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Coexistence of Single-Molecule Magnets and Spin Crossover behaviors in a new cobalt(II)-based compound

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Systems exhibiting spin crossover (SCO) or single-molecule magnets (SMMs) behavior are among the most interesting in the Molecular Magnetism area. SCO complexes are switchable materials, featuring a transition between low spin and high spin electronic configurations triggered by application of heat, pressure or irradiation. They are widely studied due to potential application as sensors or mechanical actuators.[1] SMMs are molecules that present slow relaxation of magnetization of molecular origin, with potential applications in high density data storage, data processing and quantum computing.[2] Pseudo-octahedral cobalt(II) complexes coordinated by two terpyridine-derived ligands are known to exhibit spin crossover, while many examples of high spin cobalt(II) complexes exhibiting SMM behavior have been reported in the literature.[3] Although many examples of independent behavior of SMM or SCO in cobalt(II)-based complexes have been reported so far, synergy or coexistence between SMMs and SCO behaviors are rare.[4] With this aim, the compound $[Co(terpy)_2][Co(hfac)_3]_2$ was designed, synthesized and chemically characterized, where terpy is the 2,2:6,2-Terpyridine ligand and *hfac*$^-$ is the hexafluoroacetylacetonato. The structure was solved using single crystal X-ray diffraction data and consists in cationic pseudo-octahedral complex $[Co(terpy)_2]^{2+}$ coordinated by nitrogen atoms from two three dentate terpyridine ligands. The bond lengths agree with low spin cobalt(II) ion. The counterion is the monoanionic $[Co(hfac)_3]^-$ complex, where the coordination environment of Co^{2+} is occupied by six oxygen atoms from three bidentate $hfac^-$ ligands. DC magnetic measurements have been performed between 2-360 K and indicate an incomplete and smooth spin transition starting slightly above 220 K. AC magnetic susceptibility study shows that this compound exhibit slow magnetization relaxation under an applied static magnetic field. Thus, this compound exhibit both SMM and SCO behaviors attributed to $[Co(hfac)_3]^-$ and $[Co(terpy)_2]^{2+}$, respectively. In fact, solid state EPR studies at 10 K agree with this result, showing the coexistence of high spin and low spin cobalt(II) ions. As expected, at higher temperature (100K) the signal of high spin cobalt(II) vanishes due to fast relaxation and only the low spin cobalt(II) with g nearly 2.1 is observed.

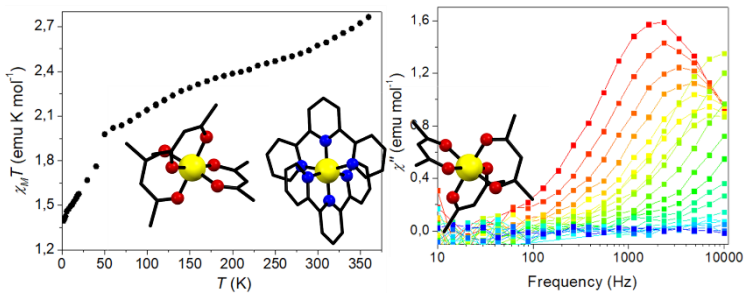

Figure 1: Structure (front), DC (left) and AC (right) magnetic measurements of the compound $[Co(terpy)_2][Co(hfac)_3]_2$

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