

EPR Facility - Publications list

Publications:

2010:

1. E. Carter, D. Collison, R. Edge, E.C. Fitzgerald, H.N. Lancashire, D.M. Murphy, J.J.W. McDouall, J. Sharples and M.W. Whiteley, "Experimental observation of spin delocalisation onto the aryl-alkynyl ligand in the complexes $[\text{Mo}(\text{C}\equiv\text{Car})(\text{Ph}_2\text{PCH}_2\text{CH}_2\text{PPh}_2)(\eta\text{-C}_7\text{H}_7)]^+$ ($\text{Ar} = \text{C}_6\text{H}_5$, $\text{C}_6\text{H}_4\text{-4-F}$; $\text{C}_7\text{H}_7 = \text{cycloheptatrienyl}$): an EPR and ENDOR investigation" *Dalton Trans.* 2010, **39**, 11424-11431. DOI: **10.1039/c0dt00642d October 2010**
2. N.J. Brown, H.N. Lancashire, M.A. Fox, D. Collison, R. Edge, D.S. Yufit, J.A.K. Howard, M.W. Whiteley and P.J. Low, "Molybdenum complexes of C,C-bis(ethynyl)carboranes: The design, synthesis and study of a weakly-coupled mixed-valence compound", *Organometallics* 2011, **30**, 884-894. DOI: **10.1021/om1010353 December 2010**
3. H.N. Lancashire, N.J. Brown, L. Carthy, D. Collison, E.C. Fitzgerald, R. Edge, M. Halliwell, M. Holden, P.J. Low, J.J.W. McDouall and M.W. Whiteley, "Synthesis, spectroscopy and electronic structure of the vinylidene and alkynyl complexes $[\text{W}(\text{C=CHR})(\text{dppe})(\eta\text{-C}_7\text{H}_7)]^+$ and $[\text{W}(\text{C=CHR})(\text{dppe})(\eta\text{-C}_7\text{H}_7)]^{n+}$ ($n = 0$ or 1)", *Dalton Trans.* 2011, **40**, 1267-1278. DOI: **10.1039/C0DT01150A December 2010**

2011:

4. G. A. Timco, T. B. Faust, F. Tuna, R. E. P. Winpenny, "Linking heterometallic rings for quantum information processing and amusement", *Chem. Soc. Rev.* 2011, **40**, 3067-3075. DOI: **10.1039/c0cs00151a January 2011 (Internal)**
5. M. L. Baker, A. Bianchi, S. Carretta, D. Collison, R. J. Docherty, E. J. L. McInnes, A. McRobbie, C. A. Muryn, H. Mutka, S. Piligkos, M. Rancan, P. Santini, G. A. Timco, P. L. W. Tregenna-Piggott, F. Tuna, H. U. Güdel and R. E. P. Winpenny, "Varying spin state composition by the choice of capping ligand in a family of molecular chains: detailed analysis of magnetic properties of chromium(III) horseshoes". *Dalton Trans.*, 2011, **40**, 2725-2734. DOI: **10.1039/C0DT01243B February 2011**
6. S. A. Sulway, D. Collison, J. J. W. McDouall, F. Tuna, R. A. Layfield, "Iron(II) cage complexes of N-heterocyclic amide and bis(trimethylsilyl)amide ligands: Synthesis, structure, and magnetic properties", *Inorg. Chem.* 2011, **50**, 2521-2526. DOI: **10.1021/ic102341a February 2011 (Internal)**
7. C.J. Cooper, M.D. Jones, S.K. Brayshaw, B. Sonnex, M.L. Russell, M.F. Mahon and D.R. Allan, "When is an imine not an imine? Unusual reactivity of a series of Cu(II) imine-pyridine complexes and their exploitation for the Henry reaction", *Dalton Trans.*, 2011, **40**, 3677-3682. DOI: **10.1039/C0DT01740J March 2011**
8. K. Butsch, A. Klein and M. Bauer, "Highly flexible O,O'N ligands and their Fe, Ni, Cu and Zn complexes", *Inorg. Chim. Acta*, 2011, **374**, 350-358. DOI: **10.1016/j.ica.2011.02.072 March 2011**

9. A.B. Boeer, A-L. Barra, L.F. Chibotaru, D. Collison, E.J.L. McInnes, R.A. Mole, G.S. Simeoni, G.A. Timco, L. Ungur, T. Unruh and R.E.P. Winpenny, "A Spectroscopic Investigation of Magnetic Exchange Between Highly Anisotropic Spin Centres", *Angew. Chem. Int. Ed.* 2011, **50**, 4007-4011. DOI: **10.1002/anie.201100306 April 2011**
10. A.M. Collins, G.J. Blanchard, J. Hawkett, D. Collison, F. Marken, "Liquid|liquid|electrode triple phase boundary photovoltaic photovoltammetry of pentoxyresorufin in 4-(3-phenylpropyl)pyridine", *Langmuir* 2011, **27**, 6471-6477. DOI: **10.1021/la2010584 April 2011**
11. L.J. Batchelor, M. Sander, F. Tuna, M. Helliwell, F. Moro, J. van Slageren, E. Burzurí, O. Montero, M. Evangelisti, F. Luis and E.J.L. McInnes, "Chromium(III) stars and butterflies: synthesis, structural and magnetic studies of tetra-metallic clusters", *Dalton Trans.* 2011, **40**, 5278-5284. DOI: **10.1039/c1dt10172b April 2011**
12. A. McRobbie, A. R. Sarwar, S. Yeninas, H. Nowell, M. Baker, D. Alan, M. Luban, C. A. Muryn, R. G. Pritchard, R. Prozorov, G. A. Timco, F. Tuna, G. F. S. Whitehead, R. E. P. Winpenny, "Chromium chains as polydentate fluoride ligands for lanthanides", *Chem Commun.* 2011, **47**, 6251-6253. DOI: **10.1039/c1cc11516b May 2011**
13. H.N. Roberts, N. J. Brown, R. Edge, R. Lewin, D. Collison and P. J. Low and M.W. Whiteley, "Synthesis, Redox Chemistry and Electronic Structure of the Alkynyl Cyclopentadienyl Molybdenum Complexes $[Mo(C\equiv CR)(CO)(L_2)Cp']^{n+}$ ($n = 0$ or 1 ; $R = Ph$ or C_6H_4-4-Me , $L_2 = Ph_2PCH_2CH_2PPh_2$ or $2PMMe_3$, $Cp' = Cp$ or Cp^*)", *Organometallics*, 2011, **30**, 3763-3778. DOI: **10.1021/om200229c June 2011**
14. R.J. Blagg, C.A. Muryn, E.J.L. McInnes, F. Tuna, R.E.P. Winpenny, "Single pyramid magnets: Dy 5 pyramids with slow magnetic relaxation to 40 K", *Angew. Chem. Int. Ed.* 2011, **50** (29), 6530-6533. DOI: **10.1002/anie.201101932 June 2011 (Internal)**
15. M.L. Baker, S. Piligkos, A. Bianchi, S. Carretta, D. Collison, J.J.W. McDouall, E.J.L. McInnes, H. Mutka, G. A. Timco, F. Tuna, P. Vadivelu, H. Weihe, H.U. Güdel and R.E.P. Winpenny, "Modification of the magnetic properties of a heterometallic wheel by inclusion of a Jahn–Teller distorted Cu(II) ion." *Dalton Trans.*, 2011, **40**, 8533–8539. DOI: **10.1039/c1dt10547g July 2011**
16. H.N. Miras, D. Stone, D-L. Long, E.J.L. McInnes, P. Kögerler and L. Cronin, "Transition metal templated $\{M_{17}V_3\}$ Dawson-like capsules: mechanistic insights, electrochemical studies and catalytic properties", *Inorg. Chem.* 2011, **50** (17), 8384–8391. DOI: **10.1021/ic200943s July 2011**
17. D. Woodruff, M. Bodensteiner, D.O. Sells, R.E.P. Winpenny and R.A. Layfield "Synthesis and structure of cationic guanidinate-bridged bimetallic $\{Li_7M\}$ cubes ($M = Mn, Co, Zn$) with inverse crown counter anions" *Dalton Trans.*, 2011, **40** 10918–10923. DOI: **10.1039/c1dt10999e July 2011**
18. E.C. Fitzgerald, A. Ladjarafi, N.J. Brown, D. Collison, K. Costuas, R. Edge, J.-F. Halet, F. Justaud, P.J. Low, H. Meghezzi, T. Roisnel, M.W. Whiteley and C. Lapinte, "Spectroscopic Evidence for Redox Isomerism in the 1,4-Diethynylbenzene Bridged Heterobimetallic Cation $\{\{Fe(dppe)Cp^*\}(\mu-C\equiv CC_6H_4C\equiv C)\{Mo(dppe)(\eta-C_7H_7)\}\}PF_6^-$ ", *Organometallics* 2011, **30**, 4180-4195, DOI: **10.1021/om200488b July 2011**

