

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

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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 55** and **166 publications** with over **14,400 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: 2025 APS Physics Global Summit, Anaheim, USA (upcoming)
Dept.: 2025 University of California, Irvine, USA (upcoming)
Invited: 2025 AIP Condensed Matter and Materials Meeting, Brisbane, Australia (upcoming)
Invited: 2024 RACI Inorganic Chemistry Conference, Sydney, Australia (upcoming)
Invited: 2024 Advances in Functional Solids, Kharagpur, India (upcoming)
Keynote: 2024 Modern Trends in Molecular Magnetism, Bangalore, India (upcoming)

Dept.: 2024 The University of Sydney, Australia

Contributed: 2024 European Conference on Molecular Magnetism, Krakow, Poland
Invited: 2024 Young European Conference on Molecular Magnetism, Krakow, Poland
Dept.: 2024 The University of New South Wales, Australia
Invited: 2024 From Fundamentals of Molecular Spin Qubit Design to Molecule-Enabled Quantum Information, Telluride, USA
Tutorial: 2024 Winter School on Quantum Information Science for Chemistry, Los Angeles, USA

Contributed: 2024 RACI Rare Earths Meeting, 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
Invited: 2021 CECAM paramagnetic NMR workshop, Toulouse, France
Dept.: 2021 Nottingham Trent University, Nottingham, UK
Invited: 2021 Rhur EPR colloquium, Germany
Invited: 2021 PTC Virtual Seminar, Chemical Institute of Canada
Invited: 2021 OpenMolcas Developers Conference, Loughborough, UK
Invited: 2021 1st Association de Magnétisme Moléculaire meeting, France
Invited: 2021 Angular Momentum, USA
Invited: 2020 Global Inorganic Discussion Weekdays, Chemical Institute of Canada
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 Univerisitat de Barcelona, Barcelona, Spain
Tutorial: 2014 Univerisitat 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

166. G. K. Gransbury, H. M. Nicholas, S. R. Murphy, J. Emerson-King, M. Vonci, C. A. P. Goodwin, R. E. P. Winpenny, N. F. Chilton, M. J. Giansiracusa and D. P. Mills, [Trigonal planar heteroleptic lanthanide\(III\) bis\(silyl\)amide complexes containing aminoxyl radicals and anions](#), *Inorg. Chem.*, 2024, accepted.

165. J. Du, B. E. Atkinson, J. A. Seed, R. F. Sheppard, F. Tuna, A. J. Wooles, N. F. Chilton and S. T. Liddle, [Strong uranium-phosphorus antiferromagnetic exchange coupling in a crystalline diphosphorus radical trianion actinide complex](#), *Chem.*, 2024, doi: 10.1016/j.chempr.2024.10.004.

164. R. Nabi, B. E. Atkinson, J. K. Staab, J. M. Skelton and N. F. Chilton, [The impact of low-energy phonon lifetimes on the magnetic relaxation in a dysprosocenium single-molecule magnet](#), *Chem. Commun.*, 2024, doi: 10.1039/D4CC03768E.

163. G. M. Richardson, T. Rajeshkumar, F. M. Burke, S. A. Cameron, B. D. Nicholls, J. E. Harvey, R. A. Keyzers, T. Butler, S. Granville, L. Liu, J. Langley, L. F. Lim, N. Cox, N. F. Chilton, J. Hicks, N. J. L. K. Davis, L. Maron and M. D. Anker, [Four-Electron Reduction of Benzene by a Simple Samarium\(II\)-Alkyl](#), *Nature Chem.*, 2024, accepted.

