21, **2011**.
Keynote lecture – “Design, Assembly and Characterisation of Discrete Porous Systems”
- 37 PACIFICHEM – the 2010 International Chemical Congress of Pacific Basin Societies Honolulu, Hawaii, USA, December 15-20, **2010**.
Invited lecture – “Structure-Property Relationships of Some Diyne-Diol Compounds”
- 36 South African Chemical Institute Conference on Inorganic Chemistry (INORG2009) Bloemfontein, South Africa, September 13-17, **2009**.
Keynote lecture – “Porosity in Flexible Metal-Organic Systems”
- 35 25th European Crystallographic Association Meeting Istanbul, Turkey, August 16-21, **2009**.
Invited lecture – “Structure-Property Relationships of Two Host-Guest Systems”
- 34 International Symposium on Macrocyclic and Supramolecular Chemistry Maastricht, the Netherlands, June 20-25, **2009**.
Invited lecture – “Porosity in Flexible Metal-Organic Systems”
- 33 XIX International Conference on the Chemistry of the Organic Solid State Sestri Levante, Italy, June 14-19, **2009**.
Invited lecture – “Structure-Property Relationships of Dumbbell-Shaped Diyne Compounds”
- 32 XXI Congress of the International Union of Crystallography Osaka, Japan, August 23-31, **2008**.
Invited lecture – “Porosity in flexible metal-organic systems”
- 31 Fourth International Conference of the African Materials Research Society Dar es Salaam, Tanzania, December 10-14, **2007**.
Invited lecture – “Porous Crystals: Discovery and Design”
Session chair
- 30 Carman National Physical Chemistry Symposium Cape Town, South Africa, September 23-27, **2007**.
Invited lecture – “Porosity in crystals”

- 29 24th European Crystallographic Association Meeting
Marrakech, Morocco, August 22-27, **2007**.
Invited lecture – “The Influence of Intermolecular Interactions in Host-Guest Systems”
- 28 24th European Crystallographic Association Meeting
Marrakech, Morocco, August 22-27, **2007**.
Plenary lecture – “From small molecules to extended structures”
- 27 2007 Meeting of the American Crystallographic Association
Salt Lake City, USA, July 21-26, **2007**.
Keynote lecture – “Porous Crystals: Discovery and Design”
- 26 XI International Seminar on Inclusion Compounds
Kiev, Ukraine, June 10-15, **2007**.
Invited lecture – “Porous Crystals: Discovery and Design”
- 25 37th International Conference on Coordination Chemistry
Cape Town, South Africa, August 13-18, **2006**.
Invited lecture - “Assembly of porous materials using zero-dimensional metal-organic systems”
Session chair
- 24 23rd European Crystallographic Association Meeting
Leuven, Belgium, August 6-11, **2006**.
Invited lecture – “Single crystal transformations”
Session chair
- 23 Carman National Physical Chemistry Symposium
Midrand, South Africa, November 16-18, **2005**.
Invited lecture – “Porosity in crystals”
- 22 X International Seminar on Inclusion Compounds
Kazan, Russia, September 19-23, **2005**.
Invited lecture – “Porosity in molecular crystals”
Session chair
- 21 Third International Workshop on Advanced Materials (WAM-III)
Stellenbosch, South Africa, September 5-8, **2005**.
Invited lecture – “Porosity in molecular crystals”
Session chair
- 20 XX Congress of the International Union of Crystallography
Florence, Italy, August 23-31, **2005**.
Invited lecture – “Porosity in molecular crystals”
- 19 Nanotechnology – The Building Block for Tomorrow's Advanced Technology
Perth, Australia, July 17-20, **2005**.
Plenary lecture – “Self-assembled Structures”
- 18 International Hydrogen Energy Congress
Istanbul, Turkey, July 13-15, **2005**.
Invited lecture – “Organic Crystals for Hydrogen Sorption”
- 17 South African Chemical Institute Conference on Inorganic Chemistry
Pietermaritzburg, South Africa, April 10-13, **2005**.
Invited lecture - “Supramolecular Coordination Chemistry: Porous Frameworks, Helices and Rotaxanes”
- 16 22nd European Crystallographic Association Meeting
Budapest, Hungary, August 24-29, **2004**.
Invited lecture – “Enclosing Chemical Space”
Session chair
- 15 38th Midwest Regional Meeting of the American Chemical Society
Columbia, Missouri, November 5-7, **2003**.
Invited lecture - “Guest Diffusion in Nonporous Organic Solids”

- 14 21st European Crystallographic Association Meeting
Durban, South Africa, August 24-29, **2003**.
Invited lecture – “Guest Diffusion in a Nonporous Organic Solid”
- 13 223rd American Chemical Society National Meeting
Orlando, Florida, April 7–11, **2002**.
Poster presentation
- 12 11th Royal Australian Chemical Institute Convention
Australian National University, Canberra, Australia, February 6–9, **2000**.
Invited lecture: “Nanoscale Spheres and Tubes”
- 11 21st Meeting of the Society for Crystallographers in Australia
Thredbo, New South Wales, Australia, February 1–4, **2000**.
Lecture: “Water Clusters in the Solid State”
- 10 28th International Summer School on Crystal Engineering: From Molecules and Crystals to Materials
Erice, Italy, May 12–23, **1999**.
Three poster presentations
- 9 American Crystallographic Association, Annual Meeting
St. Louis, Missouri, U.S.A., July 19-25, **1997**.
- 8 211th American Chemical Society National Meeting
New Orleans, Louisiana, U.S.A., March 24-28, **1996**.
- 7 8th International Symposium on Molecular Recognition and Inclusion
Ottawa, Canada, July 31 - August 5, **1994**.
- 6 14th International Symposium on Macrocyclic Chemistry
Lawrence, Kansas, U.S.A. - June 12-17, **1994**.
Poster presentation
- 5 2nd International Conference on Molecular Recognition and Synthetic Design
University of Cape Town, South Africa, February 9-11, **1994**.
Student lecture: “Kinetics of Inclusion”
- 4 4th International Summer School on Supramolecular Chemistry
Sobieszewo, Poland, June 14-25, **1993**.
Poster presentation
- 3 1st International Conference on Molecular Recognition and Synthetic Design
University of Cape Town, Rondebosch, South Africa, February 12-14, **1992**.
- 2 31st Convention of the South African Chemical Institute
Rhodes University, Grahamstown, South Africa, June 23-27, **1991**.
- 1 6th International Symposium on Molecular Recognition and Inclusion
Berlin, Federal Republic of Germany, September 10-14, **1990**.
Poster presentation