Micro-Raman spectroscopy applied to the study of spin-crossover Fe(II) compounds.

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Spin-transition compounds, also named spin-crossover (SCO) compounds, are switching materials proposed for several technological applications in molecular memories, sensors and displays[1-4]. Particular interest was attracted by the SCO of Fe(II) metal ions in an octahedral ligand field because by populating the respective t_{2g} and e_g d-orbital sets, their $3d^6$ valence shell may exists in its diamagnetic (S=0) low-spin (LS) state as well as in its paramagnetic (S=2) high-spin (HS) state. The switching process is due to the change in splitting of the d-level of the transition metal that induces the electron redistribution in d-levels. Importantly, the spin transition can be driven by external stimuli such as temperature, pressure or light radiation.

An interesting series of spin crossover compounds are bischelated iron(II) complexes of tridentate ligands based on 2,6-bis(pyrazol-1-yl)pyridine (1-bpp), which can be functionalized at its periphery with a variety of substituents. The spin change in these materials is usually very abrupt and takes place with thermal hysteresis close to room temperature. In addition, $[Fe(1\text{-}bpp)_2]^{2+}$ salts have the advantage of exhibiting SCO induced by irradiation: Light-Induced Excited Spin State Trapping effect (LIESST).

In this work we have carried out micro-Raman spectroscopy measurements on the $[Fe^{II}(bppCOOH)_2](ClO_4)_2$ compound, to be compared with previous structural and magnetic characterization. We can identify the LS state signatures at the room temperature Raman spectra and monitoring the transition towards the HS state above 380 K. High intensity signals can be obtained from isolated crystals (of a few microns diameter). As another advantage, the lateral resolution of our experimental set-up is determined by the excitation spot and focus depth (~λ), which allows obtaining spatially resolved spectra from our crystals and distinguishing undesired phases or low quality crystals. As a result, Raman spectroscopy is shown a valuable technique for the characterization of SCO compounds since we can determine the spin transition with a minor waste of synthesis products while giving insights about the compounds quality.

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