ESRF	**Experiment title:** Woodwardite structural refinement and effect of Y and Ce incorporation	**Experiment number**: EV 197
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Report:

The aim of this experiment was to apply Pair Distribution Function (PDF) technique to investigate the structural properties of the poorly crystalline mineral woodwardite [$Cu_{1-x}Al_x(SO_4)_{x/2}(OH)_2 \cdot nH_2O$] and analyse the effect of chemical substitution with Y and Ce. During our experiment we succeded in collecting enough data for our research. In order to study the effect of pH in the incorporation of Y and Ce, a total of 6 samples were analysed: a sample of pure woodwardite, a sample of woodwardite doped with Y and a sample doped with Ce synthesised at pH 8±0.3, as well as their analogues synthesised at pH 10±0.3. The measurements were carried out at room temperature. Reduction of the total scattering data to obtain $G(r)$, the PDF function, was done by the PDFgetX3 software, using Qmax = 30.0 $Å^{-1}$. Figure 1 shows the PDF functions of 3 samples selected as representative. The PDF functions evidences the typical Cu-O and Zn-O bond distance (peaks at about 2 Å); remarkably, besides the 1.6 Å peak due to the sulphate group, the PDF analysis reveals the presence of a 1.2 Å peak originated by a carbonate group, a very new result.

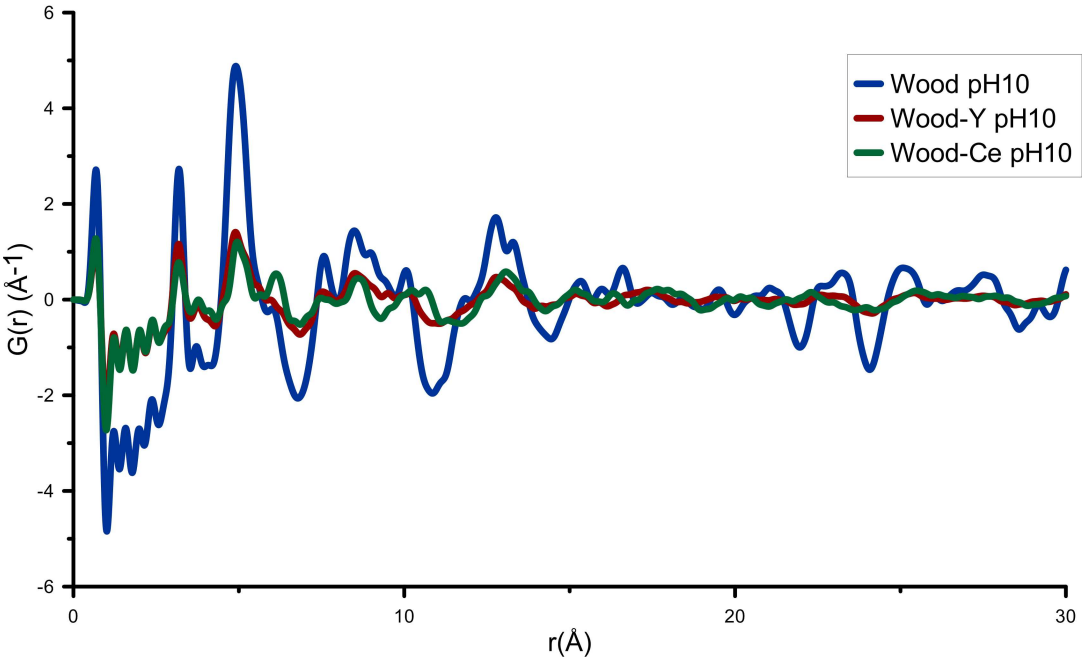

Fig. 1 – PDF data of three samples of woodwardite synthesised at pH 10

At present the investigation is still in progress and PDF data are compared with independent EXAFS mesurements. Unfortunately, the crystal structure of these poorly crystalline compounds has not yet been resolved, and hence these measurements are very important in order to build one or more structural models. By using these data we are confident to highlight the main structural properties of this family of compounds.