19. A.L. Whalley, A.J. Blake, D. Collison, E.S. Davies, H.J. Disley, M. Helliwell, F.E. Mabbs, J. McMaster, C. Wilson and C.D. Garner, "Synthesis, structure and redox properties of bis(cyclopentadienyl)dithiolene complexes of molybdenum and tungsten", *Dalton Trans.* 2011, **40**, 10457–10472. **DOI: 10.1039/c1dt10663e July 2011**
20. E. Stephen, D. Huang, J.L. Shaw, A.J. Blake, D. Collison, E. S. Davies, R. Edge, J. A. K. Howard, E. J. L. McInnes, C. Wilson, J. Wolowska, J. McMaster and M. Schröder, "Redox non-innocence of thioether crowns: spectroelectrochemistry and electronic structure of the mononuclear Ni(III) complexes of aza-thioether macrocycles", *Chem. Eur. J.* 2011, **17** (37), 10246 – 10258. **DOI:10.1002/chem.201100812. August 2011**
21. S. Zlatogorsky, C.A. Muryn, F. Tuna, D.J. Evans and M.J. Ingleson, "Synthesis, structures, and reactivity of chelating bis-N-heterocyclic carbene complexes of iron(II)", *Organometallics* 2011, **30**, 4974-4982. **DOI: 10.1021/om200605b August 2011**
22. P.R. Murray, D. Collison, S. Daff, R. Edge, B.W. Flynn, L. Jack, F. Leroux, E.J.L. McInnes, A.F. Murray, D. Sells, T. Stevenson, J. Wolowska, L.J. Yellowlees, "An *in situ* electrochemical cell for Q- and W-band EPR spectroscopy", *J. Magn. Reson.* 2011, **213**, 206-209. **DOI:10.1016/j.jmr.2011.09.041 September 2011**
23. R.A. Layfield, J.J.W. McDouall, M. Scheer, C. Schwarzmaier, F. Tuna, "Structure and bonding in three-coordinate N-heterocyclic carbene adducts of iron(II) bis(trimethylsilyl)-amide", *Chem. Commun.* 2011, **47** (38), 10623-10625. **DOI:10.1039/c1cc14576b September 2011**
24. S.A. Sulway, R.A. Layfield, F. Tuna, W. Wernsdorfer, R.E.P. Winpenny, "Single-molecule magnetism in cyclopentadienyl-dysprosium chlorides", *Chem. Commun.* 2012, **48** (10), 1508-1510. **DOI:10.1039/c1cc14643b September 2011**
25. R.J. Blagg, F. Tuna, E.J.L. McInnes, R.E.P. Winpenny, "Pentametallic lanthanide-alkoxide square-based pyramids: High energy barrier for thermal relaxation in a holmium single molecule magnet", *Chem. Commun.* 2011, **47** (38), 10587-10589. **DOI:10.1039/c1cc14186d September 2011 (Internal)**
26. P. Mücke, M. Zabel, R. Edge, D. Collison, S. Clément; S. Záliš, R. Winter, "Electron Delocalization in Vinylruthenium Substituted Cyclophanes: Assessment of the Through-Space and the Through-Bond Pathways", *J. Organomet. Chem.* 2011, **696**, 3186-3197. **DOI:10.1016/j.jorgancchem.2011.06.028 October 2011**
27. H.E. Barden, R.A. Wogelius, D. Li, P.L. Manning, N.P. Edwards and B.E. van Dongen, "Morphological and geochemical evidence of eumelanin preservation in the feathers of the early Cretaceous bird, *Gansus Yumenensis*", *PLoS ONE* 2011, **6**, e25494; **DOI: 10.1371/journal.pone.0025494 October 2011**
28. P. R. Murray, S. Crawford, A. Dawson, A. Delf, C. Findlay, L. Jack, E. J. L. McInnes, S. Al-Musharafi, G. S. Nichol, I. Oswald and L. J. Yellowlees, "On the electronic structure of nitro-substituted bipyridines and their platinum complexes" *Dalton Trans.*, 2012, **41**, 201-207. **DOI: 10.1039/c1dt11456e October 2011**
29. J.M. Byrne, N.D. Telling, V.S. Coker, R.A.D. Patrick, G. Van Der Laan, E. Arenholz, F. Tuna, J.R. Lloyd, "Control of nanoparticle size, reactivity and magnetic properties during the bioproduction of magnetite by *Geobacter sulfurreducens*", *Nanotechnology* 2011, **22** (45), 455709-455717. **DOI:10.1088/0957-4484/22/45/455709 October 2011**

30. T. B. Faust, V. Bellini, A. Candini, S. Carretta, G. Lorusso, D. R. Allan, L. Carthy, D. Collison, R. J. Docherty, J. Kenyon, J. Machin, E. J. L. McInnes, C. A. Muryn, H. Nowell, R. G. Pritchard, S. J. Teat, G. A. Timco, F. Tuna, G. F. S. Whitehead, W. Wernsdorfer, M. Affronte and R. E. P. Winpenny, "Chemical control of spin propagation between heterometallic rings", *Chem. Eur. J.* 2011, **17**, 14020-14030.
DOI: 10.1002/chem.201101785 November 2011
31. S. Sproules, T. Weyhermüller, R. Goddard and K. Wieghardt, "The Rhenium Tris(dithiolene) Electron Transfer Series: Calibrating Covalency", *Inorg. Chem.* 2011, **50** (24), 12623-12631. **DOI: 10.1021/ic2016534 November 2011**
32. C. C. Scarborough, S. Sproules, T. Weyhermüller, S. DeBeer and K. Wieghardt, "Electronic and Molecular Structures of the Members of the Electron Transfer Series $[Cr(t\text{bpy})_3]^n$ ($n = 3+, 2+, 1+, 0$): An X-ray Absorption Spectroscopic and Density Functional Theoretical Study", *Inorg. Chem.* 2011, **50** (24), 12446-12462. **DOI: 10.1021/ic201123x November 2011**
33. L.J. Batchelor, M. Sangalli, R. Guillot, N. Guihery, R. Maurice, F. Tuna, T. Mallah, "Pentanuclear cyanide-bridged complexes based on highly anisotropic CoII seven-coordinate building blocks: Synthesis, structure, and magnetic behaviour", *Inorg. Chem.* 2011, **50** (23), 12045-12052. **DOI:10.1021/ic201534e November 2011**
34. P. Surawatanawong, S. Sproules, F. Neese and K. Wieghardt, "Electronic Structures and Spectroscopy of the Electron Transfer Series $[\text{Fe}(\text{NO})\text{L}_2]^z$ ($z = 1+, 0, 1-, 2-, 3-$; $\text{L} = \text{Dithiolene}$)", *Inorg. Chem.* 2011, **50** (23), 12064-12074. **DOI: 10.1021/ic201565d November 2011**
35. T.D. Roberts, F. Tuna, T.L. Malkin, C.A. Kilner, M.A. Halcrow, "An iron(II) complex exhibiting five anhydrous phases, two of which interconvert by spin-crossover with wide hysteresis." *Chemical Science* 2012, **348** (2), 349-354. **DOI:10.1039/c1sc00584g November 2011**
36. J. Callison, R. Edge, K. R. de Cuba, R. H. Carr, J.J.W. McDouall, D. Collison, E.J.L. McInnes, W. va der Borden, K. va der Velde, J. W. Winfield and D. Lennon, "Origin of impurities formed in the polyurethane production chain. Part 1: conditions for chloride transfer from an aryl isocyanide dichloride by-product", *Ind. Eng. Chem. Res.* 2012, **51**, 2515-2523. **DOI: 10.1021/ie2013136 December 2011**
37. E.C. Fitzgerald, N.J. Brown, R. Edge, M. Helliwell, H.N. Roberts, F. Tuna, A Beeby, D. Collison, P. J. Low, and M.W. Whitley, "Orbital Symmetry Control of Electronic Coupling in a Symmetrical, All-Carbon Bridged 'Mixed Valence' Compound: Synthesis, Spectroscopy and Electronic Structure of $[\{\text{Mo}(\text{dppe})(\eta\text{-C}_7\text{H}_7)\}_2(\mu\text{-C}_4)]^{n+}$ ($n = 0, 1$ or 2)", *Organometallics* 2012, **31**, 157-169. **DOI: 10.1021/om200712m December 2011**
38. Y.-Z. Zheng, M. Evangelisti, F. Tuna, R.E.P. Winpenny, "Co-Ln mixed-metal phosphonate grids and cages as molecular magnetic refrigerants", *J. Amer. Chem. Soc.* 2012, **134** (2), 1057-1065. **DOI:10.1021/ja208367k December 2011**
39. A.L. Abdelhady, M.A. Malik, P. O'Brien, F. Tuna, "Nickel and iron sulfide nanoparticles from thiobiurets" *J. Phys. Chem. C.* 2012; **116** (3), 2253-2259. **DOI:10.1021/jp2078659 December 2011**

2012:

40. F. Piga, F. Moro, I. Krivokapic, A.J. Blake, R. Edge, E.J.L. McInnes, F. Luis, M. Evangelisti, J. McMaster and J. van Slageren, "Magnetic properties of a novel family of ferrous cubanes", *Chem. Commun.* 2012, **48**, 2430-2432. DOI: **10.1039/C2CC16853G January 2012**
41. Y. Yan, P. Chandrasekaran, J. T. Mague, S. DeBeer, S. Sproules and J. P. Donahue, "Redox-Controlled Interconversion between Trigonal Prismatic and Octahedral Geometries in a Monodithiolene Tetracarbonyl Complex of Tungsten", *Inorg. Chem.* 2012, **51** (1), 346-361. DOI: **10.1021/ic201748v January 2012**
42. E. Stephen, A. Blake, E. Carter, D. Collison, E. Davies, R. Edge, W. Lewis, D. Murphy, C. Wilson, R. Gould, A. Holder, J. McMaster and M. Schroder, "Redox Non-innocence of Thioether Crowns: Elucidation of the Electronic Structure of the Mononuclear Pd(III) Complexes $[Pd([9]aneS_3)_2]^{3+}$ and $[Pd([18]aneS_6)]^{3+}$ " *Inorg. Chem* 2012, **51**, 1450-1461. DOI: **10.1021/ic2017006 January 2012**
43. J.S. Maass, Z. Chen, M. Zeller, F. Tuna, R.E.P. Winpenny, R.L. Luck, "Syntheses, X-ray structural characterizations, and thermal stabilities of two nonclassical trinuclear vanadium(IV) complexes", *Inorg. Chem.* 2012, **51** (5), 2766-2776
DOI:**10.1021/ic201259u February 2012**
44. C.J. Wedge, G.A. Timco, E.T. Spielberg, R.E. George, F. Tuna, S. Rigby, E.J.L. McInnes, R.E.P. Winpenny, S.J. Blundell and A. Ardavan, "Chemical engineering of molecular qubits", *Phys. Rev. Lett.* 2012, **108**, 107204/1-107204/5 DOI: **10.1103/PhysRevLett.108.107204 March 2012**
45. R. Docherty, F. Tuna, C.A. Kilner, E.J.L. McInnes and M.A. Halcrow, "Suppression of Jahn-Teller distortion in a six-coordinate copper(II) lattice by doping it into a host lattice", *Chem. Commun.*, 2012, **48**, 4055-4057. DOI: **10.1039/C2CC30873H March 2012**
46. A. C. Bowman, S. Sproules and K. Wieghardt, "Electronic Structure of the $[V(^t\text{bpy})_3]^z$ ($z = 3+, 2+, 0, 1-$) Electron Transfer Series", *Inorg. Chem.* 2012, **51**, 3707-3717. DOI: **10.1021/ic202711s March 2012**
47. C. C. Scarborough, K. M. Lancaster, S. DeBeer, T. Weyhermüller, S. Sproules and K. Wieghardt, "Experimental Fingerprints for Redox-Active Terpyridine in $[Cr(tpy)_2](PF_6)_n$ ($n = 3-0$), and the Remarkable Electronic Structure of $[Cr(tpy)_2]^{1-}$ ", *Inorg. Chem.* 2012, **51**(6), 3718-3732. DOI: **10.1021/ic2027219 March 2012**
48. H.N. Miras, M. Sorus, J. Hawkett, D.O. Sells, E.J.L. McInnes, L. Cronin, "Oscillatory Template Exchange in Polyoxometalate Capsules: A Ligand-Triggered, Redox-Powered, Chemically Damped Oscillation", *J. Amer. Chem. Soc.*, 2012, **134**, 6980–6983. DOI: **10.1021/ja302861z April 2012**
49. O.J. McGann, P.A. Bingham, R.J. Hand, A.S. Gandy, M. Kavcic, M. Zitnik, K. Bucar, R. Edge, N.C. Hyatt, "The effects of γ -radiation on model vitreous wasteforms intended for the disposal of intermediate and high level radioactive wastes in the United Kingdom", *J. Nuclear Mat.* 2012, **429**, 353-367. DOI: **10.1016/j.jnucmat.2012.04.007 April 2012**

