	Experiment title: STRUCTURAL CHARACTERISATION OF SELECTED MEMBERS OF THE AERINITE SERIES WITH VERY DIFFERENT Fe2+ CONTENT.	**Experiment number**: CH-1859
Beamline: **ID31**	**Date of experiment**: from: 15 Sept. 2004 to: 17 Sept. 2004	**Date of report**: 15 Jul 2005
Shifts: 6	**Local contact(s)**: Dr. Irene Margiolaki	*Received at ESRF:*

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Report:

The powder X-ray diffraction measurements of different aerinite samples was carried out as planned. The patterns for the following limiting Fe2+/Fe3+ ratios were adquired:

Sample A: ratio =4.0
Sample B: ratio = 0.61
Sample C: ratio= 0.37

The pattern of sample C, i.e. the same sample used in Rius et. al. (2004), was measured for control. The Rietveld refinement with the published coordinates on the new data set confirmed the previous results.

Currently, the structure of sample A coming from Tartareu (Ctalunya, Spain) has been solved and we are still finishing the refinement of the channel content. It has been found that the structure type is similar but that the cation distribution is very different from that found in the control sample C. The Mössbauer spectrum of sample A is rather complex and its detailed interpretation only has been possible with the help of the diffraction data. The experimental

data also confirm the initial Fe^{2+}/Fe^{3+} ratio. A manuscript containing all this information will be sent to publication to the "European Journal of Mineralogy", surely in the last trimester of 2005.
Once the characterisation of the structure of sample A is finished, we will concentrate on the structure solution of sample B.

The experiment CH-1859 was performed after experiment CH-1947and the authors of both proposals were the same (although in different order). This allowed completing experiment CH-1947 devoted to the structural characterisation of zeolites from high resolution powder diffraction data with the measurement of two patterns of zeolite ITQ-32. With these two patterns, one including the template molecules and a second one with them removed by calcination, a new method for solving complex crystal structures by direct methods has been developed. A paper entlitled "Solving centrosymmetrical zeolites from powder diffraction data by combining the direct methods origin-free modulus sum function with the isomorphous replacement technique.X." and having our local contact as co-author has been sent to "Journal Of Applied Crystallography" for its publication.