

Understanding the effect of structural changes on slow magnetic relaxation in mononuclear octahedral copper(II) complexes

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Streszczenie

Current advances in molecular magnetism are aimed at the construction of molecular nanomagnets and spin qubits for their utilization as high-density data storage materials and quantum computers. Mononuclear coordination compounds with low spin values of $S = \frac{1}{2}$ are excellent candidates for this endeavour, but knowledge of their construction *via* rational design is limited. This particularly applies to the single copper(II) spin center, having been only recently demonstrated to exhibit slow relaxation of magnetisation in the appropriate octahedral environment. We have thus prepared a unique organic scaffold that would allow one to gain in-depth insight into how purposeful structural differences affect the slow magnetic relaxation in monometallic, transition metal complexes. As a proof-of-principle, we demonstrate how one can construct two, structurally very similar complexes with isolated Cu(II) ions in an octahedral ligand environment, the magnetic properties of which differ significantly. The differences in structural symmetry effects and in magnetic relaxation are corroborated with a series of experimental techniques and theoretical approaches, showing how symmetry distortions and crystal packing affect the relaxation behaviour in these isolated Cu(II) systems. Our unique organic platform can be efficiently utilized for the construction of various transition-metal ion systems in the future, effectively providing a model system for investigation of magnetic relaxation *via* targeted structural distortions.

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