

Prof. Nicholas F. Chilton FRSC FHEA

Professor of Chemistry

Research School of Chemistry, The Australian National University

Professor of Computational and Theoretical Chemistry

Department of Chemistry, The University of Manchester

www.nfchilton.com; nicholas.chilton@anu.edu.au; nicholas.chilton@manchester.ac.uk

Summary

General expertise concerning Quantum Mechanics, electronic structure, computational chemistry, molecular magnetism, theoretical magnetism and EPR and optical spectroscopies. Author of *PHI* and *MAGELLAN* codes for magnetic analysis and determination of magnetic anisotropy. **H-index of 52** and **153 publications** with over **13,400 citations** in journals such as *Science*, *Nature*, *Nature Chem.*, *J. Am. Chem. Soc.*, *Nature Commun.*, *Angew. Chem.*, and *Chem. Sci.* International recognition with numerous invited lectures. **Total grant income £3.3M.**

Education

2013 – 2015

Ph.D.

School of Chemistry, The University of Manchester, UK

Prof. E. J. L. McInnes and Prof. R. E. P. Winpenny

“Magnetic Anisotropy of Transition Metal Complexes”

2008 – 2011

B.Sc. Adv. Hons. (1st class)

School of Chemistry, Monash University, Australia

Prof. S. R. Batten and Prof. K. S. Murray

Employment

2023 – current

Professor of Chemistry

Research School of Chemistry, The Australian National University, Australia

2022 – current

Professor of Computational and Theoretical Chemistry

Department of Chemistry, The University of Manchester, UK

2019 – 2022

Senior Lecturer

Department of Chemistry, The University of Manchester, UK

2019 – 2023

Royal Society University Research Fellow

Department of Chemistry, The University of Manchester, UK

2018 – 2019

Presidential Fellow

School of Chemistry, The University of Manchester, UK

2016 – 2018

Ramsay Memorial Fellow

School of Chemistry, The University of Manchester, UK

2016 – 2016

Research Fellow

School of Chemistry, The University of Manchester, UK

2015 – 2015

Post-Doctoral Research Associate

EPSRC EPR National Facility, The University of Manchester, UK

2012 – 2012

Research Assistant

School of Chemistry, Monash University, Australia

2008 – 2010 **Research Assistant**
School of Chemistry, Monash University, Australia

Awards

2023 Zasshikai Lectureship Prize, The University of Tokyo, Japan
2022 Philip Leverhulme Prize, The Leverhulme Trust
2021 Harrison-Meldola Memorial Prize, Royal Society of Chemistry, UK
2020 Distinguished Achievement Medal: Teacher of the Year, The University of Manchester, UK
2019 – 2023 University Research Fellowship, The Royal Society, UK
2019 Olivier Kahn International Award, European Institute of Molecular Magnetism
2018 – 2022 Presidential Fellowship, The University of Manchester, UK
2018 Wilsmore Fellowship and Honorary Lecturer, University of Melbourne, Australia
2016 – 2018 British Ramsay Memorial Fellowship, Ramsay Memorial Trust, UK
2016 Reaxys Ph.D. Prize Finalist
2015 Dalton Division Delegation to SILQCOM, Royal Society of Chemistry, UK
2015 Dalton Young Researchers Award, Royal Society of Chemistry, UK
2015 Young Scientist, 65th Lindau Nobel Laureates Meeting
2013 – 2015 President's Doctoral Scholar Award, The University of Manchester, UK
2011 Jubilee Honours Scholarship, Monash University, Australia
2008 Summer Research Scholarship, Monash University, Australia

Grants

2023 – 2026 Leverhulme Trust "Defining the Electronic Structures of (Hetero)Metallocene Anions", UK
2023 – 2026 Leverhulme Trust "Next-generation molecule-based magnetic materials", UK
2023 – 2026 Philip Leverhulme Prize, The Leverhulme Trust, UK
2022 – 2023 Royal Society URF Enhancement Funds, UK
2020 – 2025 ERC Starting Grant (ERC-2019-STG-851504) "Chemical Control of Vibronic Coupling for Magnetic Materials", EU
2019 – 2024 EPSRC (EP/S033181/1) "Magnetic Properties Measurement System for Manchester and National EPR Facility", UK
2019 – 2024 Royal Society URF (URF191320) "Chemical Control of Vibronic Coupling", UK
2018 – 2021 EPSRC (EP/R02605X/1) "Targeting Molecular Magnetic Hysteresis at Liquid Nitrogen Temperatures", UK
2016 – 2018 Ramsay Memorial Trust "Wavefunction engineering in lanthanide complexes", UK
2016 – 2019 EPSRC (EP/P002560/1) "Designing Highly Axial Lanthanide Single Molecule Magnets", UK
2016 – 2019 EPSRC (EP/N007034/1) "Non-classical paramagnetic susceptibility and anisotropy in lanthanide coordination complexes: a combined experimental and theoretical study", UK

Lectures

Invited: 2024 Asian Conference on Molecular Magnetism, Busan, South Korea (upcoming)
Contributed: 2024 European Conference on Molecular Magnetism, Krakow, Poland (upcoming)
Invited: 2024 Young European Conference on Molecular Magnetism, Krakow, Poland (upcoming)
Invited: 2024 From Fundamentals of Molecular Spin Qubit Design to Molecule-Enabled Quantum Information, Telluride, USA (upcoming)

Tutorial: 2024 Winter School on Quantum Information Science for Chemistry, Los Angeles, USA

Contributed: 2024 Australian Rare Earths Meeting 2024 (OZRE24), Perth, Australia

Prize: 2023 The University of Tokyo, Japan

Tutorial: 2023 The University of Tokyo, Japan

Dept.: 2023 University of Rennes, Rennes, France

Invited: 2023 RSC Joliot-Curie Conference, Southampton, UK

Invited: 2023 Copenhagen Molecular Quantum Information Discussions, Denmark

Dept.: 2023 The Australian National University, Canberra, Australia

RSC Prize: 2023 University of Oxford, Oxford, UK

RSC Prize: 2022 University of St Andrews, St Andrews, UK

RSC Prize: 2022 Durham University, Durham, UK

Contributed: 2022 Actinides Revisited, Dresden, Germany

Dept.: 2022 Florida State University, Tallahassee, USA

Plenary: 2022 29th Rare Earth Research Conference, Philadelphia, USA

Tutorial: 2022 Rare Earth Research Conference Summer School, Philadelphia, USA

Dept.: 2022 University of California, Santa Barbara, USA

Invited: 2022 Molecular Spin Qubit Design and Quantum Information, Telluride, USA

Invited: 2022 ACS Spring Meeting, San Diego, USA

Dept.: 2021 Ohio State University, Ohio, USA (Zoom)

Invited: 2021 CECAM paramagnetic NMR workshop, Toulouse, France

Dept.: 2021 Nottingham Trent University, Nottingham, UK

Invited: 2021 Rhur EPR colloquium, Germany (Zoom)

Invited: 2021 PTC Virtual Seminar, Chemical Institute of Canada (Zoom)

Invited: 2021 OpenMolcas Developers Conference, Loughborough, UK (Zoom)

Invited: 2021 1st Association de Magnétisme Moléculaire meeting, France (Zoom)

Invited: 2021 Angular Momentum, USA (Zoom)

Invited: 2020 Global Inorganic Discussion Weekdays, Chemical Institute of Canada (Zoom)

Invited: 2019 International Conference on Functional Molecular Materials, Krakow, Poland

OKIA prize: 2019 European Conference on Molecular Magnetism, Florence, Italy

Invited: 2019 52nd International meeting of the RSC ESR Group, Glasgow, UK

Dept.: 2019 University of California, Irvine, USA

Dept.: 2019 University of California, Davis, USA

Dept.: 2019 University of California, Berkeley, USA

Invited: 2019 APS March Meeting, Boston, USA

Tutorial: 2018 University of Melbourne, Melbourne, Australia

Plenary: 2018 RACI Inorganic Chemistry Symposium, Melbourne, Australia

Dept.: 2018 University of Melbourne, Melbourne, Australia

Keynote: 2018 ANSTO Neutron Scattering Symposium, Sydney, Australia

Plenary: 2018 RACI Inorganic Chemistry Symposium, Sydney, Australia

Plenary: 2018 International Conference on Bimetallic Complexes, Karlsruhe, Germany