50. D.P. Mills, O.J. Cooper, F. Tuna, E.J.L. McInnes, E.S. Davies, J. McMaster, F. Moro, W. Lewis, A.J. Blake, and S. Liddle "Synthesis of a uranium(VI)-carbene: reductive formation of uranyl(V)-methanides, oxidative preparation of a $[R_2C=U=O]^{2+}$ analogue of the $[O=U=O]^{2+}$ uranyl ion ($R = Ph_2PNSiMe_3$), and comparison of the nature of $UIV=C$, $UV=C$ and $UVI=C$ double bonds", *J. Amer. Chem. Soc.*, 2012, **134**, 10047-10054. DOI: **10.1021/ja301333f May 2012**
51. K. M. Lancaster, M.-E. Zaballa, S. Sproules, M. Sundararajan, S. DeBeer, J. H. Richards, A. J. Vila, F. Neese and H. B. Gray, "Outer-Sphere Contributions to the Electronic Structure of Type Zero Copper Proteins", *J. Am. Chem. Soc.* 2012, **134**, 8241-8253. DOI: **10.1021/ja302190r May 2012**
52. S. Scheuermayer, F. Tuna, M. Bodensteiner, M. Scheer and R.A. Layfield, "Spin crossover in phosphorus- and arsenic-bridged cyclopentadienyl-manganese(II) dimers", *Chem. Commun.* 2012, **48**, 8087-8089. DOI:**10.1039/C2CC32893C May 2012**
53. D. Gingasu, I. Mindru, L. Patron, G. Marinescu, F. Tuna, S. Preda, J.M. Calderon-Moreno, C. Andronescu, "Synthesis of $CuGa_2O_4$ nanoparticles by precursor and self-propagating combustion methods", *Ceramics Int.* 2012, **38**(8), 6739-6751.
DOI:**10.1016/j.ceramint.2012.05.067 May 2012**
54. F. Tuna, C. A. Smith, M. Bodensteiner, L. F. Chibotaru, E. J. L. McInnes, L. Ungur, R. E. P. Winpenny, D. Collison, R. A. Layfield, "A high anisotropy barrier in a sulphur-bridged organo-dysprosium single-molecule magnet", *Angew. Chem. Int.*, 2012, **51**, 6976-6980. DOI:**10.1002/ange.201202497 June 2012**
55. D. M. King, F. Tuna, E. J. L. McInnes, J. McMaster, W. Lewis, A. J. Blake, S. T. Liddle, "Synthesis and Structure of a Terminal Uranium Nitride Complex", *Science*, 2012, **337**, 717-720. DOI:**10.1126/science.1223488 June 2012**
56. C. C. Scarborough, S. Sproules, C. J. Doonan, K. S. Hagen, T. Weyhermüller, and K. Wieghardt, "Scrutinizing Low-Spin Cr(II) Complexes", *Inorg. Chem.*, 2012, **51**, 6969–6982. DOI: **10.1021/ic300882r June 2012**
57. J. England, C. C. Scarborough, T. Weyhermüller, S. Sproules and K. Wieghardt, "Electronic Structure of the Electron Transfer Series: $[M(bpy)_3]^n$, $[M(tpy)_2]^n$, and $[Fe^{t}bpy_3]^n$ ($M = Fe, Ru$; $n = 3+, 2+, 1+, 0, 1-$). A Mössbauer Spectroscopic and Density Functional Theory Study", *Eur. J. Inorg. Chem.* 2012, **29**, 4605–4621
DOI: **10.1002/ejic.201200232 June 2012**
58. T.B. Faust, F. Tuna, G.A. Timco, M. Affronte, V. Bellini, W. Wernsdorfer, R.E.P. Winpenny, "Controlling magnetic communication through aromatic bridges by variation in torsion angle", *Dalton Trans.* 2012, **41**, 13626-13631. DOI: **10.1039/c2dt31292a June 2012**
59. M. Akhtar, J. Akhtar, M.A. Malik, F. Tuna, M. Helliwell, P. O'Brien, "Deposition of iron selenide nanocrystals and thin films from tris(N,N-diethyl-N ϵ^2 -naphthoylselenoureato)iron(iii)", *J. Mat. Chem.* 2012, **22** (30), 14970-14975.
DOI:**10.1039/C2JM31291C June 2012**
60. A. Silakov, M. T. Olsen, S Sproules, E. J. Reijerse, T. B. Rauchfuss, and W. Lubitz, "EPR/ENDOR, Mössbauer, and Quantum-Chemical Investigations of Diiron Complexes Mimicking the Active Oxidized State of [FeFe]Hydrogenase", *Inorg. Chem.* 2012, **51** (15), 8617-28. DOI: **10.1021/ic3013766 July 2012**

61. D.N. Woodruff, E.J.L. McInnes, D.O. Sells, R.E.P. Winpenny and R.A. Layfield, "Synthesis, structure and paramagnetism of manganese(II) imidophosphate complexes", *Inorg. Chem.*, 2012, **51** (16), 9104-9109, DOI: **10.1021/ic3014046 August 2012**
62. K. Butsch, A. Klein, S. Nitsche, K. Stirnat, J.R. Hawkett, E.J.L. McInnes and M. Bauer, "Structural, physical and kinetic parameters of the Galactose Oxidase model [Cu(triaz)₂] (triaz- = O,N chelating triazole-phenolate ligand)", *Dalton Trans.*, 2012, **41**, 11464-11475, DOI: **10.1039/c2dt31369c August 2012**
63. M.L. Baker, O. Waldmann, S. Piligkos, R. Bircher, O. Cador, S. Carretta, D. Collison, F. Fernandez-Alonso, E.J.L. McInnes, H. Mutka, A. Podlesnyak, F. Tuna, S. Ochsenbein, R. Sessoli, A. Sieber, G.A. Timco, H. Weihe, H.U. Güdel and R.E.P. Winpenny, "Inelastic neutron scattering studies on the odd-membered antiferromagnetic wheel Cr₈Ni", *Phys. Rev. B*. 2012, **86**, 064405/1-064405/11. DOI:**10.1103/PhysRevB.86.064405 August 2012**
64. H.N. Roberts, N.J. Brown, R. Edge, E.C. Fitzgerald, Y.T. Ta, D. Collison, P.J. Low and M.W. Whiteley, "Synthesis, Redox Chemistry and Electronic Structure of the Butadiynyl and Hexatriynyl Complexes [Mo{(C≡C)_n-C≡CR}{(L₂)_{{(n-C_7H_7)}}]^{z+} (n = 1 or 2; z = 0 or 1; R = SiMe₃ or H; L₂ = 2,2'-bipyridine or Ph₂PCH₂CH₂PPPh₂)", *Organometallics*, 2012, **31** (17), 6322–6335 DOI: **10.1021/om3005756 August 2012**}
65. M.M. Roessler, R.M. Evans, R.A. Davies, J. Harmer, F.A. Armstrong, "EPR spectroscopic studies of the Fe-S clusters in the O₂-tolerant [NiFe]-hydrogenase Hyd-1 from Escherichia coli and characterization of the unique [4Fe-3S] cluster by HYSCORE", *J. Amer. Chem. Soc.* 2012, **134**(37), 15581-94. **September 2012**
66. G.A. Timco, E.J.L. McInnes and R.E.P. Winpenny, "Physical studies of heterometallic rings: an ideal system for studying magnetically-coupled systems", *Chem. Soc. Rev.* 2013, **42**, 1796-1806 DOI:**10.1039/C2CS35232J September 2012**
67. K.V. Shuvaev, S. Sproules, J.M. Rautiainen, E.J.L. McInnes, D. Collison, C.E. Anson and A.K. Powell, "A self-assembled Cu(II)₄ [2x2] grid with organic radicals", *Dalton Trans.* 2013, **42**, 2371-81. DOI: **10.1039/c2dt31946b September 2012**
68. K. Abdulwahab, M. A. Malik, P. O'Brien, K. Govender, C. A. Muryn, G. A. Timco, F. Tuna and R. E. P. Winpenny, "Synthesis of Monodispersed Magnetite Nanoparticles via Iron Pivalate Clusters", *Dalton Transactions*. 2013; **42**, 196-206. DOI: **10.1039/c2dt32478d October 2012**
69. C.A. Smith, F. Tuna, M. Bodensteiner, M. Helliwell, D. Collison, R.A. Layfield. "Exchange-coupled oxygen- and sulfur-bridged cyclopentadienyl-manganese(II) cages", *Dalton Trans.* 2013, **42**, 71-74. DOI: **10.1039/c2dt32262e October 2012**
70. M.L. Baker, G.A. Timco, S. Piligkos, J. Mathieson, F. Tuna, P. Kozłowski, M. Antkowiak, T. Guidi, T. Gupta, G. Kamieniarz, R.G. Pritchard, H. Mutka, H. Weihe, L. Cronin, G. Rajaraman, D. Collison, E.J.L. McInnes and R.E.P. Winpenny, "A classification of spin frustration in molecular magnets from a physical study of large odd-numbered-metal, odd electron rings", *Proc. Natl. Acad. Sci. U.S. A.* 2012, **109** (47), 19113-19118. DOI: **10.1073/pnas.1213127109 November 2012**.
71. H. Helten, B. Dutta, J.R. Vance, M.E. Sloan, M.F. Haddow, S. Sproules, D. Collison, G. R. Whittell, G.C. Lloyd-Jones, and I. Manners, "Paramagnetic Ti(III) and Zr(III) Metallocene Complexes as Precatalysts for the Dehydrocoupling/Dehydrogenation of Amine-

Boranes”, *Angew. Chem. Int. Ed.*, 2013, **52**, 437–440 DOI: [10.1002/anie.201207903](https://doi.org/10.1002/anie.201207903)
November 2012

