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 $[Mo(C{\equiv}Car)(Ph_2PCH_2CH_2PPh_2)(\eta\text{-}C_7H_7)]^+$ (Ar = C_6H_5, C_6H_4-4-F; C_7H_7 = 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 $[W(C{=}CHR)(dppe)(\eta\text{-}C_7H_7)]^+$ and $[W(C{=}CHR)(dppe)(\eta\text{-}C_7H_7)]^{n+}$ (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 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 $2PMe_3$, 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 $[\{Fe(dppe)Cp^*\}(\mu\text{-}C{\equiv}CC_6H_4C{\equiv}C)\{Mo(dppe)(\eta\text{-}C_7H_7)\}]PF_6$", *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.jorganchem.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 eumelamin 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. Pattrick, 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 $[Cr(^{t}bpy)_3]^n$ (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 $[Fe(NO)L_2]^z$ (z = 1+, 0, 1-, 2-, 3-; L = 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. Whiteley, "Orbital Symmetry Control of Electronic Coupling in a Symmetrical, All-Carbon Bridged 'Mixed Valence' Compound: Synthesis, Spectroscopy and Electronic Structure of $[\{Mo(dppe)(\eta\text{-}C_7H_7)\}_2(\mu\text{-}C_4)]^{n+}$ (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. Speilberg, 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 $[V(^{t}bpy)_3]^{z}$ (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 [R2C=U=O]2+ analogue of the [O=U=O]2+ uranyl ion (R = Ph2PNSiMe3), 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 $[Fe(^tbpy)_3]^n$ (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-Nâ€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 $[Mo\{(C\equiv C)_n\text{-}C\equiv CR\}(L_2)(\eta\text{-}C_7H_7)]^{z+}$ (n = 1 or 2; z = 0 or 1; R = $SiMe_3$ or H; L_2 = 2,2'-bipyridine or $Ph_2PCH_2CH_2PPh_2$)", *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 O_2-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** **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** **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** **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** **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** **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** **December 2012**

2013:

77. V.A. Milway, F. Tuna, A.R. Andrew, L.E. Sharp, S. Parsons, M. Murrie. "Directed Synthesis of $\{Mn_{18}Cu_6\}$ Heterometallic Complexes", *Angew. Chem. Int. Ed.* 2013, **52** (7), 1949 -1952. **DOI: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** **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** **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** **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** **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 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 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 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**. **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**. **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. 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 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**. **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 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 K_3 analogue phthiocol", *J. Mol. Struct.* 2013, **1048**, 223-229. **DOI: 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.bbalip.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 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{$(C\equiv C)_nC\equiv CR$}(R'N=CH-CH=NR')(η-C_7H_7)], (n = 0 or 1*)", J. Organomet. Chem*. 2013 **745-746**, 251-257. **DOI:10.1016/j.jorganchem.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][Cu_2{(μ-$O_2CC_6H_3$(*o*-OH)(*o*-$C_{15}H_{31}$)}$_4$(NC_5H_5)$_2$]", *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)μ_3-η^2:η^2:η^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. MacLaren, 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, **16**, 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. Amoretti, 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 $\{Cr_7M\}$ 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**. **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 a peroxidase" *Science* 2014, **345**, 193-197. **DOI: 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 Cr_3 triangles through phosphonates and lanthanides: synthetic, structural, magnetic and EPR studies", *Dalton Trans*. 2014, **43**, 13242-13249. **DOI**: **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 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 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**. **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 $\{TbCu_3\}$ and $\{DyCu_3\}$ single-molecule magnets", *Inorg. Chem.* 2014, **53**, 8970-8978. **DOI: 10.1021/ic500885r Aug 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**. **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**. **Sept 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, "$[U^{III}\{N(SiMe_2tBu)_2\}_3]$: A structurally authenticated trigonal planar actinide complex", *Chem. Eur. J.* 2014, **20**, 14579-14583. **DOI: 10.1002/chem.201404864 Sept 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. Sept 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 Oct 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 Oct 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 Cr_7Ni molecular nanomagnets", *Phys. Rev. B* 2014, **90**, 4419. **DOI: 10.1103/PhysRevB.90.184419**. **Oct 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 Nov 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 Nov 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**. **Jan 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 μ-η^5:η^5-cyclo-P_5 complex supported by U-P_5 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**. **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**. **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. 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. 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 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**. **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**. **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)Cl2-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**. **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. 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. 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. 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. June 2015**

159. J.O. Moilanen, B.J. Day, T. Pugh and R.A. Layfield, "Open shell doublet character in a hexaazatrinapthylene trianion complex" *Chem. Commun.* 2015, **51**, 11478. **DOI: 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 C3v and D3h 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 $[Mn\{C(SiMe_3)_3\}_2]^-$ 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 cyclotricatechylene, a macrocyclic *tris*-dioxelene", *Chem. Sci.* 2015, **6**, 6935-6948. **DOI: 10.1039/c5sc02776. Aug 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/npjqi.2015.12** arXiv:1510.01694, **Sept 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 Oct 2015**

168. B.M. Gardner, G. Balázs, M. Scheer, A.J. Wooles, 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 Oct 2015**

169. L. Chatelain, J. Pecaut, F. Tuna and M. Mazzanti, **'**Heterometallic Fe_2^{II}–U^{V} and Ni_2^{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 Oct 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. Oct 2015**

171. 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, AArdavan, R.E.P. Winpenny, "Making hybrid [n]-rotaxanes as supramolecular arrays of molecular electron spin qubit', *Nature Commun*. 2015, **6**: 10240, 1-6. **DOI: 10.1038/ncomms10240 Nov 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, advanced article. **DOI: 10.1039/C5SC03111G. Nov 2015**

173. F. Ortu, 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. Nov 2015**

174. 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.* 2015, in press.

175. J.P.S. Walsh, S. Meadows, A. Ghirri, F. Moro, 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, in press.