162. N. M. Saji, M. R. Taylor, D. M. Mazzucato, P. J. Low, L. F. Lim, N. Cox, N. F. Chilton, S. A. Moggach, G. F. Turner, M. J. Giansiracusa, C. Boskovic, C. C. Ho, S. C. Thickett, M. K. Stanfield, A. C. Bissember and R. O. Fuller, [Synthesis, structure and redox properties of non-symmetric 6-oxoverdazyls](#), *Org. Lett.*, 2024, accepted.
161. F. Benner, E. R. Pugliese, R. Q. Marsden, R. J. Staples, N. F. Chilton and S. Demir, [An Organometallic Erbium Bismuth Cluster Complex Comprising a \$\text{Bi}_6^{6-}\$ Zintl Ion](#), *Inorg. Chem.*, 2024, doi:10.1021/acs.inorgchem.4c02636.
160. R. L. Frkic, Y. J. Tan, A. Maleckis, N. F. Chilton, G. Otting and C. J. Jackson, [1.3 Å Crystal Structure of *E. coli* Peptidyl-Prolyl Isomerase B with Uniform Substitution of Valine by \(2S,3S\)-4-Fluorovaline Reveals Structure Conservation and Multiple Staggered Rotamers of \$\text{CH}_2\text{F}\$ Group](#), *Biochemistry*, 2024, doi: 10.1021/acs.biochem.4c00345.
159. W. T. Morrillo, H. I. J. Cumming, A. Mattioni, J. K. Staab and N. F. Chilton, [Ab Initio Design of Molecular Qubits with Electric Field Control](#), *J. Am. Chem. Soc.*, 2024, 146, 25841.
158. J. A. Seed, P. A. Cleaves, G. R. Hatton, D. M. King, F. Tuna, A. J. Wooles, N. F. Chilton, S. T. Liddle, [Reactivity of a triamidoamine terminal uranium\(VI\)-nitride with 3d-transition metal metallocenes](#), *Chem. Commun.*, 2024, 60, 9990.
157. R. E. MacKenzie, T. Hajdu, J. A. Seed, G. F. S. Whitehead, R. W. Adams, N. F. Chilton, D. Collison, E. J. L. McInnes and C. A. P. Goodwin, [\$\delta\$ -Bonding Modulates the Electronic Structure of Formally Divalent \$\text{nd}^1\$ Rare Earth Arene Complexes](#), *Chem. Sci.*, 2024, 15, 15160.
156. B. L. L. Réant, F. J. Mackintosh, G. K. Gransbury, C. Andrea Mattei, B. Alnami, B. Atkinson, D. Bonham, J. Baldwin, A. J. Wooles, I. J. Vitorica-Yrezabal, D. Lee, N. F. Chilton, S. T. Liddle and D. P. Mills, [Tris-Silanide f-Block Complexes: Insights into Paramagnetic Influence on NMR Chemical Shifts](#), *J. Am. Chem. Soc. Au*, 2024, 4, 2695.
155. H. Kwon, K. R. McClain, J. G. C. Kragoskow, J. K. Staab, M. Ozerov, K. R. Meihaus, B. G. Harvey, E. S. Choi, N. F. Chilton and J. R. Long, [Coercive Fields Exceeding 30 T in the Mixed-Valence Single-Molecule Magnet \$\(\text{Cp}^*\text{Pr}_5\)_2\text{Ho}_2\text{I}_3\$](#) , *J. Am. Chem. Soc.*, 2024, 146, 18714.
154. J. K. Staab, M. K. Rahman and N. F. Chilton, [Intramolecular bridging strategies to suppress two-phonon Raman spin relaxation in dysprosocenium single-molecule magnets](#), *Phys. Chem. Chem. Phys.*, 2024, 26, 17539.
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 \$\text{Ln}^{\text{III}}\$ -\[\$\text{Ag}^{\text{I}}\$ \(CN\) \$_2\$ \] Networks](#), *Inorg. Chem. Front.*, 2024, 11, 3906.
152. L. E. Nodarakı, 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, 146, 15000.
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, 146, 14660.
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, 63, 9552.
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, 63, 9562.

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. Walisinghe 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. Kragoskow and N. F. Chilton, Ab initio prediction of high-temperature magnetic relaxation rates in single-molecule magnets, *J. Am. Chem. Soc.*, 2021, 143, 5943.
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