

Prof. Nicholas F. Chilton MRSC FHEA

Professor of Computational and Theoretical Chemistry

Royal Society University Research Fellow

Department of Chemistry, School of Natural Sciences, 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 45** and **124 publications** with over **9200 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 over £3M.**

Skills

SQUID magnetometry (DC and AC for regular and air-sensitive solids and solutions)

EPR spectroscopy (CW X-, K-, Q- and W-band for regular and air-sensitive solids and solutions)

CASSCF *ab initio* calculations (including two-component relativistic approaches)

DFT calculations (both molecular and periodic boundary conditions)

Spin Hamiltonian methods (numerical and analytical)

Coding (Fortran, C++, Python)

High-Performance Computing (use of local and centralised infrastructure)

XRD (single crystal and powder, including use of synchrotron facilities and full refinement of data)

Standard analytical chemistry (IR, NMR, UV-Vis-IR, MS, TGA, HPLC, GC)

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

“Synthesis, Structure and Magnetic Anisotropy of Lanthanoid-Based Single Ion Magnets”

Employment

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 – current

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

Supervision (Department of Chemistry, The University of Manchester, UK)

- 2016 – current **PDRA (5 current, 3 former)**
- 2016 – current **Ph.D. (7 current, 1 graduated)**
- 2018 – current **M.Sc. (1 current, 1 graduated)**
- 2016 – current **M.Chem. (2 current, 7 graduated)**

Awards

- 2021 Harrison-Meldola Memorial Prize, Royal Society of Chemistry, UK
- 2020 Distinguished Achievement Medal: Teacher of the Year, The University of Manchester, UK
- 2019 – 2024 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

- 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
- 2013 NSCCS computational support, UK

Teaching (Department of Chemistry, The University of Manchester, UK)2017 – current “Computational Chemistry” in “Core Physical Chemistry” (2nd year)2015 – current “Molecular Magnetism” (4th year M.Chem.)**Lectures**

Plenary: 2022 “29th Rare Earth Research Conference”, Philadelphia, USA (upcoming)
 Dept.: 2022 University of California, Santa Barbara, USA (upcoming)
 Invited: 2022 “Molecular Spin Qubit Design and Quantum Information”, Telluride Science Centre, USA (upcoming)

Invited: 2022 ACS Spring Meeting, San Diego, USA
 Dept.: 2021 Ohio State University, USA (Zoom)
 Invited: 2021 CECAM paramagnetic NMR workshop, Toulouse, France
 Dept.: 2021 Nottingham Trent University, UK
 Invited: 2021 Rhur EPR colloquium, Germany (Zoom)
 Invited: 2021 PTC Virtual Seminar, Chemical Institute of Canada (Zoom)
 Invited: 2021 OpenMolcas Developers Conference, 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 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

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.*, accepted.
123. J. G. C. Kragsskow, J. Marbey, C. D. Buch, J. Nehrkorn, 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 dlanthanide 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*, 2021, doi: 10.1016/j.chempr.2021.11.007
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 {Cr₂M} 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.
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, *[Cr₂Ni]₂ 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 sp³ 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_{3h}@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. Kragsskov, 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 {EuCu} metallacrown*, *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. Hamden, 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-Fe 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 [Fe₂M]²⁺ (M = Pd, Co, Ni, 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, Metallocrowns as templates for diabolite-like {LnCu} 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 C₂-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 U-E-U Cores (E = S, Se, Te): Implications for Determining the Presence or Absence of Actinide-Actinide Magnetic Exchange, *Chem. Sci.*, 2017, 8, 6207.

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