Pressure-induced high-spin/low-spin transition of octahedral Fe²⁺ centres in [Fe(PX)₃](BF₄)₂ · PC single crystals

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The spin cross over (SCO) behavior of single crystals of [Fe(PX)₃](BF₄)₂ · PC *(PX = 1,4-bis((1H-tetrazole-1-yl)methyl)benzene)*[1] has been investigated by in-situ techniques under hydrostatic high-pressure conditions. The experiments were performed in a diamond anvil cell (DAC) and analyzed by means of single-crystal X-ray diffraction (XRD), Raman spectroscopy and UV-VIS-NIR spectroscopy. All applied analytical methods provide evidence for a continuous spin transition occurring between ~0.4 and ~0.9 GPa. However, the SCO is most obvious in the trigonal lattice parameters as determined by high-precision XRD. While the compressional behavior of the a-axis does not show any anomalies in the corresponding pressure range, the c-axis shows an unusual negative compression behavior before and after the pressure interval which is attributed to the continuous SCO transition (Figure 1a and b). The volume properties of the lattice (Figure 1c) reveal a small but significant discontinuity as expected for the SCO effect.
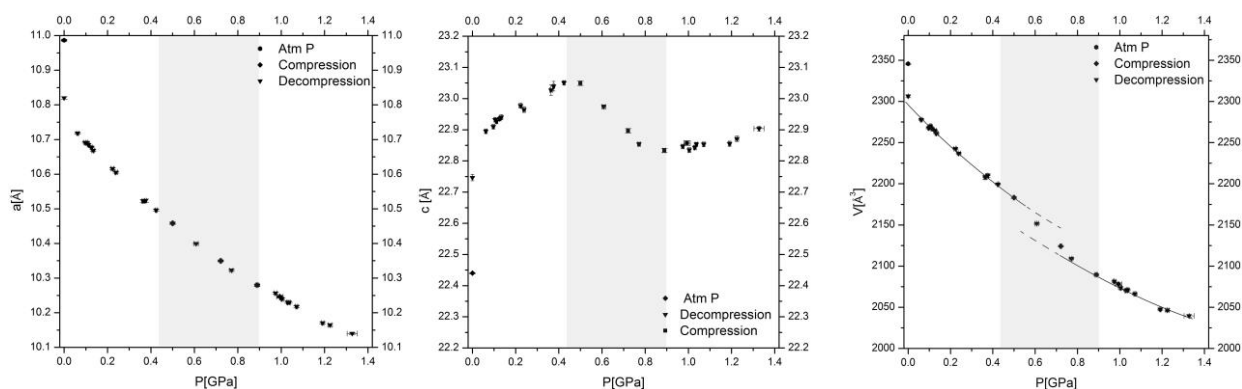

Figure 1 crystal lattice parameters during compression and decompression of [Fe(PX)₃](BF₄)₂ · PC; a and b: change in the length of the a- respective c-axis;

c: change in the unit-cell volume. The inserted lines are guide lines for the eyes.

1 Coronado, E., Giménez-Marqués, M., Mínguez Espallargas, G., Rey, F., & Vitórica-Yrezábal, I. J., *Journal of the American Chemical Society*, **2013**, *135*(43), 15986-15989