72. L.J. Kershaw Cook, F. Tuna, M.A. Halcrow, “Iron(II) and cobalt(II) complexes of tris-azinyl analogues of 2,2':6',2”-terpyridine”, *Dalton Trans.* 2013, **42**, 2254-2265. DOI: [10.1039/c2dt31736b](https://doi.org/10.1039/c2dt31736b) **November 2012**
73. G.W. Morley, P. Lueders, M.H. Mohammady, S.J. Balian, G. Aeppli, C.W.M. Kay, W.M. Witzel, G. Jeschke, T.S. Monteiro. “Quantum control of hybrid nuclear-electronic qubits”, *Nature Materials*, 2012, **12**, 103-107. DOI:[10.1038/nmat3499](https://doi.org/10.1038/nmat3499) **December 2012**
74. A. Venugopal, F. Tuna, T.P. Spaniol, L. Ungur, L.F. Chibotaru, J. Okuda, R.A. Layfield. “A hydride-ligated dysprosium single-molecule magnet”, *Chem. Commun.* 2013, **49**, 901-903. DOI: [10.1039/c2cc38036f](https://doi.org/10.1039/c2cc38036f) **December 2012**
75. D.N. Woodruff, F. Tuna, M. Bodensteiner, R.E.P. Winpenny, R.A. Layfield, “Single-molecule magnetism in tetrametallic terbium and dysprosium thiolate cages”, *Organometallics* 2013, **32** (5), 1224-1229. DOI:[10.1021/om3010096](https://doi.org/10.1021/om3010096) **December 2012**
76. S. Lindsay, S. K. Lo, O. R. Maguire, E. Bill, M. R. Probert, S. Sproules and C. R. Hess, “Syntheses and Electronic Structure of Bimetallic Complexes Containing a Flexible Redox-Active Bridging Ligand”, *Inorg. Chem.*, 2013, **52**, 898-909. DOI: [0.1021/ic302087f](https://doi.org/10.1021/ic302087f) **December 2012**

2013:

77. V.A. Milway, F. Tuna, A.R. Andrew, L.E. Sharp, S. Parsons, M. Murrie. “Directed Synthesis of {Mn₁₈Cu₆} Heterometallic Complexes”, *Angew. Chem. Int. Ed.* 2013, **52** (7), 1949 -1952. DOI:[10.1002/anie.201208781](https://doi.org/10.1002/anie.201208781) **January 2013**
78. T. S. Sheriff, S. Cope and D. S. Varsani, “Kinetics and mechanism of the manganese(II) catalysed Calmagite dye oxidation using in situ generated hydrogen peroxide”, *Dalton Trans.* 2013, **42**, 5673-5681, DOI: [10.1039/C3DT32873B](https://doi.org/10.1039/C3DT32873B) **February 2013**
79. A. C. Bowman, J. England, S. Sproules, T. Weyhermüller and K. Wieghardt, “Electronic Structures of Homoleptic [Tris(2,2'-bipyridine)M]ⁿ Complexes of the Early transition Metals (M = Sc, Y, Ti, Zr, Hf, V, Nb, Ta; n = 1+, 0, 1-, 2-, 3-): An Experimental and Density Functional Theoretical Study”, *Inorg. Chem.*, 2013, **52**, 2242-2256. DOI: [10.1021/ic302799s](https://doi.org/10.1021/ic302799s) **February 2013**
80. C.R. Pudney, R. S. K. Lane, A. J. Fielding, S. W. Magennis, S. Hay, N. S. Scrutton, “Enzymatic single-molecule kinetic isotope effects”, *J. Am. Chem. Soc.* 2013, **135**, 3855-3864. DOI: [10.1021/ja309286r](https://doi.org/10.1021/ja309286r) **February 2013**
81. D. Patel, F. Tuna, E.J.L. McInnes, J. McMaster, W. Lewis, A.J. Blake, S.T. Liddle, “A triamido-uranium(V) inverse-sandwich 10π-toluene tetraanion complex, *Dalton Trans.* 2013, **42**, 5224–5227. DOI: [10.1039/C3DT50255D](https://doi.org/10.1039/C3DT50255D) **February 2013**
82. A.H. Essa , R.I. Lerrick , F. Tuna, R.W. Harrington, W. Clegg, M.J. Hall, “Reduction of 2,2,2-trichloro-1-arylethanones by RMgX: mechanistic investigation and the synthesis of substituted α,α-dichloroketones”. *Chem. Commun.* 2013, **49**, 2756-2758. DOI:[10.1039/C3CC39147G](https://doi.org/10.1039/C3CC39147G) **February 2013**

83. S. Scheuermayer, F. Tuna, E. Moreno Pineda, M. Bodensteiner, M. Scheer, R. A. Layfield, "Transmetalation of chromocene by lithium-amide, -phosphide, and -arsenide nucleophiles", *Inorg. Chem.* 2013, **52**(7), 3878-3883. DOI: [10.1021/ic3025815](https://doi.org/10.1021/ic3025815) March 2013
84. R.T. McBurney, A. Eisenschmidt, A.M.Z. Slawin, J.C. Walton, "Rapid and selective spiro-cyclisations of O-centred radicals onto aromatic acceptors", *Chemical Science*, 2013, **4**, 2028–2035. DOI: [10.1039/c3sc50500f](https://doi.org/10.1039/c3sc50500f) March 2013
85. D. M. King, F. Tuna, J. McMaster, W. Lewis, A.J. Blake, E.J.L. McInnes, S. T. Liddle, "Single-molecule-magnetism in a single-ion triamidoamine uranium(V) terminal mono-oxo complex", *Angew. Chem. Int. Ed.* 2013, **52**, 4921–4924. DOI:[10.1002/anie.201301007](https://doi.org/10.1002/anie.201301007). April 2013
86. O.J. Cooper, D.P. Mills, J. McMaster, F. Tuna, E.J.L. McInnes, W. Lewis, A.J. Blake and S.T. Liddle, "The nature of the U=C double bond: pushing the stability of high oxidation state uranium-carbenes to the limit", *Chem. Eur. J.* 2013, **19**, 7071–7083. DOI:[10.1002/chem.201300071](https://doi.org/10.1002/chem.201300071). April 2013
87. P. Håkansson, T. Nguyen, P. B. Nair, R. Edge and E. Stulz, "Cu(II)-porphyrin molecular dynamics as seen in a novel EPR/Stochastic Liouville equation study", *Phys. Chem. Chem. Phys.*, 2013, **15**, 10930-10941. DOI: [10.1039/c3cp50788b](https://doi.org/10.1039/c3cp50788b). April 2013
88. R. T. McBurney, J. C. Walton, "Dissociation or Cyclization: Options for a Triad of Radicals Released from Oxime Carbamates", *J. Am. Chem. Soc.*, 2013, **135**, 7349–7354. DOI: [10.1021/ja402833w](https://doi.org/10.1021/ja402833w) April 2013
89. D.M. King, F. Tuna, E.J.L. McInnes, J. McMaster, W. Lewis, A.J. Blake and S.T. Liddle, "Isolation and characterization of a uranium(VI)-nitride triple bond", *Nature Chem.* 2013, **5**, 482-488. DOI:[10.1038/nchem.1642](https://doi.org/10.1038/nchem.1642). May 2013
90. Y. Yan, C. Keating, P. Chandrasekaran, U. Jayarathne, J. T. Mague, S. DeBeer, K. M. Lancaster, S. Sproules, I. V. Rubtsov, and J. P. Donahue, "Ancillary Ligand Effects upon Dithiolene Redox Noninnocence in Tungsten Bis(dithiolene) Complexes", *Inorg. Chem.* 2013, **52**, 6743-6751. DOI: [10.1021/ic4009174](https://doi.org/10.1021/ic4009174) May 2013
91. L. Kathawate, S. Sproules, O. Pawar, G. Markad, S. Haram, V. Puranik and S. Salunke-Gawali, "Synthesis and molecular structure of a zinc complex of the vitamin K₃ analogue phthiocol", *J. Mol. Struct.* 2013, **1048**, 223-229. DOI: [10.1016/j.molstruc.2013.05.057](https://doi.org/10.1016/j.molstruc.2013.05.057) May 2013
92. C. Koch, G. Tria, A. J. Fielding, F. Brodhun, O. Valerius, K. Feussner, G. H. Braus, D. I. Svergun, M. Bennati, I. Feussner. "A structural model of PpoA derived from SAXS-analysis. Implications for substrate conversion". *Biochimica et Biophysica Acta (BBA) - Molecular and Cell Biology of Lipid*,. 2013, **1831**, 1449-1457. DOI:[10.1016/j.bbapap.2013.06.003](https://doi.org/10.1016/j.bbapap.2013.06.003) June 2013
93. R.T. McBurney, J.C. Walton, "Interplay of ortho- with spiro-cyclisation during iminyl radical closures onto arenes and heteroarenes", *Beilstein J. Org. Chem.*, 2013, **9**, 1083–1092. DOI: [10.3762/bjoc.9.120](https://doi.org/10.3762/bjoc.9.120) June 2013

94. R.J. Blagg, L. Ungur, F. Tuna, J. Speak, P. Comar, D. Collison, W. Wernsdorfer, E.J.L. McInnes, L.F. Chibotaru and R.E.P. Winpenny, "Magnetic relaxation pathways in lanthanide single-molecule magnets", *Nature Chem.* 2013, **5**, 673-678. DOI: **10.1038/NCHEM.1707 July 2013**
95. K. Arumugam, C.D. Varnado, Jr., S. Sproules, V.M. Lynch and C.W. Bielawski, "Redox-switchable ring-closing metathesis: catalyst design, synthesis, and study", *Chem. Eur. J.* 2013, **19**, 10866-10875. DOI: **10.1002/chem.201301247 July 2013**
96. H.A. Alturaifi, J. Faulkner, J. Raftery, F. Tuna, D. Collison, M.W. Whiteley, "Synthesis and redox chemistry of cycloheptatrienyl-molybdenum carbon-carbon-chain complexes featuring diimine support ligands:[Mo{(C≡C)_nC≡CR}{(R'N=CH-CH=NR')(η-C₇H₇)}, (n = 0 or 1)", *J. Organomet. Chem.* 2013 **745-746**, 251-257.
DOI:**10.1016/j.jorgancchem.2013.07.073 August 2013**
97. M.A Malik, P. O'Brien, F. Tuna, R. Pritchard, J. Buchweishaija, E. Kimambo, E. Mbofu, "The synthesis, spectroscopy and X-ray single crystal structure of catena-[(μ-anacardato)-copper(II)bipyridine][Cu₂{(μ-O₂CC₆H₃(o-OH)(o-C₁₅H₃₁)}₄(NC₅H₅)₂}", *Dalton Trans.* 2013, **42**, 14438-14444. DOI: **10.1039/C3DT51634B August 2013**
98. F. Moro, S. Tang, F. Tuna, E. J. L. McInnes, E. Lester, "Magnetic Properties of Cobalt Oxide Nanoparticles Synthesised by a Continuous Hydrothermal Method" *J. Magn. Magn. Mat.* 2013, **348**, 1-7. DOI: **10.1016/j.jmmm.2013.07.064 August 2013**
99. A. Upadhyay, N. Komatireddy, A. Ghirri, F. Tuna, S. Langley, A. Kumar S. E. C. Sañudo, B. Moubaraki, K.S. Murray, E.J. L. McInnes, M. Affronte and M. Shanmugam, "Synthesis and magnetothermal properties of a ferromagnetically coupled Ni^{II}-Gd^{III}-Ni^{II} cluster", *Dalton Trans.* 2013, **43**, 259-266. DOI: **10.1039/C3DT52384E August 2013**
100. A. F. R. Kilpatrick, J.C. Green, F.G.N. Cloke, N. Tsoureasa, "Bis(pentalene)di-titanium: a bent double-sandwich complex with a very short Ti-Ti bond", *Chem. Commun.* 2013, **49**, 9434-9436. DOI: **10.1039/c3cc45187a August 2013**
101. S. Ghosh, G. T. Silber, A. J. P. White, N. Robertson, R. Vilar , "Synthesis of a self-assembled copper(II) metallo-rectangle with a guanosine-substituted terpyridine", *Dalton Trans.* 2013, **42**, 12813. DOI:**10.1039/c3dt51845k. August 2013**
102. A. J. Fielding, K. Parey, U. Ermler, S. Scheller, B. Jaun, M. Bennati, "Advanced electron paramagnetic resonance on the catalytic iron–sulfur cluster bound to the CCG domain of heterodisulfide reductase and succinate: quinone reductase", *J Biol Inorg Chem*, 2013, **18(8)**, 905-915. DOI:**10.1007/s00775-013-1037-x September 2013**
103. A. Upadhyay, N. Komatireddy, A. Ghirri, F. Tuna, S.K. Langley, A.K. Srivastava, E.C. Sañudo, B. Moubaraki, K.S. Murray, E.J.L. McInnes, M. Affronte, and M. Shanmugam, "Synthesis and magnetothermal properties of a ferromagnetically coupled Ni^{II}-Gd^{III}-Ni^{II} cluster", *Dalton Trans.* 2014, **43**, 259-266. DOI:**10.1039/C3DT52384E September 2013**
104. J.L. Loughrey, S. Sproules, E.J.L. McInnes, M.J. Hardie and M.A. Halcrow, "Synthesis and electronic structures of new bis- and tris-dioxolene complexes, and their delocalized mixed-valent redox product'. Abstracts of Papers, 246th ACS National Meeting &Exposition, Indianapolis, IN, United States, **September 2013**, INOR-391.