Keynote: 2018 International Conference on f-Elements, Lausanne, Switzerland

Keynote: 2018 International Conference on Coordination Chemistry, Sendai, Japan

Dept.: 2018 University of Oxford, Oxford, UK

Dept.: 2018 Durham University, Durham, UK

Dept.: 2018 Xi'an Jiaotong University, Xi'an, China

Tutorial: 2018 Xi'an Jiaotong University, Xi'an, China

Dept.: 2018 Guangzhou University, Guangzhou, China

Dept.: 2018 Sun Yat-Sen University, Guangzhou, China

Tutorial: 2018 Sun Yat-Sen University, Guangzhou, China

Dept.: 2018 Cardiff University, Cardiff, UK

Dept.: 2017 University of Melbourne, Melbourne, Australia

Dept.: 2017 Monash University, Melbourne, Australia
Invited: 2017 Driving magnetic molecules, Bielefeld, Germany
Contributed: 2017 European Conference on Molecular Magnetism, Bucharest, Romania
Tutorial: 2017 University of Glasgow, Glasgow, UK
Dept.: 2016 Aarhus University, Aarhus, Denmark
Tutorial: 2016 Aarhus University, Aarhus, Denmark
Contributed: 2016 European Conference on Molecular Spintronics, Bologna, Italy
Invited: 2016 RSC Early Career Symposium, Glasgow, UK
RSC Prize: 2016 University of Nottingham, Nottingham, UK
RSC Prize: 2016 University of Glasgow, Glasgow, UK
RSC Prize: 2016 University of Brighton, Brighton, UK
RSC Prize: 2016 University of Kent, Canterbury, UK
Contributed: 2015 5th Latin American Symposium on Coordination and Organometallic Chemistry, Rio de Janeiro, Brazil
Dept.: 2015 Universidade Federal Fluminense, Rio de Janeiro, Brazil
Dept.: 2015 Universidade Federal do Rio de Janeiro, Rio de Janeiro, Brazil
Tutorial: 2015 Universidade Federal do Rio de Janeiro, Rio de Janeiro, Brazil
Invited: 2015 ThUL school on f-element chemistry, Karlsruhe, Germany
Invited: 2015 International Conference on the f-Elements, Oxford, UK
Invited: 2014 Functionalized molecule-based magnetic materials, Bielefeld, Germany
Dept.: 2014 CNRS Bordeaux, Bordeaux, France
Tutorial: 2014 CNRS Bordeaux, Bordeaux, France
Invited: 2014 International Conference on Molecule-Based Magnets, St. Petersburg, Russia
Contributed: 2014 f-Element Workshop, Manchester, UK
Dept.: 2014 Universitat de Barcelona, Barcelona, Spain
Tutorial: 2014 Universitat de Barcelona, Barcelona, Spain
Contributed: 2013 European Conference on Molecular Magnetism, Karlsruhe, Germany
Tutorial: 2013 University of Manchester, Manchester, UK
Tutorial: 2012 Monash University, Melbourne, Australia

Publications

153. G. Li, O. Stefanczyk, K. Kumar, Y. Mineo, L. Wang, K. Nakabayashi, S. Chorazy, N. F. Chilton and S.-I. Ohkoshi, [Modulation on Terahertz Absorption Properties in Ln^{III}-\[Ag\(CN\)₂\] Networks](#), *Inorg. Chem. Front.*, 2024, accepted.

152. L. E. Nodaraki, A.-M. Ariciu, D. N. Huh, J. Liu, D. O. T. A. Martins, F. Ortu, R. E. P. Winpenny, N. F. Chilton, E. J. L. McInnes, D. P. Mills, W. J. Evans and F. Tuna, [Ligand Effects on the Spin Relaxation Dynamics and Coherent Manipulation of Organometallic La\(II\) Potential Qudits](#), *J. Am. Chem. Soc.*, 2024, doi: 10.1021/jacs.3c12827.

151. L. Birnoschi, M. S. Oakley, E. J. L. McInnes and N. F. Chilton, [A Relativistic Quantum Chemical Investigation of Actinide Covalency Measured by EPR Spectroscopy](#), *J. Am. Chem. Soc.*, 2024, doi: 10.1021/jacs.4c01930.

150. S. C. Corner, G. K. Gransbury, I. J. Vitorica-Yrezabal, G. F. S. Whitehead, N. F. Chilton and D. P. Mills, [Halobenzene adducts of a dysprosocenium single-molecule magnet](#), *Inorg. Chem.*, 2024, doi: 10.1021/acs.inorgchem.3c04105.

149. S. C. Corner, G. K. Gransbury, I. J. Vitorica-Yrezabal, G. F. S. Whitehead, N. F. Chilton and D. P. Mills, [Synthesis and Magnetic Properties of Bis-Halobenzene Decamethyldysprosocenium Cations](#), *Inorg. Chem.*, 2024, doi: 10.1021/acs.inorgchem.3c04106

148. L. Nodaraki, J. Liu, A.-M. Ariciu, F. Ortu, M. S. Oakley, L. Birnoschi, G. K. Gransbury, P. Cobb, J. Emerson-King, N. F. Chilton, D. P. Mills, E. J. L. McInnes and F. Tuna, Metal-carbon bonding in early lanthanide substituted cyclopentadienyl complexes probed by pulsed EPR spectroscopy, *Chem. Sci.*, 2024, 15, 3003.
147. J. Emerson-King, G. K. Gransbury, G. F. S. Whitehead, I. J. Vitorica-Yrezabal, M. Rouzières, R. Clérac, N. F. Chilton and D. P. Mills, Isolation of a bent dysprosium bis(amide) single-molecule magnet, *J. Am. Chem. Soc.*, 2024, 146, 3331.
146. J. Murillo, J. A. Seed, A. J. Wooles, M. S. Oakley, C. A. P. Goodwin, M. Gregson, D. Dan, N. F. Chilton, A. J. Gaunt, S. A. Kozimor, S. T. Liddle and B. L. Scott, Carbene Complexes of Plutonium: Structure, Bonding, and Divergent Reactivity to Lanthanide Analogs, *J. Am. Chem. Soc.*, 2024, 146, 4098.
145. A. Mattioni, J. K. Staab, W. J. A. Blackmore, D. Reta, J. Iles-Smith, A. Nazir and N. F. Chilton, Vibronic Effects on the Quantum Tunnelling of Magnetisation in Kramers Single-Molecule Magnets, *Nature Commun.*, 2024, 485.
144. P.-B. Jin, Q.-C. Luo, G. K. Gransbury, I. J. Vitorica-Yrezabal, T. Hajdu, I. Strashnov, E. J. L. McInnes, R. E. P. Winpenny, N. F. Chilton, D. P. Mills and Y.-Z. Zheng, Thermally stable Terbium(II) and Dysprosium(II) Bis-Amidinate Complexes, *J. Am. Chem. Soc.*, 2023, 145, 27993.
143. R. Nabi, J. K. Staab, A. Mattioni, J. G. C. Kragoskow, D. Reta, J. M. Skelton and N. F. Chilton, Accurate and efficient spin-phonon coupling and spin dynamics calculations for molecular solids, *J. Am. Chem. Soc.*, 2023, 145, 24558.
142. G. K. Gransbury, S. C. Corner, J. G. C. Kragoskow, P. Evans, H. M. Yeung, W. J. A. Blackmore, G. F. S. Whitehead, I. J. Vitorica-Yrezabal, M. S. Oakley, N. F. Chilton and D. P. Mills, AtomAccess: A predictive tool for molecular design and its application to the targeted synthesis of dysprosium single-molecule magnets, *J. Am. Chem. Soc.*, 2023, 145, 22814.
141. J. G. C. Kragoskow, A. Mattioni, J. K. Staab, D. Reta, J. M. Skelton and N. F. Chilton, Spin-phonon coupling and magnetic relaxation in single-molecule magnets, *Chem. Soc. Rev.*, 2023, 52, 4567.
140. W. J. A. Blackmore, G. K. Gransbury, P. Evans, J. G. C. Kragoskow, D. P. Mills and N. F. Chilton, Characterisation of magnetic relaxation on extremely long timescales, *Phys. Chem. Chem. Phys.*, 2023, 25, 16735.
139. R. Alotaibi, A. Booth, E. Little, A. Brookfield, A. Achari, S. J. Lockyer, G. A. Timco, G. F. S. Whitehead, I. Vitorica-yrezabal, N. F. Chilton, R. R. Nair, D. Collison and R. E. P. Winpenny, Synthesis and Characterization of Heterometallic Rings Templated through Alkylammonium or Imidazolium Cations, *Dalton Trans.*, 2023, 52, 7473.
138. B. Alnami, J. G. C. Kragoskow, J. K. Staab, J. M. Skelton and N. F. Chilton, Structural evolution of paramagnetic lanthanide compounds in solution compared to time- and ensemble-average structures, *J. Am. Chem. Soc.*, 2023, 145, 13632.
137. G. Li Manni, I. Fdez. Galván ..., L. Birnoschi ..., N. F. Chilton ..., J. K. Staab *et al.*, The OpenMolcas Web: A Community-Driven Approach to Advancing Computational Chemistry, *J. Chem. Theor. Comput.*, 2023, 19, 6933.
136. K. R. McClain, H. Kwon, K. Chakarawet, R. Nabi, J. G. C. Kragoskow, N. F. Chilton, R. D. Britt, J. R. Long and B. G. Harvey, A Trinuclear Gadolinium Cluster with a Three-Center One-Electron Bond and an $S = 11$ Ground State, *J. Am. Chem. Soc.*, 2023, 145, 8996.

