
# International conference Functional Materials

# ICFM-2001

## *ABSTRACTS*

Ukraine, Crimea, Partenit
2001

## EQ – 11/9 STUDY OF THE ELECTRIC FIELDS GRADIENTS IN POROUS CRYSTALS

*Sapiga A. V., Sergeev* N. A, Yatsenko A. V.*
*Faculty of Physics, Tavrida National University, Crimea, Ukraine*
**Institute of Physics, University of Szczecin, Poland*

The mineral natrolite $Na_2Al_2Si_3O_{10}2H_2O$ (space group Fdd2) is the typical channel-type compound with the porous structure (zeolite). The zeolites have a number of interesting properties, such as lose/regain water, ion exchange and molecular sieve properties and other. The natrolite framework consists of chains $AlO_4$ and $SiO_4$ tetrahedra linked together via common oxygen atoms. The sodium ions and water molecules are located into zeolite channels. Each sodium ion is coordinated by four framework's oxygen atoms and by two water molecules $W_1$ and $W_2$ [1]. From NMR data it follows that water molecules diffuse along the vacancies whose positions coincide with the regular positions of water molecules [2]. The temperature dependencies of NMR spectra of $^{23}Na$, $^{27}Al$ and $^1H$ nuclei in have been studied. The obtained values of a second moment $M_2$ of $^1H$ and quadrupolar coupling constant ($C_{zz}= e^2qQ/h$) $^{23}Na$ and $^{27}Al$ nuclei are given in a fig. 1. The $M_2$ of $^1H$ spectra is decreased at $T > 350$ K as a result of water molecules diffusion. One can see from Fig. 1 that the $C_{zz}$ for the $^{27}Al$, $^{23}Na$ nuclei does not depend on the temperature for $T < 450$ K. The increasing of the $C_{zz}$ of $^{27}Al$ nuclei at $T > 620$ K is probably connected with the complete dehydration of natrolite. The observed decreasing of the $C_{zz}$ of $^{23}Na$ nuclei at $T > 450$ K may be accounted for by diffusion of water molecules. Using the model of the point electric charges, we calculated the components of electric field gradient (EFG) tensor at the position of $^{27}Al$ and $^{23}Na$ (Tab. 1).

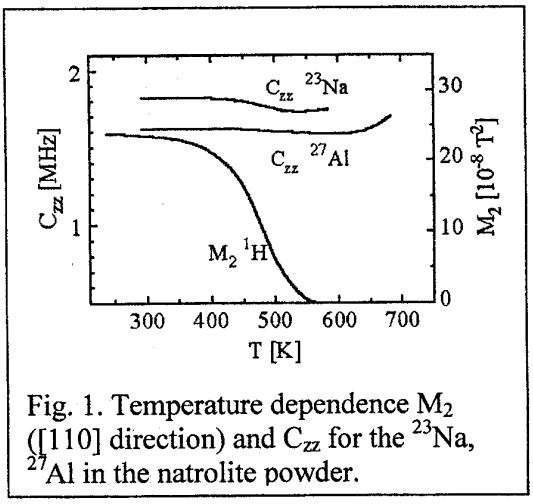


Fig. 1. Temperature dependence $M_2$ ([110] direction) and $C_{zz}$ for the $^{23}Na$, $^{27}Al$ in the natrolite powder.

Table 1: The theoretical values of main component of the EFG tensor (*eq*).

| $^{23}Na$, *eq* ($10^{20}$ V/m$^2$) | | | | | $^{27}Al$, *eq* ($10^{20}$ V/m$^2$) | |
|---|---|---|---|---|---|---|
| a | b | c | d | e | a | b |
| -1.11 | 2.64 | 1.50 | 1.47 | 2.52 | 3.45 | 3.48 |

a – the value *eq* of the whole lattice; b - the value *eq* of the whole lattice minus of all water molecules; c- the value *eq* of the whole lattice minus of the water molecule $W_1$; d - the value *eq* of the whole lattice minus of the $W_2$; c - the value *eq* of the whole lattice minus the electric charges of the water molecules $W_1$ and $W_2$.

Using for the $^{23}Na$ $\gamma_\infty = -4.65$ we have obtained the value of the quadrupolar coupling constant $e^2qQ/h = 1626$ kHz and $\eta = 0.5$. These theoretical values are in good agreement with experimental values. It has been established that the internal mobility of aluminium and sodium ions does not occur in natrolite. The influence of the water molecule diffusion on the NMR spectra of $^{23}Na$ and $^{27}Al$ has been discussed.

References.

1. Pechar, F., Schafer, W. and Will, G.: Z. Kristallog., (1983), **164** 19.
2. Sapiga, A. V., Sergeev, N. A., Shcherbakov, V. N. et. al.: J. Struk. Chem., (1986), **27**, 183.