105. L. Turyanska, F. Moro, A. N. Knott, M. W. Fay, T. D. Bradshaw and A. Patanè, "Paramagnetic, near-infrared fluorescent Mn-doped PbS colloidal nanocrystals", *Part. Part. Syst. Charact.* 2013, **30**, 945-949. DOI: **10.1002/ppsc.201300184**. September 2013
106. G. Pascu, C. Deville, S.E. Clifford, L. Guenée, C. Besnard, K.W. Krämer, S-X. Liu, S. Decurtins, F. Tuna, E.J.L. McInnes, R.E.P. Winpenny and A.F. Williams, "The coordination chemistry of tartronic acid with copper: magnetic studies of a quasi-equilateral tricopper triangle", *Dalton Trans.* 2013, **43**, 656-662. DOI: **10.1039/C3DT51838H** October 2013.
107. T. R. Bartlett, S. Ahmed, F. Tuna, D. Collison, G. J. Blanchard, and F. Marken, "Liquid | Liquid Interfacial Photoelectrochemistry of Chromoionophore I Immobilised in 4-(3-Phenylpropyl)-Pyridine Microdroplets", *ChemElectroChem.* 2014, **1**, 400-406. DOI:**10.1002/celc.201300090** October 2013.
108. D. Patel, F. Tuna, E.J.L. McInnes, W. Lewis, A.J. Blake and S.T. Liddle, "An actinide-zintl cluster: a tris-(triamidouranium) $\mu_3\text{-}\eta^2\text{:}\eta^2\text{:}\eta^2$ -hepta-phophanotricycle and its diverse synthetic utility", *Angew. Chem. Int. Ed.* 2013, **52**, 13334-13337. DOI: **10.1002/anie.201306492** October 2013
109. F. J. Douglas, D.A. McLaren, F. Tuna, W. M. Holmes, C.C. Berry and M. Murrie, "Formation of octapod MnO nanoparticles with enhanced ferromagnetism through kinetically-controlled thermal decomposition of polynuclear manganese complexes", *Nanoscale*, 2014, **6**, 172-176. DOI: **10.1039/c3nr04832b** October 2013
110. V. Mougel, L. Chatelain, J. Hermle, R. Caciuffo, E. Colineau, F. Tuna, N. Magnani, A. Degeyer, J. Pécaut and M. Mazzanti, "A uranium based UO_2^{+} - Mn^{2+} single chain magnet assembled trough cation-cation interaction", *Angew. Chem. Int. Ed.* 2014, **53**, 819-823. DOI: **10.1002/anie.201307366** November 2013
111. F. Moro, D. Kaminski, F. Tuna, G.F.S. Whitehead, G.A. Timco, D. Collison, R.E.P. Winpenny, A. Ardavan and E.J.L. McInnes, "Coherent electron spin manipulation in a dilute oriented ensemble of molecular nanomagnets: pulsed EPR on doped single crystals", *Chem. Commun.* 2014, **50**, 91-93. DOI: **10.1039/c3cc46326e** November 2013
112. R. Pievo, B. Angerstein, A.J. Fielding, C. Koch, I. Feussner, M.A Bennati, "Rapid Freeze-Quench Setup for Multi-Frequency EPR Spectroscopy of Enzymatic Reactions", *ChemPhysChem.* 2013, **14**, 4094-4101. DOI:**10.1002/cphc.201300714** November 2013

2014:

113. L. Gala, M. Lawson, K. Jomova, L. Zelenicky, A. Congradyova, M. Mazur and M. Valko, "EPR Spectroscopy of a Clinically Active (1:2)Copper(II)-Histidine Complex Used in the Treatment of Mekes Disease: A Fourier Transform Analysis of a Fluid CW-EPR Spectrum", *Molecules* 2014, **19**, 980-991. DOI: **10.3390/molecules.19010980** Jan 2014

114. J.L. Loughrey, S. Sproules, E.J.L. McInnes, M.J. Hardie and M.A. Halcrow, "Stable mixed-valent radicals from platinum(II) complexes of a bis-dioxolene ligand", *Chem. Eur. J.* 2014, **21**, 6272-6276. DOI: **10.1002/chem.201304848** Feb 2014
115. B.M. Gardner, G. Balázs, M. Scheer, F. Tuna, E.J.L. McInnes, J. McMaster, W. Lewis, A. J. Blake and S.T. Liddle, "Triamidoamine-uranium(IV) stabilised terminal parent phosphide and phosphinidine complexes", *Angew. Chem. Int. Ed.* 2014, **53**, 4484-4488. DOI: **10.1002/anie.201400798** March 2014
116. F. Moro, R. de Miguel, M. Jenkins, C. Gómez-Moreno, D. Sells, F. Tuna, E.J.L. McInnes, A. Lostao, F. Luis and J. van Slageren, "Magnetic anisotropy of polycrystalline magnetoferritin investigated by SQUID and electron magnetic resonance", *J. Magn. Magn. Mat.* 2014, **361**, 188-196. DOI: **10.1016/j.jmmm.2014.02.053** March 2014
117. S.T. Liddle, D. King, B. Gardner, A. Wooles, P. Cleaves, J. McMaster, W. Lewis, A. Blake, E.J.L. McInnes, F. Tuna, Recent Progress in molecular nitride chemistry, Abstracts of Papers, 247th ACS National Meeting &Exposition, Dallas, TX, United States, **March 2014**, NUCL-49.
118. S. Sproules, "Tris(dithiolene) chemistry: a golden jubilee", *Prog. Inorg. Chem.* 2014, **58**, 1-186. ISBN: **978-1-118-79282-7** April 2014
119. 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 splitting effects of the ground state spin arising from antisymmetric exchange effects in heterometallic triangles", *Angew. Chem. Int. Ed.* 2014, **53**, 5310-5313. DOI: **10.1002/anie.201400655**. April 2014
120. D. King, J. McMaster, F. Tuna, E.J.L. McInnes, W. Lewis, A. Blake, S.T. Liddle, "Synthesis and Characterization of an f-Block Terminal Parent Imido [U=NH] Complex: A Masked Uranium(IV)-Nitride Analogue", *J. Am. Chem. Soc.* 2014, **136**, 5619-5622. DOI: **10.1021/ja502405e**. April 2014
121. E. Lu, O. J. Cooper, J. McMaster, F. Tuna, E. J. L. McInnes, W. Lewis, A. J. Blake, S. T. Liddle, "Synthesis, Characterisation, and Reactivity of a Uranium(VI) Carbene Imido Oxo Complexes", *Angew. Chem. Int. Ed.* 2014, **53**, 6696-6700. DOI:**10.1002/anie.201403892**. May 2014
122. L.J. Batchelor, I. Cimatti, R. Guillot, F. Tuna, W. Wernsdorfer, L. Ungur, L. F. Chibotaru, V. E. Campbell, T. Mallah, "Chemical tuning of the magnetic relaxation in dysprosium(III) mononuclear complexes", *Dalton Trans.* 2014, **43**, 12146-12149. DOI: **10.1039/C4DT00846D**. May 2014
123. P. Cucos, F. Tuna, L. Sorace, I. Matei, C. Maxim, S. Shova, R. Gheorghe, A. Caneschi, M. Hillebrand, M. Andruh, "Magnetic and luminescent binuclear double stranded helicates", *Inorg. Chem.* 2014, **53**, 7738-7747. DOI:**10.1021/ic501051q**. June 2014
124. E. Garlatti, M. Albring, M. Baker, R. Doherty, H. Mutka, T. Guidi, G. Whitehead, R. Pritchard, G. Timco, F. Tuna, G. Moretti, S. Carretta, P. Santini, G. Lorusso, M. Affronte, E.J.L. McInnes, D. Collison, R.E.P. Winpenny, 'A detailed study of the magnetism of chiral {Cr₇M} rings: an investigation into parameterization and transferability of parameters', *J. Am. Chem. Soc.* 2014, **136**, 9763-9772
DOI:**10.1021/ja5047445** June 2014.

