

MS27-P2 Antiferromagnetic exchange interactions in a Cu(II) alternated chain. Manuela Ramos Silva,^a Pedro Sidónio P. Silva,^a Bruce Milne^b, Laura C. J. Pereira^c, José António Paixão,^a ^aCEMDRX, Physics Department, University of Coimbra, P-3004-516 Coimbra, Portugal, ^bCFC, Physics Department, University of Coimbra, P-3004-516 Coimbra, Portugal, ^cITN, UTL, Estrada Nacional 10, 2686-953 Sacavém, Portugal
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Single-molecule magnets are coordination clusters with magnetic properties that rely on superexchange, the magnetic coupling between two nearest neighbour cations through a non-magnetic anion. In the solid state structure of copper(II) nitrophenylacetate, there is the formation of alternated chains where one of the bridging paths between the metal centres is made by four carboxylic groups, in a paddle-wheel configuration.

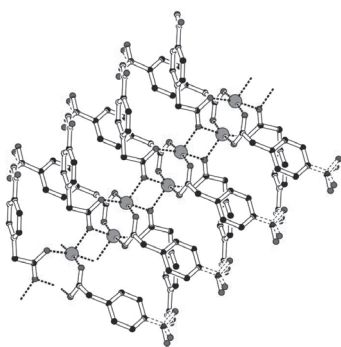


Figure 1. Chain formation in Catena-(bis(m₃-4-nitrophenylacetato-O,O,O'))-(bis(m₂-4-nitrophenylacetato-O,O'))-copper(II). H atoms were omitted for clarity.

Magnetic susceptibility measurements were performed on a powder sample of copper(II) nitrophenylacetate. A Bleaney-Bowers expression was used to fit the susceptibility curve yielding a value of -424 K (-302 cm⁻¹) for the coupling constant. The magnetic exchange couplings constants have also been investigated by means of a methodology based on broken-symmetry unrestricted density functional theory, with the TPSS0 hybrid meta-GGA functional [1] and the multiply-polarized def2-TZVPP triple- ζ basis set [2]. The calculations yielded a value of $2J = -299.6$ cm⁻¹ for the main exchange path.

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Keywords: Cu(II) complex; paddle-wheel ; molecular magnet

MS28-P1 Hyperspectral X-ray imaging using scattered radiation. Robert Cernik, Christopher Egan and Simon Jacques *School of Materials, Grosvenor St, Manchester, M1 7HX, UK*
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We report the development of laboratory based material-specific X-ray imaging system using a recently developed hyper-spectral X-ray sensitive camera⁽¹⁻⁵⁾. The camera coupled to CdTe detector slab allows the recording of photons in the energy range 5-250 keV with an energy resolution of 1%. This enables the discrimination of fluorescence and absorption edges of elements adjacent to one another with $Z > 28$. We demonstrate elemental imaging in an integrated circuit component as an indication of its use in security scanning. We also demonstrate how the camera may have applications for medical diagnosis by imaging a brain phantom.

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Keywords: Imaging; X-ray scattering; security scanning