Magnetic Fingerprint of Planar Bistable Molecule-Based Magnets

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Theoretical predictions of magnetic properties of bistable purely organic molecule-based magnets have experienced an incredible development during the last years. Some of these compounds present peculiarities that cannot yet be explained with the *state-of-the-art* theoretical models. Our attention is devoted to dithiazolyl (DTA, see Figure 1a)-based compounds, namely TTTA[1], PDTA, TDPDTA, and 4NCBDTA[2]. They are, in principle, the best candidates for potential technological applications, like storage devices, sensors and quantum computers. The study addresses three main issues. First, to evaluate by means of FPBU working strategy[3] which pairs of radicals are magnetically non-negligible in order to identify the magnetic topology of the molecule-based crystals. Second, to assess whether structural (geometrical) as well as the electronic (DTA-ring, substituent interactions) factors affect the magnitude of the overall radical···radical J_{AB} magnetic coupling. Finally, we aim at providing a magneto-structural map as a function of the substituents of the DTA-moiety to highlight which is the static ferromagnetic fingerprint region. At this point, we would like to stress that this magneto-structural map could be used as a practical tool to help experimentalists to design more stable and efficient purely organic radicals with ferromagnetic properties in the solid state.

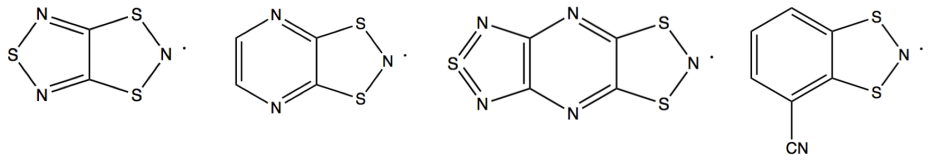

Figure 1. DTA-based compounds investigated.

[1] Brusso et al., *J. Am. Chem. Soc.*. 2004, 126, 8256-8265

[2] Vela et al., *Chem. Eur. J*. 2017, 23, 3479 – 3489

[3] Vela et al., *Phys.Chem.Chem.Phys.,* 2015, 17, 16306