MS14-P129 - LATE | MULTI-SCALE CHARACTERISATION OF THE CATIONIC DISORDER IN THE NOVEL BORATE $Sr_6Tb_{0.94}Fe_{1.06}(BO_3)_6$

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The remarkable magnetic-optical properties of Tb-based compounds focused a number of works on the tailoring of novel crystals [1-2].

Millimetre sized single crystals of $Sr_6Tb_{0.94}Fe_{1.06}(BO_3)_6$ were prepared by crystal growing from high-temperature solution. The crystal structure of this new borate was resolved by single-crystal X-ray diffraction with the trigonal *R-3* space group: a = 12.2164(2) Å, c = 9.1943(2) Å. The refinement of the crystal structure led to a final model with a long range disorder relative to the Tb and Fe statistical distribution over the *3a* and *3b* sites. Previously, the ^{57}Fe Mössbauer spectroscopy revealed the only presence of Fe^{3+} with two different environments. Diffuse reflectance experiments showed no luminescence under excitation, consistent with a point disorder in the Tb/FeO_6 octahedra and a local loss of the centre of symmetry. Finally, XPS and magnetic susceptibility measurements excluded the presence of Tb^{4+} and helped to settle down the cationic distribution in the final structure model. The cationic disorder in $Sr_6Tb_{0.94}Fe_{1.06}(BO_3)_6$ is discussed in comparison with the structure of a close phase, synthesised in different conditions [3].

[1] P. Veber, M. Velázquez, G. Gadret, D. Rytz, M. Peltz, R. Decourt, *CrystEngComm*, **2015**, 17, 492.
[2] K. Shimamura et al., *Cryst. Growth Des*., **2010**, 10, 3466.
[3] H. Inoue, Y. Doi, Y. Hinatsu, *J. Alloys Comp*., **2016**, 681, 115-119.