135. P. Zhang, R. Nabi, J. K. Staab, N. F. Chilton and S. Demir, Taming Super-Reduced Bi_2^{3-} Radicals with Rare Earth Cations, *J. Am. Chem. Soc.*, 2023, 145, 9152.
134. M. J. Giansiracusa, M. Vonci, Y. L. Whyatt, C. Williams, K. Mason, D. Parker, E. J. L. McInnes and N. F. Chilton, Determination of molecular hydration in solution via changes in magnetic anisotropy, *Chem. Commun.*, 2023, 59, 4531.
133. T. Han, Y.-S. Ding, M. J. Giansiracusa, N. F. Chilton, R. E. P. Winpenny and Y.-Z. Zheng, Determinative Effect of Axial Linearity on Single-Molecule Magnet Performance in Dinuclear Dysprosium Complexes, *Chem. Eur. J.*, 2023, 29, e202300256.
132. W. J. A. Blackmore, A. Mattioni, S. C. Corner, P. Evans, G. K. Gransbury, D. P. Mills and N. F. Chilton, Measurement of the Quantum Tunnelling Gap in a Dysprosocenium Single-Molecule Magnet, *J. Phys. Chem. Lett.*, 2023, 14, 2193.
131. V. S. Parmar, A. M. Thiel, R. Nabi, G. K. Gransbury, M. S. Norre, P. Evans, S. C. Corner, J. M. Skelton, N. F. Chilton, D. P. Mills and J. Overgaard, Influence of pressure on the structure, phonon spectrum and magnetic properties of a dysprosocenium Single Molecule Magnet, *Chem. Commun.*, 2023, 59, 2656.
130. A. Vincent, Y. L. Whyatt, N. F. Chilton and J. R. Long, Strong Axiality in a Dysprosium(III) Bis(borolide) Complex Leads to Magnetic Blocking at 65 K, *J. Am. Chem. Soc.*, 2023, 145, 1572.
129. G. K. Gransbury, B. L. L. Réant, A. J. Wooles, J. Emerson-King, N. F. Chilton, S. T. Liddle and D. P. Mills, Electronic Structure Comparisons of Isostructural Early d- and f-Block Metal(III) Bis(cyclopentadienyl) Silanide Complexes, *Chem. Sci.*, 2023, 14, 621.
128. J. K. Staab and N. F. Chilton, An analytic linear vibronic coupling method for first-principles spin-dynamics calculations in single-molecule magnets, *J. Chem. Theor. Comput.*, 2022, 11, 6588.
127. M. Godsall and N. F. Chilton, Investigation of the Electronic Structure and Optical Spectra of Uranium-(IV), -(V) and -(VI) Complexes Using Multi-configurational Methods, *J. Phys. Chem. A*, 2022, 36, 6059.
126. L. Birnoschi and N. F. Chilton, HYPERION: A New Computational Tool for Relativistic Ab Initio Hyperfine Coupling, *J. Chem. Theor. Comput.*, 2022, 18, 4719.
125. N. F. Chilton, Molecular Magnetism, *Annu. Rev. Mater. Res.*, 2022, 52, 79.
124. T. Pei, J. O. Thomas, S. Sopp, M.-Y. Tsang, N. Dotti, J. Baugh, N. F. Chilton, S. Cardona-Serra, A. Gaita-Ariño, H. L. Anderson and L. Bogani, Exchange-induced spin polarization in a single magnetic molecule junction, *Nature Commun.*, 2022, 4506.
123. J. G. C. Kragsskow, J. Marbey, C. D. Buch, J. Nehr Korn, M. Ozerov, S. Piligkos, S. Hill and N. F. Chilton, Analysis of vibronic coupling in a 4f molecular magnet with FIRMS, *Nature Commun.*, 2022, 13, 825.
122. C. A. Gould, K. R. McClain, D. Reta, J. G. C. Kragsskow, D. A. Marchiori, E. Lachman, E.-S. Choi, J. G. Analytis, R. D. Britt, N. F. Chilton, B. G. Harvey and J. R. Long, Ultrahard magnetism from mixed-valence dilanthanide complexes with metal-metal bonding, *Science*, 2022, 375, 198.
121. Y.-S. Ding, W. J. A. Blackmore, Y.-Q. Zhai, M. J. Giansiracusa, D. Reta, I. Vitorica-Yrezabal, R. E. P. Winpenny, N. F. Chilton and Y.-Z. Zheng, Studies of the Temperature-Dependence of the Structure and Magnetism of a Hexagonal Bipyramidal Dysprosium(III) Single-Molecule Magnet, *Inorg. Chem.*, 2022, 61, 227.

