**[MS14-P06] Computer Simulation of Diffuse Scattering in [Fe(CH3CN)4(Pyz)](ClO4)2 Compound**

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$[Fe(CH_3CN)_4(Pyz)](ClO_4)_2$ (Pyz = pyrazine) belongs to the family of Fe(II) complex compounds exhibiting the spin crossover (SCO) phenomena, which may be caused by changes of the temperature, pressure or laser light irradiation [1]. The studied compound is the first example of the SCO complex, in which four nitrile based ligands belong to the Fe(II) coordination sphere [2]. The compound is also very interesting due to the fact that observed spin transition has three step behaviour. The $[Fe(CH_3CN)_4(Pyz)](ClO_4)_2$ complex compound crystallizes in the orthorhombic crystal system in *Pccn* space group. Studied compound possesses a chain structures and in the unit cell there is only one symmetrically independent iron(II) ion position. In the structure there are no direct bonds between adjacent chains and the interactions between chains are mediated by $ClO^-$ anions arranged in *bc* layers. At temperatures below 140 K structural disorder is observed associated with appearance of alternatively oriented pyrazine rings and perchlorate anions. The occupancy of the alternative positions increases with decreasing temperature. Analysis of the X-ray measurements showed that below 140 K a diffuse scattering is observed on *kl* and *hl* planes in the form of one- dimensional stripes along the *l* direction. The intensity of diffuse scattering is temperature dependent and also decreases with the distance in reciprocal space. The proposed model of the short-range order in the crystal structure is based on the formation of layers in the structure in which the pyrazine rings and $ClO^-$ anions occupy only one of the two alternative positions. This model is characterized by five parameters describing the value of the occupancy factor of the low temperature alternative positions and four parameters defining the correlation between pyrazine rings in one of the high or low temperature alternative positions. Simulations of diffuse scattering and refinement of the parameters describing short-range order using differential evolution algorithm was carried out by means of DISCUS software package [3,4]. Distribution and intensity of the diffuse scattering obtained from the calculations based on the proposed model of the real crystal structure is in good agreement with the observed diffraction patterns. This work was funded by the Polish National Science Centre Grant No. DEC-2011/01/B/ST5/06311

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**Keywords:** diffuse X-ray scattering, disordered molecular crystals, computer simulation