Poster

Unconventional charge transfer transition in KCo[Fe] Prussian Blue Analogue

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Prussian blue analogues (PBAs) are versatile metal–cyanide framework materials with a broad range of potential applications. Besides mass transport and mass-storage applications enabled by their microporosity, many PBAs also experience electronic and magnetic bistability [2]. This bistability allows an optical and magnetic switching of PBAs between two distinct states by external stimuli, such as temperature, light, pressure, or electric field. The process responsible for switching between these two electronic configurations involves the transfer of an electron from one metal to another and is known as charge transfer (CT) [2]. Upon cooling from room temperature down to 200K, KCo[Fe]-PBA switches from a cubic paramagnetic $Fe^{III}Co^{II}$ to a cubic diamagnetic $Fe^{II}Co^{III}$ state, with metal-ligand bond shortening by 0.2 Å. CT transitions are known to follow one of two routes: *first order* or *crossover type* transition [3]. The first order transition is characterized by the high degree of cooperativity and an abrupt change of the unit cell parameters, while crossover type transition happens through a gradual change of unit cell parameters. Typically, these transitions are considered mutually exclusive. In our work, we report a mixed-type scenario in KCo[Fe]-PBA. The transition begins as the crossover type and continues as the first order transition. We also observe a self-healing effect, a recovery of crystallinity, during the subsequent warming-up cycle.

[1] Tokoro, H., & Ohkoshi, S. I. (2011). *Dalton Trans.*, **40**, 6825.

[2] Sato, O., Iyoda, T., Fujishima, A., & Hashimoto, K. (1996). *Science*, **272**, 704.

[3] Collet, E., & Guionneau, P. (2018). *C. R. Chim.*, **12**, 1133.