
Date: December 13th (Wednesday)

Room: G103 of Graduate School of Science (Shiomi memorial room)

Part I 13:30-14:50

Prof. Joel S. Miller (Department of Chemistry, University of Utah)

Seminar Title:

Extraordinarily Long 2-Electron - 4-Center (2e-/4c) 2.9-A and
2e-/6c 3.04-A Carbon-Carbon Bonds - What is a Chemical Bond?

Part 2 15:00-16:20

Prof. Javier Campo (Materials Science Institute of Aragon, CSIC

University of Zaragoza)

Seminar Title:

Neutron scattering experiments in a new multiferroic molecular magnet

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Extraordinarily Long 2-Electron - 4-Center ($2e^-/4c$) 2.9-Å and $2e^-/6c$ 3.04-Å Carbon-Carbon Bonds - What is a Chemical Bond?

Joel S. Miller

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Carbon-carbon (CC) bonding is a key essence of organic and biochemistry. The length of a CC bond, *i.e.* 1.54 Å found in the diamond allotrope of carbon and ethane, is among the essential information learned by all chemistry students. This is the length of a single bond (σ) between sp^3 -hybridized carbons and is the longest of all common CC bonds. Our studies of the π -[TCNE] $_2^{2-}$ (TCNE = tetracyanoethylene) dimers reveal that 2.89 ± 0.05 Å 2 electron/4 center ($2e^-/4c$) CC bonds are present. Structural, spectroscopic, magnetic, and computational data supporting this multicenter formulation will be presented. These unusual bonds lead to unusual physical properties that will be discussed, as well as *what is a chemical bond?* Furthermore, examples of long, multicenter C-C bonds existing for other dianions, *e.g.*, [cyanil] $_2^{2-}$, as well as dications, *e.g.*, [TTF] $_2^{2+}$ (TTF = tetrathiafulvalene), and neutral homo-, *e.g.*, [tri-*t*-butylphenalenyl] $_2$ and zwitterionic heterodimers *e.g.*, TTF $^{\delta+}$ •••TCNE $^{\delta-}$ ($\delta \sim 0.5$). In addition, several applications related to control of network structural motifs as well as bistable devices will be discussed.

Neutron scattering experiments in a new multiferroic molecular magnet

Javier Campo

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The family of antiferromagnetic $A_2[\text{FeCl}_5(\text{H}_2\text{O})]$ compounds (A = alkali metal or ammonium ion) has awakened a renewed interest owing to the recent observation of multiferroicity in some of its members.[1], [2] We have recently investigated by means of single crystal and powder neutron diffraction the magnetic structure of $(\text{ND}_4)_2[\text{FeCl}_5(\text{D}_2\text{O})]$ (with properties completely equivalent to the hydrogenated form) in order to understand the underlying mechanism of multiferroicity in this compound. This material orders antiferromagnetically at $T_N = 7.25$ K and multiferroicity arises below ca. 6.9 K with the onset of ferroelectric order. We have observed at zero magnetic field a cycloidal magnetic structure propagating in the c -axis with $\mathbf{k} = (0, 0, 0.23)$ and with the magnetic moments lying in the ac plane (Fig.1). This cycloid would be at the origin of the magneto-electric coupling via inverse Dzyaloshinsky–Moriya interaction [3]. Also the evolution of the magnetic structure with increasing the magnetic field has been determined by the use of neutron diffraction under applied magnetic field. It shows three different regions including a lock-in of the propagation vector for fields between 2.5 and 5 T.

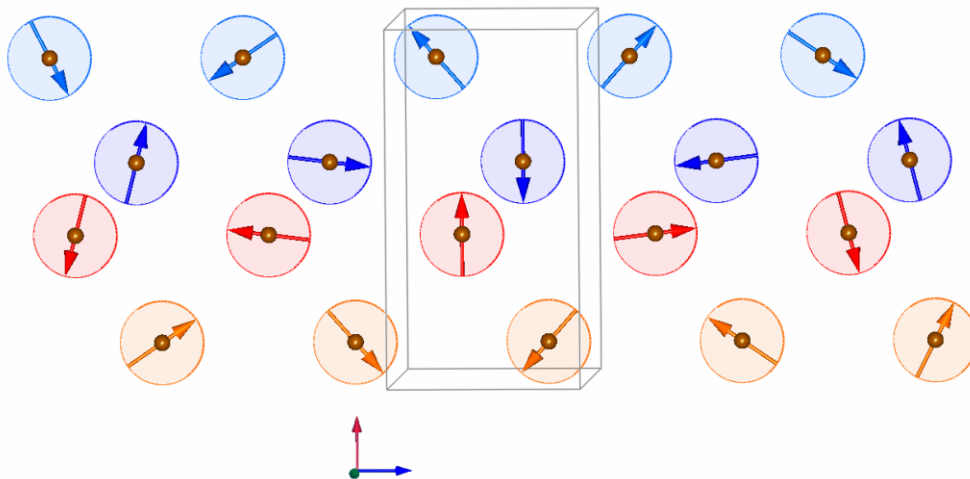


Figure 1: View along the ac plane of magnetic structures of $(\text{ND}_4)_2[\text{FeCl}_5(\text{D}_2\text{O})]$. For the sake of clarity only Fe atoms have been represented.

References

- [1] Ackermann M, Brüning D, Lorenz T, Becker P and Bohatý L 2013 *New J. Phys.* **15** 123001
- [2] Ackermann M, Lorenz T, Becker P and Bohatý L 2014 ArXiv :1408.3997v1
- [3] Rodríguez-Velamazán J.A., Fabelo O, Campo J, Millán A, Chapon L, Johnson R, *Scientific Reports* | 5:14475 | DOI: 10.1038/srep14475