125. L. Turyanska, R.J.A. Hill, O. Makarovsky, F. Moro, A.N. Knott, O.J. Larkin, A. Patanè, A. Meaney, P.C.M. Christianen, M.W. Fay and R.J. Curry, "Tuneable paramagnetic susceptibility and exciton g-factor in Mn-doped PbS colloidal nanocrystals", *Nanoscale* 2014, **6**, 8919-8925. DOI: [10.1039/c4nr02336f](https://doi.org/10.1039/c4nr02336f). June 2014
126. C.M. Casadei, A. Gumiero, C.L. Metcalfe, E.J. Murphy, J. Basran, M.G. Concilio, S.C.M. Teixeira, T.E. Schrader, A.J. Fielding, A. Ostermann, M.P. Blakeley, E.L. Raven, P.C.E. Moody, "Neutron cryo-crystallography captures the protonation state of ferryl heme in a peroxidase" *Science* 2014, **345**, 193-197. DOI: [10.1126/science.1254398](https://doi.org/10.1126/science.1254398). July 2014.
127. K.H. Zangana, E. Moreno Pineda, I.J. Vitorica-Yrezabal, E.J.L. McInnes and R.E.P. Winpenny, "Linking Cr₃ triangles through phosphonates and lanthanides: synthetic, structural, magnetic and EPR studies", *Dalton Trans.* 2014, **43**, 13242-13249. DOI: [10.1039/C4DT01264J](https://doi.org/10.1039/C4DT01264J) July 2014
128. 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 di-nickel carboxylate complexes", *Inorg. Chem.* 2014, **53**, 8464-8472. DOI: [10.1021/ic501036h](https://doi.org/10.1021/ic501036h) July 2014
129. P. Cleaves, D. King, C. Kefalidis, L. Maron, F. Tuna, E.J.L. McInnes, J. McMaster, W. Lewis, A. Blake, S. Liddle, "Two-electron reductive carbonylation of terminal uranium(V) and uranium(VI) nitrides to cyanate by carbon monoxide", *Angew. Chem. Int. Ed.* 2014, **53**, 10412-10415. DOI: [10.1002/anie.201406203](https://doi.org/10.1002/anie.201406203) July 2014
130. A. Witt, F. W. Heinemann, S. Sproules, M. M. Khusniyarov, "Modulation of magnetic properties at room temperature: coordination-induced valence tautomerism in a cobalt dioxolene complex", *Chem Eur. J.* 2014, **20**, 11149. DOI:[10.1002/chem.201402129](https://doi.org/10.1002/chem.201402129). July 2014
131. F.J. Kettles, V. A. Milway, F. Tuna, R. Valiente, L. H. Thomas, W. Wernsdorfer, S. T. Ochsenbein, M. Murrie, "Exchange interactions at the origin of slow relaxation of the magnetization in {TbCu₃} and {DyCu₃} single-molecule magnets", *Inorg. Chem.* 2014, **53**, 8970-8978. DOI: [10.1021/ic500885r](https://doi.org/10.1021/ic500885r) August 2014
132. L. Chatelain, J.P.S. Walsh, J. Pecaut, F. Tuna, M. Mazzanti, "Self-assembly of a 3d-5f trinuclear single-molecule magnet from a pentavalent uranyl complex", *Angew. Chem. Int. Ed.* 2014, **53**, 13434-13438. DOI: [10.1002/ange.201407334](https://doi.org/10.1002/ange.201407334). August 2014
133. D.J. Lewis, P. Deshmukh, F. Tuna, P. O'Brien, 'On the Interaction of copper(II) with disulfiram", *Chem. Commun.* 2014, **50**, 13334-13337. DOI: [10.1039/c4cc04767b](https://doi.org/10.1039/c4cc04767b). September 2014
134. C.A.P. Goodwin, F. Tuna, E.J.L. McInnes, S.T. Liddle, J. McMaster, I.J. Vitorica-Yrezabal and D.P. Mills, "[U^{III}{N(SiMe₂tBu)₂}₃]: A structurally authenticated trigonal planar actinide complex", *Chem. Eur. J.* 2014, **20**, 14579-14583. DOI: [10.1002/chem.201404864](https://doi.org/10.1002/chem.201404864) September 2014
135. J.W. Sharples, D. Collison, E.J.L. McInnes, J. Schnack, E. Palacio, M. Evangelisti, "Quantum signatures of a molecular nanomagnet in direct magnetocaloric measurements", *Nature. Commun.* 2014, **5**, DOI: [10.1038/ncomms6321](https://doi.org/10.1038/ncomms6321). September 2014
136. T. Nguyen, P. Håkansson, R. Edge, D. Collison, B.A. Goodman, J.R. Burns, E. Stulz, "EPR

- based distance measurement in Cu-porphyrin-DNA”, *New J. Chem.* 2014, **38**, 5254-5259. DOI: **10.1039/c4nj00673a October 2014**
137. 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. DOI: **10.1038/ncomms6243 October 2014**
138. D. Kaminski, A.L. Webber, C.J. Wedge, J. Liu, G.A. Timco, I.J. Vitorica-Yrezabal, E.J.L. McInnes, R.E.P. Winpenny and A. Ardavan, “Quantum spin coherence in halogen-modified Cr₇Ni molecular nanomagnets”, *Phys. Rev. B* 2014, **90**, 4419. DOI: **10.1103/PhysRevB.90.184419. October 2014**
139. A.J. Fielding, M.G. Concilio, G. Heaven and M.A. Hollas, “New developments in spin labels for pulsed dipolar EPR”, *Molecules* 2014, **19**, 16998-17025. DOI: **10.3390/molecules191016998. October 2014**.
140. S. Vaidya, A. Upadhyay, S.K. Singh, T. Gupta, S. Tewary, S.K. Langley, J.P.S. Walsh, K.S. Murray, G. Rajaraman and M. Shanmugam, “Synthetic strategy for switching the single ion anisotropy in tetrahedral Co(II) complexes”, *Chem. Commun.* 2015, DOI: **10.1039/C4CC08305A. October 2014**
141. D. Jeanmaire, G.A. Timco, A. Gennari, S. Sproules, K.J. Williams, R.E.P. Winpenny and N. Tirelli, “Binary behaviour of an oxidation-responsive MRI nano contrast agent”, *Chem. Commun.* 2015, **51**, 1074. DOI:**10.1039/C4CC08024F November 2014**
142. F. Moro, L. Turyanska, J. Granwehr and A. Patanè, “Spin manipulation and spin-lattice relaxation in magnetic colloidal quantum dots”, *Phys. Rev. B* 2014, **90**, 205428. DOI:**10.1103/PhysRevB.90.205428 November 2014**
143. J. Goura, J.P.S. Walsh, F. Tuna, V. Chandrasekhar, “Synthesis, structure, and magnetism of non-planar heptanuclear lanthanide(III) complexes”, *Dalton Trans.* 2015, **44**, 1142-1149. DOI: **10.1039/c4dt01603c November 2014**

2015:

144. C.E. Tait, P. Neuhaus, H.L. Anderson, C.R. Timmel, D. Carbonera and M. Di Valentin, “HYSCORE on photoexcited triplets”, *Appl. Magn. Reson.* 2015, **46**, 389-409. DOI:**10.1007/s00723-014-0624-5. January 2015**
145. S. Sanz, H.M. O’Connor, E.M. Pineda, K.S. Pederson, G.S. Nichol, O. Mønsted, H. Weihe, S. Piligkos, E.J.L. McInnes, P.J. Lusby and E.K. Brechin, “[Cr^{III}₈M^{II}₆]¹²⁺ (M^{II} = Cu, Co) coordination cubes”, *Angew. Chem. Int. Ed.* 2015, **54**, 6761-6764. DOI: **10.1002/anie.201501041. April 2015**
146. B.M. Gardner, F. Tuna, E.J.L. McInnes, J. McMaster, W. Lewis, A.J. Blake and S.T. Liddle, “An inverted sandwich diuranium $\mu\text{-}\eta^5\text{:}\eta^5$ -cyclo-P₅ complex supported by U-P₅ bonding”, *Angew. Chem. Int. Ed.* 2015, **54**, 7068-7072. DOI: **10.1002/anie.201501728. April 2015**
147. C.E. Tait, P. Neuhaus, H.L. Anderson and C.R. Timmel, “Triplet state delocalisation in a conjugated porphyrin dimer probed by transient electron paramagnetic resonance

- techniques”, *J. Amer. Chem. Soc.* 2015, **137**, 6670-6679. DOI: [10.1021/jacs.5b03249](https://doi.org/10.1021/jacs.5b03249). April 2015
148. J. Goura, J. P.S. Walsh, F. Tuna, R. Halder, T. K. Maji, V. Chandrasekhar, “P-C Bond Cleavage-assisted lanthanide phosphate coordination polymers”, *Crystal Growth. Design* 2015, **15**, 2555-2560. DOI:[10.1021/cg5017005](https://doi.org/10.1021/cg5017005). April 2015
149. A. Baldansuren, “Structure and magnetic properties of six-atom silver clusters supported on LTA zeolite”, arXiv.org, *e-Print Archive, Condensed Matter* 2015, 1-10. DOI: [arXiv:1504.00893v1](https://arxiv.org/abs/1504.00893v1). April 2015 (Internal)
150. J. Goura, A. Chakraborty, J. P. Walsh, F. Tuna, V. Chandrasekhar, “Hexanuclear 3d-4f Neutral Co₂Ln₄ clusters: synthesis, structure and magnetism”, *Crystal Growth. Design* 2015, **15**, 3157-3165. DOI:[10.1021/acs.cgd.5b00588](https://doi.org/10.1021/acs.cgd.5b00588). May 2015
151. B.M. Gardner, G. Balazs, M. Scheer, F. Tuna, E.J.L. McInnes, J. McMaster, W. Lewis, A.J. Blake, S.T. Liddle, “Triamidoamine uranium(IV)-arsenic complexes containing one-, two- and threefold U-As bonding interactions”, *Nature Chem.* 2015, **7**, 582-590. DOI:[10.1038/nchem.2279](https://doi.org/10.1038/nchem.2279) June 2015
152. A. Fernandez, E.M. Pineda, J. Ferrando-Soria, E.J.L. McInnes, G.A. Timco and R.E.P. Winpenny, “A hybrid organic-inorganic daisy chain”, *Chem. Commun.* 2015, **51**, 11126-11129. DOI: [10.1039/C5CC02216A](https://doi.org/10.1039/C5CC02216A). June 2015
153. F. Moro, L. Turyanska, J. Wilman, A.J. Fielding, M.W. Fray, J. Granwehr and A. Patanè, “Electron spin coherence near room temperature in magnetic quantum dots”, *Scientific Reports* 2015, **5**, 10855. DOI:[10.1038/srep10855](https://doi.org/10.1038/srep10855). June 2015
154. E.V. Puttock, P. Banerjee, M. Kaspar, L. Drennen, D.S. Yufit, E. Bill, S. Sproule, C.R. Hess, “A series of [Co(Mabiq)Cl_{2-n}] (n = 0, 1, 2) compounds and evidence for the elusive bimetallic form” *Inorg. Chem.* 2015, **54**, 5864-5873. DOI:[10.1021/acs.inorgchem.5b00636](https://doi.org/10.1021/acs.inorgchem.5b00636). June 2015
155. A.T. Murray, M.J.H. Dowley, F.P. Caggiano, A. Baldansuren, A. J. Fielding, F. Tuna, C.H. Hendon, A. Walsh, G.C. Lloyd-Jones, M.P. John, D.R. Carbery, “Catalytic Amine Oxidation under Ambient Aerobic Conditions: Mimicry of Monoamine Oxidase B”, *Angew. Chem. Int. Ed.* 2015, **54**, 8997-9000. DOI: [10.1002/anie.201503654](https://doi.org/10.1002/anie.201503654). June 2015
156. L. Chatelain, F. Tuna, J. Pecaut, M. Mazzanti, “A zig-zag uranyl(V)-Mn(II) single chain magnet with a high relaxation barrier”, *Chem. Commun.* 2015, **51**, 11309-11312. DOI: [10.1039/C5CC02945G](https://doi.org/10.1039/C5CC02945G). June 2015
157. J. Ferrando-Soria, A. Fernandez, E. Moreno Pineda, S. A. Varey, R. W. Adams, I. J. Vitorica-Yrezabal, F. Tuna, G. A. Timco, C. A. Muryn, R. E. P. Winpenny, “Controlled Synthesis of Nanoscopic Metal Cages”, *J. Amer. Chem. Soc.* 2015, **137**, 7644-7647. DOI:[10.1021/jacs.5b04664](https://doi.org/10.1021/jacs.5b04664). June 2015
158. E. Moreno Pineda, N. F. Chilton, F. Tuna, R. E. P. Winpenny, E.J.L. McInnes, “Systematic study of a family of butterfly-like {M₂Ln₂} molecular magnets”, *Inorg. Chem.* 2015, **54**, 5930-5941. DOI:[10.1021/acs.inorgchem.5b00746](https://doi.org/10.1021/acs.inorgchem.5b00746). June 2015
159. J.O. Moilanen, B.J. Day, T. Pugh and R.A. Layfield, “Open shell doublet character in a hexaaazatrinaphylene trianion complex” *Chem. Commun.* 2015, **51**, 11478. DOI: [10.1039/c5cc04004c](https://doi.org/10.1039/c5cc04004c) June 2015

