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Semi-quantitation of VT-XPS spectra of Fe(II) spin-crossover complexes

The study of spin-crossover (SCO) phenomena between high-spin (HS) and low-spin (LS) states of octahedral 3d4-3d7 transition-metal ions represents an important area of coordination chemistry. The SCO compounds in this study comprise Fe(II) complexes in an octahedral ligand field with a LS to HS transition triggered by temperature. These complexes have several potential applications, however, design and synthesis of SCO systems with the required properties represents a significant challenge. This investigation sought to identify if the Fe2p splitting could be observed *in situ* using variable temperature X-ray photoelectron spectroscopy (VT-XPS) and to test if the spectral changes could be semi-quantified by calibrating to magnetic susceptibility data performed using a SQUID magnetometer. We are also interested in how these XPS spectra differed when the number of Fe(II) metal centres in the complex changed from mononuclear to dinuclear. A dinuclear triple-stranded helicate iron(II) complex that displays a complete spin transition with a gradual-abrupt character at high $T_{1/2}$ is also reported [1, 2]. The ability of XPS to identify the SCO transition temperature serves as a strong advantage over a bulk measurement technique such as SQUID, as XPS is better suited to measure potential electronic or sensing SCO devices.

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