Experimental report

05/03/2024

Proposal: **EASY-1204** **Council:** 4/2023

Title: Nuclear structure of mesolite compound

Research area: Materials

This proposal is a new proposal

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Experimental team:

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Samples: Na2Ca2(Al2Si3O10)3·8H2O

Instrument	Requested days	Allocated days	From	To
D19	72	72	01/09/2023	04/09/2023

Abstract:

The aim of the present experiment is to test several mesolite samples in order to prepare an official proposal to properly localize the hydrogen atoms of the structure

Experimental Report - Proposal EASY-1204
Si/Al-ordering, H-bonding scheme and real symmetry of the zeolite mesolite, ideally $Na_2Ca_2Al_6Si_9O_{30}\cdot 8H_2O$

The experiment was performed in order to acquire a comprehensive structural model of the zeolite mesolite (Fig. 1). This will enable us to accurately identify the structural characteristics mentioned earlier. We asked for D19 instrument to collect a complete data set at low-*T* (20 K) to reduce the ADP's and better locate light atoms. With the combination of chemical, X-ray and neutron data, we expected to provide:

a) the real Si/Al-ordering in the tetrahedral framework

b) an unambiguous location of all the proton sites, their anisotropic displacement regime, and the description of the complex H-bonding network

c) a description of the crystal chemistry of this natural zeolite based on modern analytical protocols, with a particular attention to the potential framework and extra-framework substituents.

The single-crystal neutron data collection was performed at 20 K. The unit-cell parameters proved a metrically orthorhombic lattice (with a=18.3955(3), b=56.6265(4), c=6.5566(3) Å), with reflection conditions compatible to the *Fdd*2 space group. A total number of 15343 reflections were collected ($-33 \le h \le 33$, $-103 \le k \le 62$, $-1 \le l \le 10$, Max. 2-theta = 121.48°, lambda 0.95083 Å), out of which 5893 were unique with R(int) = 0.0493 and R(sigma) = 0.0405. The structure refinement is in progress.

Figure 1. A view of the crystal structure of mesolite, down [001], and configuration of the T_5O_{10} units forming infinite chains //[001] (structural model of Stuckenschmidt & Kirfel 2000).