Electronic Supplementary Material (ESI) for RSC Advances.
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High pressure studies of Eu^{2+} and Mn^{2+} doped $NaScSi_2O_6$ clinopyroxenes

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Supplementary data

The details of XRD measurements are described in the text of the publication. The phase analysis of the samples was performed using Diffrac.EVA evaluation software compiled with PDF (Powder Diffraction File) 4+/2014 data base. The semi-quantitative phase analysis was carried out using method that consists of the comparison of I/I_{cor} ratio (given in PDF card) of all evaluated phases with their signal intensities.

$NaScSi_2O_6$:Eu(5%)

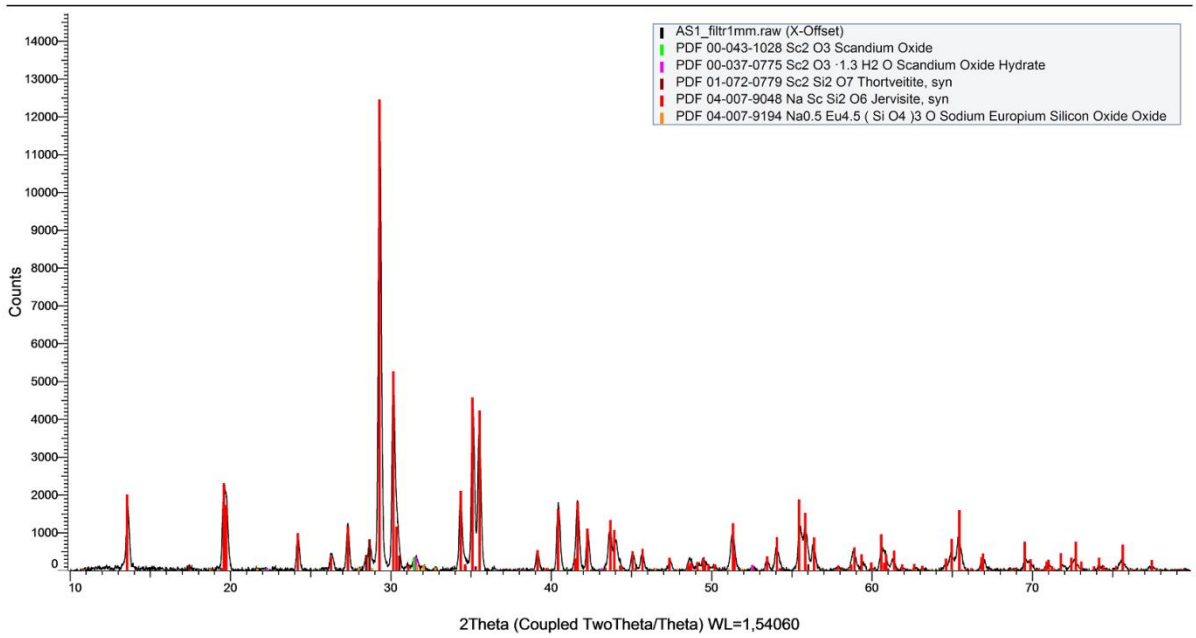

Fig. 1. The XRD pattern of $NaScSi_2O_6$:Eu(5%) and attributed standards.

As it can be seen on the Fig. 1 the product of synthesis consists of different crystallographic phases. The sample, besides the desired phase of $NaScSi_2O_6$ (PDF 04-007-9048) contains also two different phases of scandium oxide: hydrated and unhydrated, PDF 00-037-0775 and 00-043-1028, respectively, as well as scandium pyrosilicate (PDF 04-007-9048) and $Na_{0.5}Eu_{4.5}(SiO_4)_3$ (PDF 04-007-9194). The semi-quantitative analysis could not be carried out, in this case, due to the lack of I/I_{cor} value for the $Sc_2O_3 \cdot 1.3H_2O$, (PDF 00-037-0775).

$NaScSi_2O_6$:Mn(5%)