120. P. Zhang, F. Benner, N. F. Chilton and S. Demir, Organometallic Lanthanide Bismuth Cluster Single-Molecule Magnets, *Chem*, 2022, 8, 717.
119. A. J. Walsinghe and N. F. Chilton, Assessment of minimal active space CASSCF-SO methods for calculation of atomic Slater-Condon and spin-orbit coupling parameters in d- and f-block ions, *Dalton Trans.*, 2021, 50, 14130.
118. R. T. R. Alotaibi, E. Little, J. M. Fowler, A. Brookfield, R. W. Adams, A. Achari, G. A. Timco, G. F. S. Whitehead, N. F. Chilton, R. R. Nair, D. Collison and R. E. P. Winpenny, Single Isomer Heterometallic $\{Cr^{III}_6M^{II}_2\}$ Rings Templated by Tetramethylammonium, *Inorg. Chem.*, 2021, 60, 15675.
117. E. Garlatti, A. Chiesa, P. Bonfà, E. Macaluso, I. Onuorah, V. Parmar, Y.-S. Ding, Y.-Z. Zheng, M. Giansiracusa, D. Reta, E. Pavarini, T. Guidi, D. P. Mills, N. F. Chilton, R. E. P. Winpenny, P. Santini and S. Carretta, A Cost-Effective Semi Ab-initio Approach to Model Relaxation in Rare-Earth Single-Molecule Magnets, *J. Phys. Chem. Lett.*, 2021, 12, 8826.
116. K. Kumar, O. Stefanczyk, N. F. Chilton, K. Nakabayashi, K. Imoto, R. E. P. Winpenny and S.-I. Ohkoshi, Magnetic Properties and Second Harmonic Generation of Noncentrosymmetric Cyanido-Bridged Ln(III)-W(V) Assemblies, *Inorg. Chem.*, 2021, 60, 12009.
115. D. Reta, J. G. C. Kragsskow and N. F. Chilton, Ab initio prediction of high-temperature magnetic relaxation rates in single-molecule magnets, *J. Am. Chem. Soc.*, 2021, 143, 5943.
114. J. A. Seed, L. Birnoschi, E. Lu, F. Tuna, A. J. Wooles, N. F. Chilton and S. T. Liddle, Anomalous Magnetism of Uranium(IV)-Oxo and -Imido Complexes Reveals Unusual Doubly-Degenerate Electronic Ground States, *Chem*, 2021, 7, 1666.
113. L. R. Thomas-Hargreaves, M. J. Giansiracusa, M. Gregson, E. Zanda, F. O'Donnell, A. J. Wooles, N. F. Chilton and S. T. Liddle, Correlating Axial and Equatorial Ligand Field Effects to the Single-Molecule Magnet Performances of a Family of Dysprosium Bis-Methanediide Complexes, *Chem. Sci.*, 2021, 12, 3911.
112. H. M. O'Connor, S. Sanz, A. J. Scott, M. B. Pitak, W. T. Klooster, S. J. Coles, N. F. Chilton, E. J. L. McInnes, P. J. Lusby, H. Weihe, S. Piligkos and E. K. Brechin, $[Cr^{III}_8Ni^{II}_6]^{n+}$ Heterometallic Coordination Cubes, *Molecules*, 2021, 26, 757.
111. A. J. McMillan, M. Sienkowska, P. Di Lorenzo, G. K. Gransbury, N. F. Chilton, M. Salamone, A. Ruffoni, M. Bietti and D. Leonori, Practical and Selective sp^3 C-H Bond Chlorination via Aminium Radicals, *Angew. Chem. Int. Ed.*, 2021, 60, 7132.
110. C. A. P. Goodwin, M. J. Giansiracusa, S. M. Greer, H. M. Nicholas, P. Evans, M. Vonci, S. Hill, N. F. Chilton and D. P. Mills, Isolation and electronic structures of derivatized manganocene, ferrocene and cobaltocene anions, *Nature Chem.*, 2021, 13, 243
109. L. R. Thomas-Hargreaves, D. Hunger, M. Kern, A. J. Wooles, J. van Slageren, N. F. Chilton and S. T. Liddle, Insights into D_{4h} Metal-Symmetry Single-Molecule Magnetism: The Case of a Dysprosium-bis(Boryloxide) Complex, *Chem. Commun.*, 2021, 57, 733.
108. J. Wang, Q.-W. Li, S.-G. Wu, Y.-C. Chen, R.-C. Wan, G.-Z. Huang, Y. Liu, J.-L. Liu, D. Reta, M. J. Giansiracusa, Z.-X. Wang, N. F. Chilton and M.-L. Tong, Opening magnetic hysteresis by axial ferromagnetic coupling: from mono-decker to double-decker metallacrown, *Angew. Chem. Int. Ed.*, 2021, 60, 5299.
107. D. Reta and N. F. Chilton, Extraction of "hidden" relaxation times from AC susceptibility data, *Chem. Sq.*, 2020, 4, 3.

106. M. J. Giansiracusa, S. Al-Badran, A. K. Kostopolous, G. F. S. Whitehead, E. J. L. McInnes, D. Collison, R. E. P. Winpenny and N. F. Chilton, [Magnetic Exchange Interactions in Symmetric Lanthanide Dimetallics](#), *Inorg. Chem. Front.*, 2020, 7, 3909.
105. G. Lu, Y. Liu, W. Deng, G.-Z. Huang, Y.-C. Chen, J.-L. Liu, Z.-P. Ni, M. J. Giansiracusa, N. F. Chilton and M.-L. Tong, [A Perfect Triangular Dysprosium Single-Molecule Magnet with Virtually Antiparallel Ising-like Anisotropy](#), *Inorg. Chem. Front.*, 2020, 7, 2941.
104. D. Parker, E. A. Suturina, I. Kuprov and N. F. Chilton, [How the Ligand Field in Lanthanide Coordination Complexes Determines Magnetic Susceptibility Anisotropy, Paramagnetic NMR Shift and Relaxation Behaviour](#), *Acc. Chem. Res.*, 2020, 53, 1520.
103. K.-X. Yu, J. G. C. Kragsskow, Y.-S. Ding, Y.-Q. Zhai, D. Reta, N. F. Chilton and Y.-Z. Zheng, [Enhancing magnetic hysteresis in single-molecule magnets by ligand functionalisation](#), *Chem*, 2020, 6, 1777.
102. P. Evans, D. Reta, C. A. P. Goodwin, F. Ortu, N. F. Chilton and D. P. Mills, [A Double-Dysprosocenium Single-Molecule Magnet Bound Together with Neutral Ligands](#), *Chem. Commun.*, 2020, 56, 5677.
101. V. S. Parmar, F. Ortu, X. Ma, N. F. Chilton, R. Clérac, D. P. Mills and R. E. P. Winpenny, [Probing relaxation dynamics in five-coordinate dysprosium single-molecule magnets](#), *Chem. Eur. J.*, 2020, 36, 7774.
100. A. Chiesa, F. Cugini, R. Hussain, E. Macaluso, G. Allodi, E. Garlatti, M. Giansiracusa, C. A. P. Goodwin, F. Ortu, D. Reta, J. M. Skelton, T. Guidi, P. Santini, M. Solzi, R. De Renzi, D. P. Mills, N. F. Chilton and S. Carretta, [Understanding magnetic relaxation in high blocking-temperature single-ion magnets](#), *Phys. Rev. B*, 2020, 101, 174402.
99. T. Han, M. J. Giansiracusa, Z.-H. Li, Y.-Song Ding, N. F. Chilton, R. E. P. Winpenny and Y.-Z. Zheng, [Exchange-Biasing in a Dinuclear Dysprosium\(III\) Single-Molecule Magnet with a Large Energy Barrier for Magnetization Reversal](#), *Chem. Eur. J.*, 2020, 26, 6773.
98. Y.-S. Ding, T. Han, Y.-Q. Zhai, D. Reta, N. F. Chilton, R. E. P. Winpenny and Y.-Z. Zheng, [A Study of Magnetic Relaxation in Dysprosium\(III\) Single-Molecule Magnets](#), *Chem. Eur. J.*, 2020, 26, 5893.
97. P. Evans, D. Reta, G. F. S. Whitehead, N. F. Chilton and D. P. Mills, [A Bis-Monophospholyl Dysprosium Cation Showing Magnetic Hysteresis at 48 Kelvin](#), *J. Am. Chem. Soc.*, 2019, 141, 19935.
96. D. Reta and N. F. Chilton, [Uncertainty Estimates for Magnetic Relaxation Times and Magnetic Relaxation Parameters](#), *Phys. Chem. Chem. Phys.*, 2019, 21, 23567.
95. H. M. Nicholas, M. Vonci, C. A. P. Goodwin, S. Wei Loo, S. R. Murphy, D. Cassim, R. E. P. Winpenny, E. J. L. McInnes, N. F. Chilton and D. P. Mills, [Electronic Structures of Bent Lanthanide\(III\) Complexes with Two N-Donor Ligands](#), *Chem. Sci.*, 2019, 10, 10493.
94. A. M. Ariciu, D. H. Woen, D. N. Huh, L. Nodaraki, A. Kostopoulos, C. A. P. Goodwin, N. F. Chilton, E. J. L. McInnes, R. E. P. Winpenny, W. J. Evans and F. Tuna, [Engineering electronic structure to prolong relaxation times in molecular qubits by minimising orbital angular momentum](#), *Nature Commun.*, 2019, 10, 3330.
93. M. J. Giansiracusa, S. Al-Badran, A. K. Kostopoulos, G. F. S. Whitehead, D. Collison, F. Tuna, R. E. P. Winpenny and N. F. Chilton, [A Large Barrier Single-Molecule Magnet Without Magnetic Memory](#), *Dalton Trans.*, 2019, 48, 10795.

