Elucidation of Caloric Effect in Spin Crossover Compound

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Improving refrigeration technology receives great scientific attention, leading to new efficient materials and refrigeration mechanism to replace the standard vapor compression technology. The caloric refrigeration cycle is an alternative technology. It is based on the temperature change of the material when exposed to an external magnetic, electric field, or hydrostatic pressure. Recently, spin crossover compounds have been recognized as a promising candidate to exhibit large caloric effects. Large barocaloric effects has been reported for some of these SCO compounds at fairly low hydrostatic pressures (<1.2GPa) [1]. SCO complexes in which the central metal ion switches between two different spin states from a low spin (LS) state to a high spin (HS) state by varying pressure, temperature, or irradiation of light. In the SCO compounds the entropy changes (and consequently the caloric effect) originate not only from the magnetic subsystem (accounting for only about 30% of the entropy change) [2]. The major part of the entropy change originates from changes in the intramolecular vibrations [2,3].

In this work, we are studying two SCO complexes consisting of Fe (II) as a central ion bounded to six nitrogen atoms. The first compound is Fe (PM-Bia)2(NCS)2 PM-Bia = (N-(2'-pyridylmethylene)-4-amino-bi-phenyl) which crystallizes in two polymorphs depending on the synthesis route. Polymorph (P1) has an orthorhombic space group (*Pccn*). It undergoes a thermal abrupt spin transition around 170 K. Polymorph (P2) crystallizes in the monoclinic space group ($P2_1/c$) and undergoes a gradual spin transition around 200 K [4]. The second compound is Fe(PM–AzA)2(NCS)2 PM-aza = (N-(2'-pyridylmethylene)-4-(azophenyl) aniline which crystallizes in the monoclinic space group ($P2_1/c$) and undergoes a gradual spin transition around Tsco ~ 189 K [5].

In this talk, we will present the temperature-dependent magnetization and the powder x-ray diffraction results of these two compounds. Also, I will discuss the results from ESRF temperature-dependent single crystal data.

References

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