[MS14-P07] Crystal Structure of [Fe{5-NO2-sal-N(1,4,7,10)}] Two-Step-Spin Crossover Compound Joachim Kusz[a], Maria Nowak[a] and Philipp Gütlich[b]

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Spin crossover (SCO) systems are of great interest because the switching of spin state between high spin (HS, S = 2, paramagnetic) and low spin state (LS, S = 0, diamagnetic) by varying the temperature, pressure, magnetic field or light irradiation offer the potential of practical applications [1]. In the region of SCO compounds there coexist molecules in both HS and LS states. [Fe{5-NO2-sal-N(1,4,7,10)}] compound belongs to the family of mononuclear iron(II) complex compounds exhibiting the two-step SCO with hysteresis phenomena. The first structural studies on single crystals of this compound were performed by Boinnard *et al.* [2] at 292 K, 153 K and 103 K. They found that the two-step spin transition was accompanied by a structural phase transition leading to lowering of symmetry. In the case of two-step spin transition theoretical predictions and computer simulations have shown that HS and LS complex molecules should be ordered in the plateau region [3]. From this point of view, structural studies of complex compounds with two-step spin transition have always been of particular interest of researchers from the very beginning. Only few examples of such compounds are known where two- step spin transition is accompanied by long range ordering of these molecules. Reinvestigations of this complex compound using strong X- ray sources and CCD camera show that there appear satellite reflections in the plateau region. This is evidence that the superstructure is formed in the plateau region with long range ordering of the HS and LS molecules [4]. We have shown that in the complex [Fe(5-NO2-sal- N(1,4,7,10))] there are four phases, not three as found in previous studies [2]. Only in phase III there is a plateau in the spin transition curve and only in this phase the superstructure is directly connected with ordering of HS and LS molecules. Molecules in HS and LS states create two independent alternating parallel chains along [201]. The two-step spin transition is also connected with a change of the conformer. It leads to a dramatic change in the hydrogen bonding system resulting in the stabilization of the intermediate phase. This work was partly funded by the DFG (Priority Program 1137 'Molecular Magnetism') and by the Polish National Science Centre Grant No. DEC-2011/01/B/ST5/06311.

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