92. T. Han, Y.-S. Ding, Z.-H. Li, K.-X. Yu, Y.-Q. Zhai, N. F. Chilton and Y.-Z. Zheng, Dichlorido-bridged dinuclear Dy(III) single-molecule magnet with an effective energy barrier larger than 600 K, *Chem. Commun.*, 2019, 55, 7930.
91. A. C. Harnden, E. A. Suturina, A. S. Batsanov, M. A. Fox, K. Mason, M. Vonci, E. J. L. McInnes, N. F. Chilton and D. Parker, Unravelling the Complexities of Pseudocontact Shift Analysis in Lanthanide Coordination Complexes of Differing Symmetry, *Angew. Chem. Int. Ed.*, 2019, 58, 10290.
90. E. A. Suturina, K. Mason, M. Botta, F. Carniato, I. Kuprov, N. F. Chilton, E. J. L. McInnes, M. Vonci and D. Parker, Periodic trends and hidden dynamics of magnetic properties in three series of triazacyclononane lanthanide complexes, *Dalton Trans.*, 2019, 48, 8400.
89. F. Ortu, D. Reta, Y.-S. Ding, C. A. P. Goodwin, M. P. Gregson, E. J. L. McInnes, R. E. P. Winpenny, Y.-Z. Zheng, S. T. Liddle, D. P. Mills and N. F. Chilton, Studies of Hysteresis and Quantum Tunnelling of the Magnetisation in Dysprosium(III) Single Molecule Magnets, *Dalton Trans.*, 2019, 48, 8541.
88. M. J. Giansiracusa, A. K. Kostopoulos, D. Collison, R. E. P. Winpenny and N. F. Chilton, Correlating Blocking Temperatures with Relaxation Mechanisms in Single-Molecule Magnets, *Chem. Commun.*, 2019, 55, 7025.
87. J. Liu, D. Reta, J. Cleghorn, Y. X. Yeoh, F. Ortu, C. A. P. Goodwin, N. F. Chilton and D. P. Mills, Light Lanthanide Metallocenium Cations Exhibiting Weak Equatorial Anion Interactions, *Chem. Eur. J.*, 2019, 25, 7749.
86. M. Vonci, K. Mason, E. R. Neil, D. S. Yufit, E. J. L. McInnes, D. Parker and N. F. Chilton, Sensitivity of Magnetic Anisotropy in the Solid State for Lanthanide Complexes with Small Crystal Field Splitting, *Inorg. Chem.*, 2019, 58, 5733.
85. J. Wang, Z.-Y. Ruan, Q.-W. Li, Y.-C. Chen, G.-Z. Huang, J.-L. Liu, D. Reta, N. F. Chilton, Z.-X. Wang and M.-L. Tong, Slow magnetic relaxation in a {EuCu₅} metallocrown, *Dalton Trans.*, 2019, 48, 1686.
84. C. A. P. Goodwin, D. Reta, F. Ortu, J. Liu, N. F. Chilton and D. P. Mills, Terbocenium: completing a heavy lanthanide metallocenium cation family with an alternative anion abstraction strategy, *Chem. Commun.*, 2018, 54, 9182.
83. K. Mason, A. C. Harnden, C. Patrick, A. W. J. Poh, A. S. Batsanov, E. A. Suturina, M. Vonci, E. J. L. McInnes, N. F. Chilton and D. Parker, Exquisite Sensitivity of The Ligand Field to Solvation and Donor Polarisability in Coordinatively Saturated Lanthanide Complexes, *Chem. Commun.*, 2018, 54, 8486.
82. Y.-S. Ding, K.-X. Yu, D. Reta, F. Ortu, R. E. P. Winpenny, Y.-Z. Zheng and N. F. Chilton, Field- and temperature-dependent quantum tunnelling of the magnetisation in a large barrier single-molecule magnet, *Nature Commun.*, 2018, 9, 3134.
81. E. A. Suturina, K. Mason, C. F. G. C. Geraldès, N. F. Chilton, D. Parker and Ilya Kuprov, Lanthanide-induced relaxation anisotropy, *Phys. Chem. Chem. Phys.*, 2018, 20, 17676.
80. D. Sertphon, P. Harding, K. S. Murray, B. Moubaraki, N. F. Chilton, S. Hill, J. Marbey, H. Adams, C. G. Davies, G. N. L. Jameson and D. J. Harding, Self-assembly of a mixed-valence Fe^{II}-Fe^{III} tetranuclear star, *Dalton Trans.*, 2018, 47, 7118.
79. J. Turner, N. F. Chilton, A. Kumar, A. L. Colebatch, G. R. Whittell, H. A. Sparkes, A. S. Weller and I. Manners, Iron Precatalysts with Bulky Tri(t-butyl)cyclopentadienyl Ligands for the Dehydrocoupling of Dimethylamine-Borane, *Chem. Eur. J.*, 2018, 24, 14127.

78. S. Sanz, H. M. O'Connor, P. Comar, A. Baldansuren, M. B. Pitak, S. J. Coles, H. Weihe, N. F. Chilton, E. J. L. McInnes, P. J. Lusby, S. Piligkos and E. K. Brechin, Modular $[\text{Fe}^{\text{III}}_8\text{M}^{\text{II}}_6]^{n+}$ ($\text{M}^{\text{II}} = \text{Pd}, \text{Co}, \text{Ni}, \text{Cu}$) Coordination Cages, *Inorg. Chem.*, 2018, 57, 3500.
77. M. J. Giansiracusa, E. Moreno-Pineda, R. Hussain, R. Marx, M. Martínez Prada, P. Neugebauer, S. Al-Badran, D. Collison, F. Tuna, J. van Slageren, S. Carretta, T. Guidi, E. J. L. McInnes, R. E. P. Winpenny and N. F. Chilton, Measurement of Magnetic Exchange in Asymmetric Lanthanide Dimetallics: Toward a Transferable Theoretical Framework, *J. Am. Chem. Soc.*, 2018, 140, 2504.
76. D. Reta, F. Ortu, S. Randall, D. P. Mills, N. F. Chilton, R. E.P. Winpenny, L. Natrajan, B. Edwards and N. Kaltsoyannis, The performance of density functional theory for the description of ground and excited state properties of inorganic and organometallic uranium compounds, *J. Organomet. Chem.*, 2018, 857, 58.
75. C. A. P. Goodwin, D. Reta, F. Ortu, N. F. Chilton and D. P. Mills, Synthesis and Electronic Structures of Heavy Lanthanide Metallocenium Cations, *J. Am. Chem. Soc.*, 2017, 139, 18714.
74. G.-J. Zhou, T. Han, Y.-S. Ding, N. F. Chilton and Y.-Z. Zheng, Metallacrowns as templates for diabolo-like $\{\text{LnCu}_8\}$ complexes with nearly perfect square antiprismatic geometry, *Chem. Eur. J.*, 2017, 23, 15617.
73. M. Vonci, K. Mason, E. A. Suturina, A. T. Frawley, S. G. Worswick, I. Kuprov, D. Parker, E. J. L. McInnes and N. F. Chilton, Rationalisation of anomalous pseudo-contact shifts and their solvent dependence in a series of C_3 -symmetric lanthanide complexes, *J. Am. Chem. Soc.*, 2017, 139, 14166.
72. C. A. P. Goodwin, F. Ortu, D. Reta, N. F. Chilton and D. P. Mills, Molecular magnetic hysteresis at 60 kelvin in dysprosocenium, *Nature*, 2017, 548, 439.
71. J. A. Seed, M. Gregson, F. Tuna, N. F. Chilton, A. J. Wooles, E. J. L. McInnes and S. T. Liddle, Rare Earth- and Uranium-Mesoionic Carbenes: A New Class of f-Block Carbene Complex Derived from an N-Heterocyclic Olefin, *Angew. Chem. Int. Ed.*, 2017, 56, 11534.
70. B. M. Gardner, D. M. King, F. Tuna, A. J. Wooles, N. F. Chilton and S. T. Liddle, Assessing Crystal Field and Magnetic Interactions in Diuranium- μ -Chalcogenide Triamidoamine Complexes With $\text{U}^{\text{IV}}\text{-E-U}^{\text{IV}}$ Cores (E = S, Se, Te): Implications for Determining the Presence or Absence of Actinide-Actinide Magnetic Exchange, *Chem. Sci.*, 2017, 8, 6207.
69. J. S. Uber, M. Estrader, J. Garcia, P. Lloyd-Williams, A. Sadurní, D. Dengler, J. van Slageren, N. F. Chilton, O. Roubeau, S. J. Teat, J. Ribas-Ariño and G. Aromí, Molecules Designed to Contain Two Weakly Coupled Spins with a Photo-switchable Spacer, *Chem. Eur. J.*, 2017, 23, 13648.
68. S. Sanz, H. M. O'Connor, V. Marti-Centelles, P. Comar, M. B. Pitak, S. J. Coles, G. Lorusso, E. Palacios, M. Evangelisti, A. Baldansuren, N. F. Chilton, H. Weihe, E. J. L. McInnes, P. J. Lusby, S. Piligkos and E. K. Brechin, $[\text{M}^{\text{III}}_2\text{M}^{\text{II}}_3]^{n+}$ trigonal bipyramidal cages based on diamagnetic and paramagnetic metalloligands, *Chem. Sci.*, 2017, 8, 5526.
67. C. A. P. Goodwin, N. F. Chilton, L. S. Natrajan, M.-E. Boulon, J. W. Ziller, W. J. Evans and D. P. Mills, Investigation into the Effects of a Trigonal-Planar Ligand Field on the Electronic Properties of Lanthanide(II) Tris(silylamide) Complexes (Ln = Sm, Eu, Tm, Yb), *Inorg. Chem.*, 2017, 56, 5959.
66. E. Loukopoulos, N. F. Chilton, A. Abdul-Sada, and G. E. Kostakis, Exploring the coordination capabilities of a family of flexible benzotriazole-based ligands using cobalt(II) sources, *Cryst. Growth Des.*, 2017, 17, 2718.