160. T. Pugh, F. Tuna, L. Ungur, E.J.L. McInnes, D. Collison, L. Chibotaru, R.A. Layfield, "Influencing the properties of dysprosium single-molecule magnets with phosphorus donor ligands", *Nature Commun.* 2015, DOI:10.1038/ncomms8492 **July 2015**
161. E. Moreno Pineda, C. Heesing, F. Tuna, Y.-Z. Zheng, E.J.L. McInnes, J. Schnack, R.E.P. Winpenny, "Copper lanthanide phosphonate cages: Highly symmetric {Cu₃Ln₉P₆} and {Cu₆Ln₆P₆} clusters with C_{3v} and D_{3h} symmetry, *Inorg. Chem.* 2015, **54**, 6331-6337. DOI: 10.1021/acs.inorgchem.5b00649. **July 2015**
162. O.A. Blackburn, N.F. Chilton, K. Keller, C. Tait, W.K. Meyers, E.J.L. McInnes, A.M. Kenwright, 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**, 10783-10786. DOI: 10.1002/anie.201503421. **July 2015**
163. A. Fernandez, E.M. Pineda, C.A. Muryn, S. Sproules, F. Moro, G.A. Timco, E.J.L. McInnes and R.E.P. Winpenny, "g-engineering in hybrid rotaxanes to create AB and AB₂ electron spin systems: EPR studies of weak interactions between dissimilar electron spin qubits", *Angew. Chem. Int. Ed.* 2015, **54**, 10858-10861. DOI: DOI: 10.1002/anie.201504487. **July 2015**
164. C-Y. Lin, J.C. Fettinger, N.F. Chilton, A. Formanuik, F. Grandjean, G.J. Long and P.P. Power, "Salts fo the two-coordinate homoleptic manganese(I) dialkyl anion [Mn{C(SiMe₃)₃}₂]⁻ with quenched orbital magnetism", *Chem. Commun.* 2015, **51**, 13275-13278. DOI: 10.1039/c5cc05166e **July 2015**
165. J.L. Loughrey, N.J. Patmore, A. Baldansuren, A.J. Fielding, E.J.L. McInnes, M.J. Hardie, S. Sproules and M.A. Halcrow, "Platinum(II) complexes of mixed-valent radicals derived from cyclotriflatechylene, a macrocyclic tris-dioxolene", *Chem. Sci.* 2015, **6**, 6935-6948. DOI: 10.1039/c5sc02776. **August 2015**
166. A. Ardavan, A.M. Bowen, A. Fernandez, A.J. Fielding, D. Kaminski, F. Moro, C.A. Muryn, M.D. Wise, A. Ruggi, E.J.L. McInnes, K. Severin, G.A. Timco, C.R. Timmel, F. Tuna, G.F.S. Whitehead and R.E.P. Winpenny, "Engineering coherent interactions in molecular nanomagnet dimers", *npj Quantum Information* 2015, **1**, 151012. doi:10.1038/npjqqi.2015.12 arXiv:1510.01694, **September 2015**
167. E.J.L. McInnes, G.A. Timco, G.F.S. Whitehead and R.E.P. Winpenny, "Heterometallic rings: their physics and use as supramolecular building blocks", *Angew. Chem. Int. Ed.* 2015, **54**, 14244-14269. DOI: 10.1002/anie.201502730 **October 2015**
168. B.M. Gardner, G. Balázs, M. Scheer, A.J. Wooley, F. Tuna, E.J.L. McInnes, J. McMaster, W. Lewis, A.J. Blake and S.T. Liddle, "Isolation of elusive HAsAsH in a crystalline diuranium(IV) complex", *Angew. Chem. Int. Ed.* 2015, **54**, 15250-15254. DOI: 10.1002/anie.201508600 **October 2015**
169. L. Chatelain, J. Pecaut, F. Tuna and M. Mazzanti, 'Heterometallic Fe₂^{II}-U^V and Ni₂^{II}-U^V Exchange-coupled Single-Molecule Magnets: Effect of the 3 d Ion on the Magnetic Properties', *Chem. Eur. J.* 2015, **50**, 18038–18042. DOI: 10.1002/chem.201503637 **October 2015**
170. M.J.H. Ojea, C. Wilson, S.J. Coles, F. Tuna and M. Murrie, "Directed synthesis of {Cu^{II}₂Zn^{II}₂} and {Cu^{II}₈Zn^{II}₈} heterometallic complexes ", *Dalton Trans.* 2015, **44**, 19275-19281. DOI: 10.1039/C5DT03344F. **October 2015**

171. A. Baldansuren, "EXAFS Experiments on Local Structure of NO Adsorbed on Supported Silver Clusters", arXiv.org, *e-Print Archive, Condensed Matter*. 2015, 1-4. DOI: [arXiv:1510.02648v1](https://arxiv.org/abs/1510.02648v1). October 2015
172. 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**, 155-165. DOI: [10.1039/C5SC03111G](https://doi.org/10.1039/C5SC03111G). November 2015
173. F. Ortú, H. Zhu, M.E. Boulon, D. Mills, "Synthesis and Reactivity of a Cerium(III) Scorpionate Complex Containing a Redox Non-Innocent 2,2'-Bipyridine Ligand", *Inorganics*, 2015, **3**, 534-553. DOI: [10.3390/inorganics3040534](https://doi.org/10.3390/inorganics3040534). November 2015
174. M.A. Palacios, E.M. Pineda, S. Sanz, R. Inglis, M.B. Pitak, S.J. Coles, M. Evangelisti, H. Nojiri, C. Heesing, E.K. Brechin, J. Schnack and R.E.P. Winpenny, "Copper Keplerates: high-symmetry magnetic molecules", *ChemPhysChem* 2016, **17**, 55-60. DOI: [10.1002/cphc.201500956](https://doi.org/10.1002/cphc.201500956). November 2015
175. C.J. Stevens, A. Prescimone, F. Tuna, E.J.L. McInnes, S. Parsons, C.A. Morrison, P.L. Arnold and J.B. Love, "Inter vs. intramolecular structural manipulation of a dichromium(II) Pacman complex through pressure variation", *Inorg. Chem.* 2016, **55**, 214-220. DOI: [10.1021/acs.inorgchem.5b02151](https://doi.org/10.1021/acs.inorgchem.5b02151) December 2015
176. J.P.S. Walsh, S. Meadows, A. Ghirri, M. Jennings, W. Smith, D. Graham, T. Kihara, H. Nojiri, I. Vitorica-Yrezabal, G.A. Timco, D. Collison, E.J.L. McInnes and R.E.P. Winpenny, "Electronic structure of a novel mixed-metal fluoride-centered triangle complex: a potential qubit component", *Inorg. Chem.* 2015, **54**, 12019-12026. DOI: [10.1021/acs.inorgchem.5b01898](https://doi.org/10.1021/acs.inorgchem.5b01898) December 2015
177. A.T. Murray, R. King, J.V.G. Donelly, M.J.H. Dowley, F. Tuna, D. Sells, M.P. John, D.R. Carbery, 'Symbiotic transition-metal and organocatalysis for catalytic ambient amine oxidation and alkene reduction reactions', *ChemCatChem* 2016, **8**, 510-514. DOI: [10.1002/cctc.201501153](https://doi.org/10.1002/cctc.201501153). December 2015

2016:

178. A. Fernandez, J. Ferrando-Soria, E. M. Pineda, F. Tuna, I.J. Vitorica-Yrezabal, C. Knappke, J. Ujma, C.A. Muryn, G.A. Timco, P.E. Barran, A. Adavan, R.E.P. Winpenny, "Making hybrid [n]-rotaxanes as supramolecular arrays of molecular electron spin qubit", *Nature Commun.* 2016, **7**: 10240, 1-6. DOI: [10.1038/ncomms10240](https://doi.org/10.1038/ncomms10240) January 2016
179. M.L. Baker, T. Lancaster, A. Chiesa, G. Amoretti, P.J. Baker, C. Barker, S.J. Blundell, S. Garretta, D. Collison, H.U. Guedel, T. Guidi, E.J.L. McInnes, J.S. Moeller, H. Mutka, J. Ollivier, F.L. Pratt, P. Santini, F. Tuna, P.L.W. Tregenna-Piggott, I.J. Vitorica-Yrezabal, G.A. Timco and R.E.P. Winpenny, "Studies of a large odd-numbered odd- electron metal ring: Inelastic neutron scattering and muon spin relaxation spectroscopy of Cr₈Mn", *Chem. Eur. J.*, 2016, **22**, 1779-1788. DOI: [10.1002/chem.20150343](https://doi.org/10.1002/chem.20150343). Jan 2016