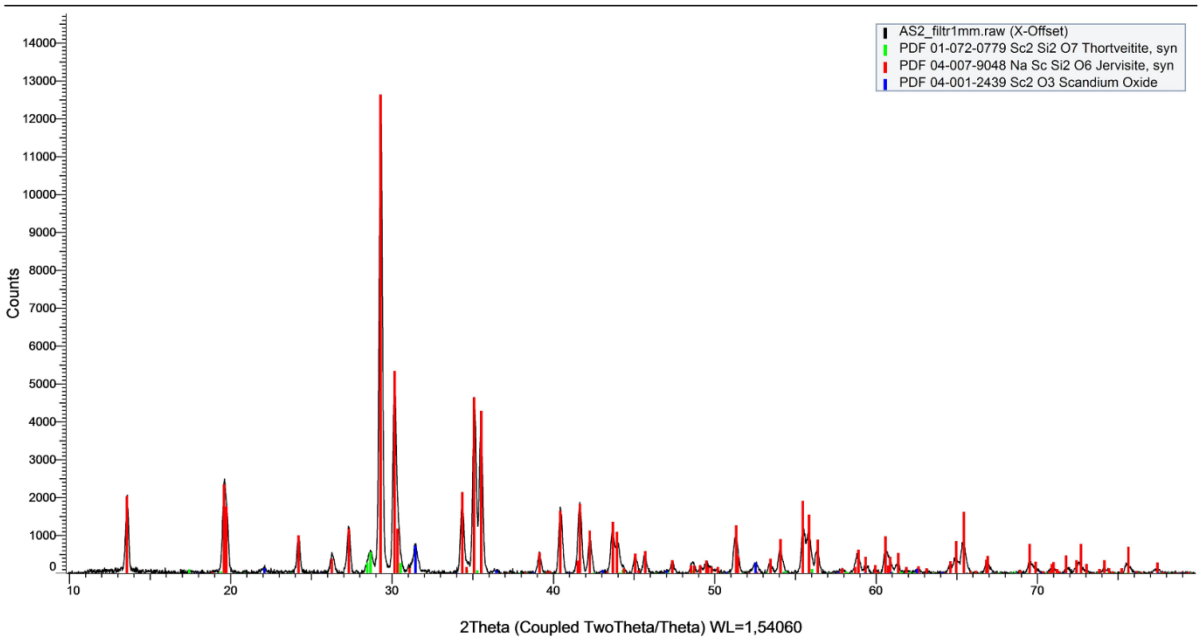

Fig. 2. The XRD pattern of $NaScSi_2O_6$:Mn(5%) and attributed standards.

The main crystallographic phase that can be seen in the XRD pattern (Fig. 2) of the material doped with manganese is attributed to $NaScSi_2O_6$ (PDF 04-007-9048). However, the sample contains also impurity phases such as scandium oxide (PDF 04-001-2439) and scandium pyrosilicate (PDF 01-072-0779). The semi-quantitative analysis is as follows: $NaScSi_2O_6$ – 95%; Sc_2O_3 – 2%; $Sc_2Si_2O_7$ – 3%.

$NaScSi_2O_6$:Eu(5%), Mn(15%)

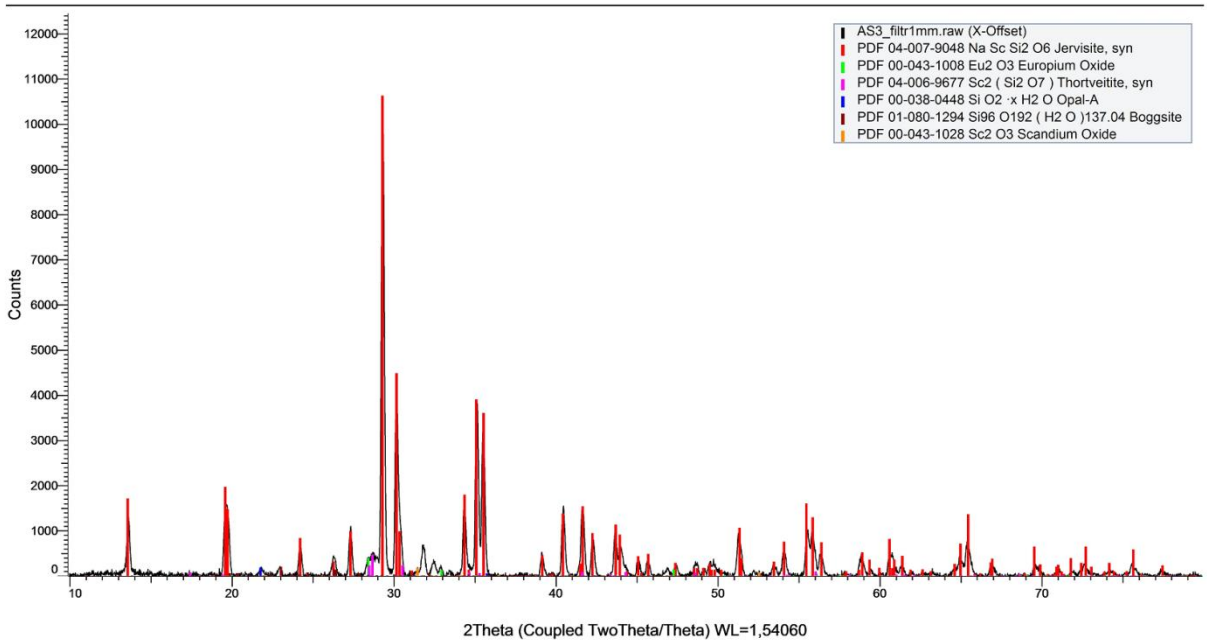

Fig. 3. The XRD pattern of $NaScSi_2O_6$:Eu(5%), Mn(15%) and attributed standards.

Fig. 3 shows the XRD pattern of the sample doped with europium and manganese. In this case, as in the previous ones the $NaScSi_2O_6$ standard is attributed to the main crystallographic phase of sample. However, the additional impurity phases can be also distinguished, such as europium oxide (PDF 00-043-1008) and scandium pyrosilicate (PDF 01-072-0779). Moreover, the signals in the range of 21 – 23.5 2 theta degree are attributed to the two different phases of hydrated silica (PDF 00-038-0448, PDF 01-080-1294), the signal at 31.5 degree is attributed to the scandium oxide (PDF 00-043-1028). The signals at 29, 31.8 and 32.5 degree have not been assigned to the any crystallographic phases using described above evaluation software.