65. E. Loukopoulos, M. Kallitsakis, N. Tsoureas, A. Abdul-Sada, N. F. Chilton, I. N. Lykakis and G. E. Kostakis, Cu(II) coordination polymers as vehicles in the A³ coupling, *Inorg. Chem.*, 2017, 56, 4898.
64. M.-E. Boulon, A. Fernandez, E. Moreno Pineda, N. F. Chilton, G. Timco, A. J. Fielding and R. E. P. Winpenny, Measuring spin-spin interactions between heterospins in a hybrid [2]rotaxane, *Angew. Chem. Int. Ed.*, 2017, 56, 3876.
63. F. Ortu, J. Liu, M. Burton, J. M. Fowler, A. Formanik, M.-E. Boulon, N. F. Chilton and D. P. Mills, Analysis of Lanthanide-Radical Magnetic Interactions in Ce(III) 2,2'-Bipyridyl Complexes, *Inorg. Chem.*, 2017, 56, 2496.
62. T. Pugh, N. F. Chilton and R. A. Layfield, Antimony-Ligated Dysprosium Single-Molecule Magnets as Catalysts for Stibine Dehydrocoupling, *Chem. Sci.*, 2017, 8, 2073.
61. Y.-S. Ding, N. F. Chilton, R. E. P. Winpenny and Y.-Z. Zheng, On Approaching The Limit of Molecular Magnetic Anisotropy: A Near-Perfect Pentagonal Bipyramidal Dy^{III} Single-Molecule Magnet, *Angew. Chem. Int. Ed.*, 2016, 55, 16071.
60. Q.-W. Li, R.-C. Wan, Y.-C. Chen, J.-L. Liu, L.-F. Wang, J.-H. Jia, N. F. Chilton and M.-L. Tong, Unprecedented Hexagonal Bipyramidal Single-Ion Magnets Based on Metallocrowns, *Chem. Commun.*, 2016, 52, 13365.
59. D. M. King, P. A. Cleaves, A. J. Wooles, B. M. Gardner, N. F. Chilton, F. Tuna, W. Lewis, E. J. L. McInnes and S. T. Liddle, Molecular and Electronic Structure of Terminal and Alkali Metal-Capped Uranium(V)-Nitride Complexes, *Nature Commun.*, 2016, 7, 13773.
58. T. Pugh, N. F. Chilton and R. A. Layfield, A Low-Symmetry Dysprosium Metallocene Single-Molecule Magnet with a High Anisotropy Barrier, *Angew. Chem. Int. Ed.*, 2016, 55, 11082.
57. K. Griffiths, P. Kumar, G. Akién, N. F. Chilton, A. Abdul-Sada, G. J. Tizzard, S. Coles and G. E. Kostakis, Tetranuclear 3d/4f coordination clusters as highly efficient catalysts for Friedel Crafts alkylation, *Chem. Commun.*, 2016, 52, 7866.
56. C. A. P. Goodwin, N. F. Chilton, G. F. Vettese, E. M. Pineda, I. F. Crowe, J. W. Ziller, W. J. Evans and D. P. Mills, Physicochemical properties of near-linear Ln(II) bis-silylamide complexes (Ln = Sm, Eu, Tm, Yb), *Inorg. Chem.*, 2016, 55, 10057.
55. J. P. S. Walsh, G. Bowling, A.-M. Ariciu, N. F. M. Jailani, N. F. Chilton, P. G. Waddell, D. Collison, F. Tuna and L. J. Higham, Evidence of Slow Magnetic Relaxation in Co(AcO)₂(py)₂(H₂O)₂, *Magnetochemistry*, 2016, 2, 23.
54. J. J. Dunsford, D. J. Evans, T. Pugh, S. N. Shah, N. F. Chilton and M. J. Ingleson, Three-Coordinate Iron(II) Expanded Ring N-heterocyclic Carbene Complexes, *Organometallics*, 2016, 35, 1098.
53. J. O. Moilanen, N. F. Chilton, B. M. Day, T. Pugh and R. A. Layfield, Strong Exchange Coupling in a Trimetallic Radical-Bridged Cobalt(II)-Hexaazatrinaphthalene Complex, *Angew. Chem. Int. Ed.*, 2016, 55, 5521.
52. M. Gregson, N. F. Chilton, A.-M. Ariciu, F. Tuna, I. F. Crowe, W. Lewis, A. J. Blake, D. Collison, E. J. L. McInnes, R. E. P. Winpenny and S. T. Liddle, A Monometallic Lanthanide Bis(methanediide) Single Molecule Magnet with a Large Energy Barrier and Complex Spin Relaxation Behaviour, *Chem. Sci.*, 2016, 7, 155.

51. S. K. Langley, D. P. Wielechowski, N. F. Chilton, B. Moubaraki and K. S. Murray, A Family of $\{Cr^{III}_2Ln^{III}_2\}$ Butterfly Complexes: Effect of the Lanthanide Ion on the Single-Molecule Magnet Properties, *Inorg. Chem.*, 2015, 54, 10497.
50. S. K. Langley, N. F. Chilton, B. Moubaraki and K. S. Murray, Single-molecule magnetism in $\{Co^{III}_2Dy^{III}_2\}$ -amine-polyalcohol-acetylacetonate complexes: Effects of ligand replacement at the Dy^{III} sites on the dynamics of magnetic relaxation, *Inorg. Chem. Front.*, 2015, 2, 867.
49. C. S. Hawes, N. F. Chilton, B. Moubaraki, G. P. Knowles, A. L. Chaffee, K. S. Murray, S. R. Batten and D. R. Turner, Coordination polymers from a highly flexible alkyldiamine-derived ligand: structure, magnetism and gas adsorption studies, *Dalton Trans.*, 2015, 44, 17494.
48. C.-Y. Lin, J.C. Fettinger, N. F. Chilton, A. Formanuk, F. Grandjean, G. J. Long, and P. P. Power, Salts of the Two-Coordinate Homoleptic Manganese(I) Dialkyl Anion $[Mn\{C(SiMe_3)_3\}_2]^-$ with Quenched Orbital Magnetism, *Chem. Commun.*, 2015, 51, 13275.
47. O. A. Blackburn, N. F. Chilton, K. Keller, C. E. Tait, W. K. Myers, E. J. L. McInnes, A. M. Kenwright, P. D. Beer, C. R. Timmel and S. Faulkner, Spectroscopic and crystal field consequences of fluoride binding by $[Yb.DTMA]^{3+}$ in aqueous solution, *Angew. Chem. Int. Ed.*, 2015, 54, 10783.
46. E. Moreno Pineda, N. F. Chilton, F. Tuna, R. E. P. Winpenny and E. J. L. McInnes, Systematic Study of a Family of Butterfly-Like $\{M_2Ln_2\}$ Molecular Magnets ($M = Mg^{II}, Mn^{III}, Co^{II}, Ni^{II},$ and Cu^{II} ; $Ln = Y^{III}, Gd^{III}, Tb^{III}, Dy^{III}, Ho^{III},$ and Er^{III}), *Inorg. Chem.*, 2015, 54, 5930.
45. N. F. Chilton, H. Lei, A. M. Bryan, F. Grandjean, G. J. Long and P. P. Power, Ligand Field Influence on the Electronic and Magnetic Properties of Quasi-Linear Two-Coordinate Iron(II) Complexes, *Dalton Trans.*, 2015, 44, 11202.
44. B. M. Day, N. F. Chilton and R. A. Layfield, Molecular and Electronic Structures of Donor-Functionalized Dysprosium Pentadienyl Complexes, *Dalton. Trans.*, 2015, 44, 7109.
43. T. Rajeshkumar, H. V. Annadata, M. Evangelisti, S. K. Langley, N. F. Chilton, K. S. Murray and G. Rajaraman, Theoretical Studies on Polynuclear $\{Cu^II_5Gd^{III}_n\}$ Clusters ($n = 4, 2$): Towards Understanding Their Large Magnetocaloric Effect, *Inorg. Chem.*, 2015, 54, 1661.
42. N. F. Chilton, Design Criteria for High-Temperature Single-Molecule Magnets, *Inorg. Chem.*, 2015, 54, 2097.
41. S. K. Langley, D. P. Wielechowski, V. Vieru, N. F. Chilton, B. Moubaraki, L. F. Chibotaru and K. S. Murray, The first 4d/4f single molecule magnet containing a $\{Ru^{III}_2Dy^{III}_2\}$ core, *Chem. Commun.*, 2015, 51, 2044.
40. N. F. Chilton, C. A. P. Goodwin, D. P. Mills and R. E. P. Winpenny, The first near-linear bis(amide) f-block complex: a blueprint for a high temperature single molecule magnet, *Chem. Commun.*, 2015, 51, 101.
39. E. Moreno Pineda, N. F. Chilton, R. Marx, M. Dörfel, D. O. Sells, P. Neugebauer, S.-D. Jiang, D. Collison, J. van Slageren, E. J. L. McInnes and R. E. P. Winpenny, Direct measurement of dysprosium(III)···dysprosium(III) interactions in a single-molecule magnet, *Nature Commun.*, 2014, 5, 5243.
38. J. P. S. Walsh, S. Sproules, N. F. Chilton, A.-L. Barra, G. A. Timco, D. Collison, E. J. L. McInnes and R. E. P. Winpenny, On the Possibility of Magneto-Structural Correlations: Detailed Studies of Dinickel Carboxylate Complexes, *Inorg. Chem.*, 2014, 53, 8464.