180. K.E.H. Frandsen, T.J. Simmons, P. Dupree, J.-C. N. Poulsen, G.R. Hemsworth, L. Ciano, E.M. Johnston, M. Tovborg, K.S. Johansen, P. von Freiesleben, L. Marmuse, S. Fort, S. Cottaz, H. Driguez, B. Henrissat, N. Lenfant, F. Tuna, A. Baldansuren, G.J. Davies, L. Lo Leggio and P. H. Walton, "The molecular basis of polysaccharide cleavage by lytic polysaccharide-monooxygenases", *Nature Chemical Biology* 2016, **12**, 298-303 (Cover). DOI:10.1038/nchembio.2029. February 2016
181. M. Gregson, E. Liu, F. Tuna, E.J.L. McInnes, C. Hennig, A.C. Schienhost, J. McMaster, W. Lewis, A.J. Blake, A. Kerridge and S.T. Liddle, "Emergence of comparable covalency in isostructural cerium(IV)- and uranium(IV)-carbon multiple bonds", *Chem. Sci.* 2016, **7**, 3286-3297. DOI: 10.1039/C6SC00278A. February 2016
182. J.S.R. Wheeler, A. Longpre, D. Sells, D. McManus, S. Lancaster, S.W. Reynolds and S.G. Yeates, "Effect of polymer branching on degradation during inkjet printing", *Poly. Degrad. Stab.*, 2016, **128**, 1-7. DOI:10.1016/j.polymdegradstab.2016.02.012. February 2016
183. 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)-hexaazatrifluorophalene complex", *Angew. Chem. Int. Ed.* 2016, **55**, 5521- 5525. DOI: 10.1002/anie.201600694. March 2016
184. L.J. Kershaw Cook, R. Kulmaczewski, R. Mohammed, S. Dudley, S.A. Barrett, M.A. Little, R. J. Deeth, and M.A. Halcrow, "A unified treatment of the relationship between ligand substituents and spin state in a family of iron(II) complexes", *Angew. Chem. Int. Ed.* 2016, **55**, 4327-4331. DOI: 10.1002/anie.201600165. March 2016
185. M. Grazia Concilio, A.J. Fielding, R. Bayliss, S.G. Burgess, "Density functional theory studies of MTSI nitroxide side chain conformations attached to an activation loop", *Theor. Chem. Acc.* 2016, **135**:97. DOI: 10.1007/s00214-016-1859-z. March 2016
186. C. Hua, B. Chan, A. Rawal, F. Tuna, D. Collison, D. Hook, D.M. D'Alessandro, "Redox tunable viologen- based porous organic polymers", *J. Mat. Chem. C.*, 2016, **4**, 2535-2544. DOI:10.1039/C6TC00132G. March 2016
187. J. Ferrando-Soria, E.M. Pineda, A. Fernandez, S.A. Magee, A. Chiesa, S. Carretta, P. Santini, I.J. Vitorica-Yrezabal, F. Tuna, G.A. Timco, E.J.L. McInnes and R.E.P. Winpenny, "A modular design of molecular qubits to implement universal quantum gates", *Nature Commun.* 2016, **7**: 11377, DOI:10.1038/ncomms11377. April 2016
188. K.S. Pedersen, A.M. Ariciu, S. McAdams, H. Heihe, J. Bendix, F. Tuna, S. Piligkos, "Toward molecular 4f single-ion magnet qubits", *J. Amer. Chem. Soc.* 2016, **138**, 5801-5804. DOI: 10.1021/jacs.6b02702. April 2016
189. J.P.S. Walsh, G. Bowling, A.M. Ariciu, N.F.M. Jailani, N.F. Chilton, P.G. Waddell, D. Collison, F. Tuna, L.J. Higham, "Evidence of slow magnetic relaxation in $\text{Co}(\text{AcO})_2(\text{py})_2(\text{H}_2\text{O})_2$ ", *Magnetochemistry* 2016, **2**, 23. DOI:10.3390/magnetochemistry2020023. April 2016
190. B. Chen, Z.-P. Lv, C. Hua, C. Leong, F. Tuna, D. D'Alessandro, D. Collison and J.-L. Zuo, "Dinuclear Ruthenium Complex Based on a π -Extended Bridging Ligand with Redox Active Tetrathiafulvalene and 1,10-Phenanthroline Units", *Inorg. Chem.* 2016, **55**, 4606-4615. DOI: ic-2016-00437a.R3 May 2016

191. K. Griffiths, P. Kumar, G.R. Akien, N.F. Chilton, A. Abdul-Sada, G.J. Tizzard, S.J. Coles and G.E. Kostakis, "Tetranuclear Zn/4f coordination clusters as highly efficient catalysts for Friedel–Crafts alkylation", *Chem. Commun.* 2016, **52**, 7866-7869. DOI: [10.1039/C6CC03608B](https://doi.org/10.1039/C6CC03608B). May 2016
192. 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, in press. DOI: [10.1021/acs.inorgchem.6b00808](https://doi.org/10.1021/acs.inorgchem.6b00808). May 2016
193. R.J. Woolfson, G. A. Timco, A. Chiesa, I.J. Vitorica-Yrezabal, F. Tuna, T. Guidi, E. Pavarini, P. Santini, S. Carretta, R.E.P. Winpenny, "[CrF(O₂C^tBu)₂]₉: Synthesis and characterisation of a regular homometallic ring with an odd number of metal centers and electrons", *Angew. Chem. Int. Ed. Engl.* 2016, **55**, 8856-8859. DOI: [10.1002/anie.201601734](https://doi.org/10.1002/anie.201601734). June 2016
194. E. Lu, O.J. Cooper, F. Tuna, A.J. Wooles, N. Kaltsoyannis, S. T. Liddle, "Uranium-carbene-imido metalla-allenes: Acillary-ligand-controlled cis/trans-isomerisation and assessment of trans influence in the R₂C=U^{IV}=NR' unit (R = Ph₂PNSiMe₃; R'=CPh₃)", *Chem. Eur. J.* 2016, **22**, 11559-11563. DOI: [10.1002/chem.201602690](https://doi.org/10.1002/chem.201602690). July 2016
195. E. Lu, F. Tuna, W. Lewis, N. Kaltsoyannis, S. T. Liddle, "Uranium metalla-allenes with carbene imido R₂C=U^{IV}=NR' units (R=Ph₂PNSiMe₃; R'=CPh₃): Alkali-metal-mediated push-pull effects with an amido auxiliary", *Chem. Eur. J.* 2016, **22**, 11554-11558. DOI: [10.1002/chem.201602603](https://doi.org/10.1002/chem.201602603). July 2016
196. C. Hua, A. Baldansuren, F. Tuna, D. Collison, D.M. D'Alessandro, "In-situ spectrochemical investigations of the redox-active tris-[4-pyridin-4-yl]phenyl]amine ligand and a Zn²⁺ coordination framework", *Inorg. Chem.* 2016, **55**, 7270-7280. DOI: [10.1021/acs.inorgchem.6b00981](https://doi.org/10.1021/acs.inorgchem.6b00981). July 2016
197. G. Timco, S. Marocchi, E. Garlatti, C. Barker, M. Albring, V. Bellini, F. Manghi, E. J. L. McInnes, R.G. Pritchard, F. Tuna, W. Wernsdorfer, G. Lorusso, G. Amoretti, S. Carretta, M. Affronte and R. E. P. Winpenny, "Heterodimers of heterometallic rings", *Dalton Trans.* 2016, in press. DOI: [10.1039/C6DT01941B](https://doi.org/10.1039/C6DT01941B). July 2016
198. A.T. Taguchi, A. Baldansuren, S.A. Dikanov, "Basic and combination cross-features in X- and Q-band HYSCORE of the ¹⁵N labeled bacteriochlorophyll a cation radical", *Z. Phys. Chem.* 2016, in press. DOI [10.1515/zpch-2016-0815](https://doi.org/10.1515/zpch-2016-0815). July 2016
199. F.J. Douglas, D.A. MacLaren, N. Maclen, I. Andreu, F.J. Kettles, F. Tuna, C.C. Berry, M. Castro, M. Murrie, "Gadolinium-doped magnetite nanoparticles from a single-source precursor", *RSC Adv.* 2016, **6**, 74500-74505. DOI: [10.1039/C6RA18095G](https://doi.org/10.1039/C6RA18095G). July 2016
200. J.-R. Jiménez, A. Mondal, L.-M. Chamoreau, P. Fertey, F. Tuna, M. Julve, A. Bousseksou, R. Lescouëzec and L. Lisnard, "An {Fe₆₀} tetrahedral cage: building nanoscopic molecular assemblies through cyanometallate and alkoxo linkers", *Dalton Trans.* 2016, in press. DOI: [10.1039/C6DT03151J](https://doi.org/10.1039/C6DT03151J). August 2016
201. K. Parey, A.J. Fielding, M. Sorgel, R. Rachel, H. Huber, C. Ziegler, C. Rajendran, "In meso crystal structure of a novel membrane-associated octaheme cytochrome c from the Crenarchaeon *Ignicoccus hospitalis*", *The FEBS Journal* 2016, in press. DOI: [10.1111/febs.13870](https://doi.org/10.1111/febs.13870). September 2016.

202. F. Moro, L. Turyanska, J. Wilman, H. E. L. Williams, A. J. Fielding, and A. Patanè, "Surface Sensing of Quantum Dots by Electron Spins", *Nano Lett.* 2016, in press. DOI: **10.1021/acs.nanolett.6b02727. September 2016**
203. E.J.L. McInnes and D. Collison, "EPR Interactions – Coupled spins", *eMagRes*, 2016, **5**, 1445-1458. DOI **10.1002/9780470034590.emrstm1502. September 2016**
204. E. Houton, B. Kelly, S. Sanz, E.J.L. McInnes, D. Collison, E.K. Brechin, A-L. Barra, A.G. Ryder and L.F. Jones, "A facile synthetic route to a family of Mn(III) monomers and their structural, magnetic and spectroscopic studies", *Eur. J. Inorg. Chem.* 2016, in press. DOI:**10.1002/ejic.201601124. October 2016**
205. D. M. King, P. A. Cleaves, A. J. Woole, 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, **accepted**.
206. Z. Lu, H.G.W. Godfrey, I. da Silva, M. Savage, T.L. Easun, F. Tuna, E.J.L. McInnes, S.J. Teat, K.J. Gagnon, M.D. Frogley, G. Cinque, P. Manuel, S. Rudić, S. Yang and M. Schröder, "Tuning CO₂ binding in a functional host *via* modulation of supramolecular interaction at a microscopic level", *Nature Commun.* 2016, **accepted**.
207. J. Ferrando-Soria, S. Magee, A. Chiesa, S. Carretta, P. Santini, I. Vitorica-Yrezabal, F. Tuna, G.F.S. Whitehead, S. Sproules, K. Lancaster, A-L. Barra, G.A. Timco, E.J.L. McInnes and R.E.P. Winpenny, "Redox-switchable electron exchange interactions in molecular double qubits: towards the physical implementation of quantum information processing", *Chem.* 2016, in press.