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Pressure induced, reversible, fourfold enhancement of the magnetic ordering temperature in transition metal monomers

Since the discovery of Single-Molecule Magnets (SMMs) in 1993 there has been extensive interest in understanding,[1] developing and tuning the nature of magnetic interactions within molecules the with emphasis on potential device miniaturisation and a bottom-up approach to building components. More recently attention has shifted from large polymetallic clusters of paramagnetic metal ions known as SMMs to include other classes of materials such as Single-Ion Magnets (SIMs),[2] where monometallic complexes are able to order via through space dipole intermolecular interactions arising from the combination of large magnetic anisotropy and spin-delocalisation from metal to ligand.[3,4]

We report a high-pressure study of two ReIV SIMs, [ReCl4(MeCN)2]·MeCN (1) and [ReBr4(bpym)] (2) (bpym = 2,2'-bipyrimidine) with the intention of investigating the role that pressure may play on their magnetic and structural properties. Both compounds display magnetic ordering at low temperatures (Tc = 6.7 K, 19.0 K respectively) via a spin canting mechanism controlled by the strength of the intermolecular interactions with the crystal structure, making it likely to be highly susceptible to pressure. Both compounds have been investigated using high-pressure SQUID magnetometer and the results correlated with high-pressure crystallography and computational analysis to reveal up to a four-fold increase in Tc despite only moderate increases in pressure (ambient to 4 GPa) that correlates directly with significant reductions in intermolecular Re-X…X interactions as pressure increases.

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