37. S. Langley, D. Wielechowski, V. Vieru, N. F. Chilton, B. Moubaraki, L. F. Chibotaru and K. S. Murray, Modulation of Slow Magnetic Relaxation by Tuning Magnetic Exchange in $\{\text{Cr}_2\text{Dy}_2\}$ Single Molecule Magnets, *Chem. Sci.*, 2014, 5, 3246.
36. A. Jozwiuk, A. L. Ingram, D. R. Powell, B. Moubaraki, N. F. Chilton, K. S. Murray and R. P. Houser, Redox and acid–base properties of asymmetric non-heme (hydr)oxo-bridged diiron complexes, *Dalton Trans.*, 2014, 43, 9740.
35. S. K. Langley, L. Ungur, N. F. Chilton, B. Moubaraki, L. F. Chibotaru and K. S. Murray, Single-Molecule Magnetism in a Family of $\{\text{Co}^{\text{III}}_2\text{Dy}^{\text{III}}_2\}$ Butterfly Complexes: Effects of Ligand Replacement on the Dynamics of Magnetic Relaxation, *Inorg. Chem.*, 2014, 53, 4303.
34. S. A. Magee, S. Sproules, A.-L. Barra, G. A. Timco, N. F. Chilton, D. Collison, R. E. P. Winpenny and E. J. L. McInnes, Large Zero-Field Splittings of the Ground Spin State Arising from Antisymmetric Exchange Effects in Heterometallic Triangles, *Angew. Chem. Int. Ed.*, 2014, 53, 5310.
33. N. F. Chilton, G. B. Deacon, O. Gazukin, P. C. Junk, B. Kersting, S. K. Langley, B. Moubaraki, K. S. Murray, F. Schleife, M. Shome, D. R. Turner and J. A. Walker, Structure, Magnetic Behavior, and Anisotropy of Homoleptic Trinuclear Lanthanoid 8-Quinolinolate Complexes, *Inorg. Chem.*, 2014, 53, 2528.
32. G. F. S. Whitehead, J. Ferrando-Soria, L. G. Christie, N. F. Chilton, G. A. Timco, F. Moro and R. E. P. Winpenny, The acid test: the chemistry of carboxylic acid functionalised $\{\text{Cr}_7\text{Ni}\}$ rings, *Chem. Sci.*, 2014, 5, 235.
31. S. Koenig, N. F. Chilton, C. Maichle-moessmer, E. M. Pineda, T. Pugh, R. Anwender and R. A. Layfield, Fast magnetic relaxation in an octahedral dysprosium tetramethyl-aluminate complex, *Dalton Trans.*, 2014, 43, 3035.
30. C.-Y. Lin, J.-D. Guo, J. C. Fettinger, S. Nagase, F. Grandjean, G. J. Long, N. F. Chilton and P. P. Power, Dispersion Force Stabilized Two-Coordinate Transition Metal–Amido Complexes of the $-\text{N}(\text{SiMe}_3)\text{Dipp}$ ($\text{Dipp} = \text{C}_6\text{H}_3-2,6-\text{Pr}_2$) Ligand: Structural, Spectroscopic, Magnetic, and Computational Studies, *Inorg. Chem.*, 2013, 52, 13584.
29. S. K. Langley, N. F. Chilton, B. Moubaraki and K. S. Murray, Magnetic properties of octa- and heptadeca-nuclear heterometallic $\text{Co}^{\text{II}}-\text{Ln}^{\text{III}}$ complexes derived from the ligand 6-chloro-2-hydroxypyridine, *Polyhedron*, 2013, 66, 48.
28. S. K. Langley, D. P. Wielechowski, V. Vieru, N. F. Chilton, B. Moubaraki, B. F. Abrahams, L. F. Chibotaru and K. S. Murray, A $\text{Cr}^{\text{II}}_2\text{Dy}^{\text{III}}_2$ Single-Molecule Magnet: Enhancing the Blocking Temperature through 3d Magnetic Exchange, *Angew. Chem. Int. Ed.*, 2013, 52, 12014.
27. N. F. Chilton, D. Collison, E. J. L. McInnes, R. E. P. Winpenny and A. Soncini, An electrostatic model for the determination of magnetic anisotropy in dysprosium complexes, *Nature Commun.*, 2013, 4, 2551.
26. M. E. Russell, C. S. Hawes, A. Ferguson, M. I. J. Polson, N. F. Chilton, B. Moubaraki, K. S. Murray and P. E. Kruger, Synthesis, structural and magnetic characterisation of iron(II/III), cobalt(II) and copper(II) cluster complexes of the polytopic ligand: N-(2-pyridyl)-3-carboxypropanamide, *Dalton Trans.*, 2013, 42, 13576.
25. H. S. Scott, T. M. Ross, N. F. Chilton, I. A. Gass, B. Moubaraki, G. Chastanet, N. Paradis, J.-F. Létard, K. R. Vignesh, G. Rajaraman, S. R. Batten and K. S. Murray, Crown-linked dipyridylamino-triazine ligands and their spin-crossover iron(II) derivatives: magnetism, photomagnetism and cooperativity, *Dalton Trans.*, 2013, 42, 16494.

