



	<b>Experiment title:</b> Temperature- & time-resolved structural investigation of the long- & short-range structures of the novel water filter materials	<b>Experiment number:</b> A31-1-200
<b>Beamline:</b> B01	<b>Date of experiment:</b> from: 10 <sup>th</sup> of May 2023 to: 15 <sup>th</sup> of May 2023	<b>Date of report:</b> 30.10.2023
<b>Shifts: 15</b>	<b>Local contact(s):</b> Vadim Diadkin	<i>Received at ESRF:</i>
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The report presents the results of the diffraction experiments conducted at the SNBL synchrotron facilities on samples of dypingite, a mineral with potential applications as a water filter. The main objective of this study was to investigate the structural properties and thermal behaviour of both minerals and synthetic dypingite materials.

Series of mineral and synthetic dypingite samples, with a different water content, were measured with a synchrotron powder X-ray diffraction (SR-PXD) instrument at room temperature. During the experiment powders were sealed in a boron-glass capillary ( $d = 0.5$  mm). The measurements revealed that the synthetic mineral had better crystallinity than the mineral one. Additionally, based on the analysis of the SR-PXD data of hydrated and dehydrated synthetic dypingite, we could confirm a systematic and water-induced variation of the Bragg peak positions in the material diffraction patterns, along with their intensity change and broadening modifications upon the sample hydration/dehydration (see Figure 1).

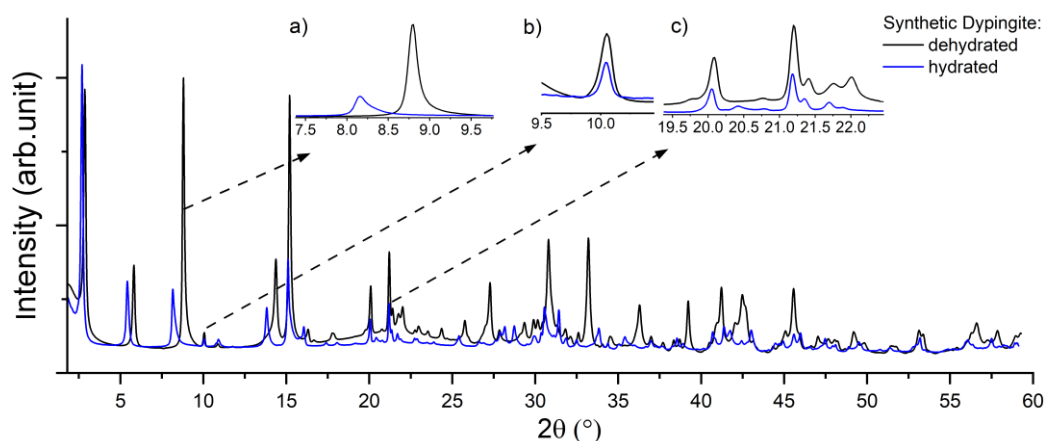


Figure 1. SR-PXD ( $\lambda = 0.70843$  Å) of hydrated and dehydrated synthetic dypingite.

The obtained results provided an important and systematic insight on the dypingite structural properties and allowed us to suggest a crystal structure model that is currently being refined.

To investigate the thermal behavior of the synthetic dypingite, the mass spectrometry analysis was conducted during the temperature-dependent *in situ* SR-PXD experiments. The experimental results showed that the decomposition of synthetic mineral involved the water release in the temperature range of 40-240°C, followed by the massive release of CO<sub>2</sub> in the temperature range of 300-500°C (see Figure 2). The further analysis of the data will be needed to describe the structural relationship between the water-poor and water-rich material samples.

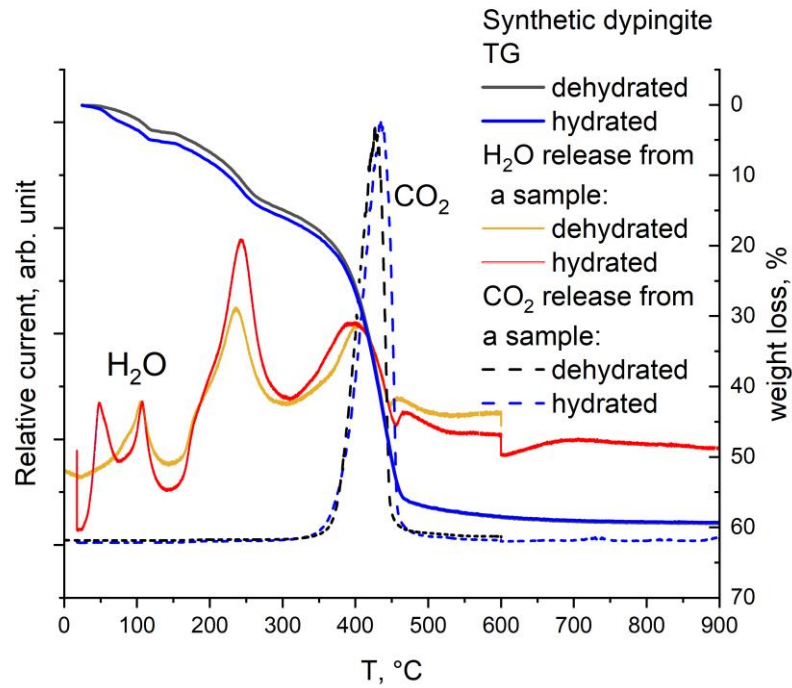


Figure 2. Thermal behaviour of synthetic dypingite with different water content.

The mineral, although discovered and known since the 70's, has not been yet systematically studied and its reported structural properties have been incomplete and ambiguous. Thus, finding a link between the material functional and structural behavior was impossible. Our experiments at SNBL synchrotron facilities have provided valuable data on the structural and thermal behaviour of dypingite samples, and based on the results obtained, we have successfully solved the mineral crystal structure.