24. S. K. Langley, N. F. Chilton, B. Moubaraki and K. S. Murray, Anisotropy barrier enhancement via ligand substitution in tetranuclear $\{\text{Co}^{\text{III}}_2\text{Ln}^{\text{III}}_2\}$ single molecule magnets, *Chem. Commun.*, 2013, 49, 6965.
23. W. A. Gobeze, V. A. Milway, N. F. Chilton, B. Moubaraki, K. S. Murray and S. Brooker, Di- and Tetranuclear Complexes of Bis-Tetradentate Pyrimidine-Based Ligands with All-Methylene-Versus Mixed Methylene/Ethylene-Linked Arms, *Eur. J. Inorg. Chem.*, 2013, 2013, 4485.
22. I. A. Gass, S. Tewary, A. Nafady, N. F. Chilton, C. J. Gartshore, M. Asadi, D. W. Lupton, B. Moubaraki, A. M. Bond, J. F. Boas, S.-X. Guo, G. Rajaraman and K. S. Murray, Observation of Ferromagnetic Exchange, Spin Crossover, Reductively Induced Oxidation, and Field-Induced Slow Magnetic Relaxation in Monomeric Cobalt Nitroxides, *Inorg. Chem.*, 2013, 52, 7557.
21. S. K. Langley, N. F. Chilton, B. Moubaraki and K. S. Murray, Single-Molecule Magnetism in Three Related $\{\text{Co}^{\text{III}}_2\text{Dy}^{\text{III}}_2\}$ -Acetylacetonate Complexes with Multiple Relaxation Mechanisms, *Inorg. Chem.*, 2013, 52, 7183.
20. N. F. Chilton, R. P. Anderson, L. D. Turner, A. Soncini and K. S. Murray, PHI: A powerful new program for the analysis of anisotropic monomeric and exchange-coupled polynuclear d- and f-block complexes, *J. Comput. Chem.*, 2013, 34, 1164.
19. M. R. Razali, N. F. Chilton, A. Urbatsch, B. Moubaraki, S. K. Langley, K. S. Murray, G. B. Deacon and S. R. Batten, Trinuclear and tetranuclear manganese clusters derived from cyano(imino(methoxy)methyl)nitrosomethanide (cmnm), *Poly.*, 2013, 52, 797.
18. Y. Han, N. F. Chilton, M. Li, C. Huang, H. Xu, H. Hou, B. Moubaraki, S. K. Langley, S. R. Batten, Y. Fan and K. S. Murray, Post-Synthetic Monovalent Central-Metal Exchange, Specific I_2 Sensing, and Polymerization of a Catalytic $[3 \times 3]$ Grid of $[\text{Cu}^{\text{I}}_4\text{L}_6] \cdot (\text{I})_2 \cdot 13\text{H}_2\text{O}$, *Chem. Eur. J.*, 2013, 19, 6321.
17. M. Schmidt, D. Wiedemann, B. Moubaraki, N. F. Chilton, K. S. Murray, K. R. Vignesh, G. Rajaraman and A. Grohmann, Iron(II) Complexes of Two Amine/Imine N_5 Chelate Ligands Containing a 1,4-Diazepane Core – To Crossover or Not To Crossover, *Eur. J. Inorg. Chem.*, 2013, 2013, 958.
16. N. F. Chilton, S. K. Langley, B. Moubaraki, A. Soncini, S. R. Batten and K. S. Murray, Single molecule magnetism in a family of mononuclear β -diketonate lanthanide(III) complexes: rationalization of magnetic anisotropy in complexes of low symmetry, *Chem. Sci.*, 2013, 4, 1719.
15. C. J. Schneider, J. D. Cashion, N. F. Chilton, C. Etrillard, M. Fuentealba, J. A. K. Howard, J.-F. Létard, C. Milsmann, B. Moubaraki, H. A. Sparkes, S. R. Batten and K. S. Murray, Spin Crossover in a 3,5-Bis(2-pyridyl)-1,2,4-triazolate-Bridged Dinuclear Iron(II) Complex $[\{\text{Fe}(\text{NCBH}_3)(\text{py})\}_2(\mu\text{-L}^1)]_2$ - Powder versus Single Crystal Study, *Eur. J. Inorg. Chem.*, 2013, 2013, 850.
14. M. R. Razali, A. S. R. Chesman, N. F. Chilton, S. K. Langley, B. Moubaraki, K. S. Murray, G. B. Deacon and S. R. Batten, Structure and magnetism of a mixed-valence octanuclear manganese(II/III) cluster derived from carbamoylcyanonitrosomethanide (ccnm), *Dalton Trans.*, 2013, 42, 1400.
13. S. K. Langley, N. F. Chilton, L. Ungur, B. Moubaraki, L. F. Chibotaru and K. S. Murray, Heterometallic Tetranuclear $[\text{Ln}^{\text{III}}_2\text{Co}^{\text{III}}_2]$ Complexes Including Suppression of Quantum Tunneling of Magnetization in the $[\text{Dy}^{\text{III}}_2\text{Co}^{\text{III}}_2]$ Single Molecule Magnet, *Inorg. Chem.*, 2012, 51, 11873.
12. M. Nematirad, W. J. Gee, S. K. Langley, N. F. Chilton, B. Moubaraki, K. S. Murray and S. R. Batten, Single molecule magnetism in a μ -phenolato dinuclear lanthanide motif ligated by heptadentate Schiff base ligands, *Dalton Trans.*, 2012, 41, 13711.

11. A. S. R. Chesman, D. R. Turner, K. J. Berry, N. F. Chilton, B. Moubaraki, K. S. Murray, G. B. Deacon and S. R. Batten, $\text{Ln}^{\text{III}}_2\text{Mn}^{\text{III}}_2$ heterobimetallic 'butterfly' complexes displaying antiferromagnetic coupling (Ln = Eu, Gd, Tb, Er), *Dalton Trans.*, 2012, 41, 11402.
10. S. K. Langley, N. F. Chilton, B. Moubaraki and K. S. Murray, Unusual oxidation state distributions observed for two mixed-valence heptanuclear manganese disc-like clusters, *Dalton Trans.*, 2012, 41, 9789.
9. S. K. Langley, N. F. Chilton, B. Moubaraki and K. S. Murray, Structure and magnetic exchange in heterometallic 3d-3d transition metal triethanolamine clusters, *Dalton Trans.*, 2012, 41, 1033.
8. S. K. Langley, N. F. Chilton, I. A. Gass, B. Moubaraki and K. S. Murray, Planar tetranuclear lanthanide clusters with the Dy_4 analogue displaying slow magnetic relaxation, *Dalton Trans.*, 2011, 40, 12656.
7. R. J. Archer, C. S. Hawes, G. N. L. Jameson, V. McKee, B. Moubaraki, N. F. Chilton, K. S. Murray, W. Schmitt and P. E. Kruger, Partial spin crossover behaviour in a dinuclear iron(II) triple helicate, *Dalton Trans.*, 2011, 40, 12368.
6. S. K. Langley, N. F. Chilton, B. Moubaraki and K. S. Murray, Self-assembled decanuclear $\text{Na}_2\text{Mn}^{\text{II}}_4\text{Mn}^{\text{III}}_4$ complexes: from discrete clusters to 1-D and 2-D structures, with the $\text{Mn}^{\text{II}}_4\text{Mn}^{\text{III}}_4$ unit displaying a large spin ground state and probable SMM behaviour, *Dalton Trans.*, 2011, 40, 12201.
5. S. K. Langley, L. Ungur, N. F. Chilton, B. Moubaraki, L. F. Chibotaru and K. S. Murray, Structure, Magnetism and Theory of a Family of Nonanuclear $\text{Cu}^{\text{II}}_5\text{Ln}^{\text{III}}_4$ -Triethanolamine Clusters Displaying Single-Molecule Magnet Behaviour, *Chem. Eur. J.*, 2011, 17, 9209.
4. S. K. Langley, R. A. Stott, N. F. Chilton, B. Moubaraki and K. S. Murray, A high nuclearity mixed valence $\{\text{Mn}_{32}\}$ complex, *Chem. Commun.*, 2011, 47, 6281.
3. S. K. Langley, N. F. Chilton, B. Moubaraki, T. Hooper, E. K. Brechin, M. Evangelisti and K. S. Murray, Molecular coolers: The case for $[\text{Cu}^{\text{II}}_5\text{Gd}^{\text{III}}_4]$, *Chem. Sci.*, 2011, 2, 1166.
2. N. F. Chilton, S. K. Langley, B. Moubaraki and K. S. Murray, Synthesis, structural and magnetic studies of an isostructural family of mixed 3d/4f tetranuclear 'star' clusters, *Chem. Commun.*, 2010, 46, 7787.
1. S. K. Langley, N. F. Chilton, M. Massi, B. Moubaraki, K. J. Berry and K. S. Murray, Synthesis and characterization of homo- and heterovalent tetra- hexa- hepta- and decanuclear manganese clusters using pyridyl functionalized β -diketone, carboxylate and triethanolamine ligands, *Dalton Trans.*, 2010, 39, 7236.