ESRF	**Experiment title:** THERMAL EXPANSION AND PHASE TRANSITIONS IN AKERMANITE-GEHLENITE-Na-MELILITE SOLID SOLUTIONS ($Ca_2MgSi_2O_7$-$Ca_2Al_2SiO_7$-$NaCaAlSi_2O_7$)	**Experiment number**: 08 02 608
Beamline: BM08	**Date of experiment**: from: 18/02/2004 to: 22/02/2004	**Date of report**:
Shifts: 12	**Local contact(s)**: Carlo Meneghini	*Received at ESRF:*

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Report:

Melilites are a group of minerals which form continuos solid solutions between the end members gehlenite (Ge, $Ca_2Al_2SiO_7$) akermanite (Ak, $Ca_2MgSi_2O_7$), soda-melilite (NaMel, $NaCaAlSi_2O_7$) and Fe-bearing end members (Fe^{2+}-gehlenite – Fe^{3+}-gehlenite / Fe^{2+}-akermanite – Fe^{3+}-akermanite). The importance of these minerals is due to the fact that almost pure terms of the series gehlenite-akermanite are among the first silicates which condensed from the solar nebula and they are found in chondritic meteorites. Melilites crystallise also in alkaline magmatic roks, whose origin is restricted to significant geodynamic environments. Therefore a modelling of their thermodynamic parameters is mandatory in order to improve the accuracy of phase equilibria calculations, which could have important implications in petrological studies (i.e. for accurate determination of the thermal history of meteorites, of the temperature of solidification of alkaline roks ...). The thermodynamic calculations involving phase equilibria of melilites are usually performed assuming the ideality of the solid solution (s.s.) [1]. Nevertheless melilite s.s. has not an ideal behaviour (fig. 1). Our results show that the unit cell volume curve in the ge-ak join has a sigmoidal shape, with a negative and a positive excess molar volume close to ge and ak end-members respectively. This is the general behaviour of non equivalent site substitution mentioned by Newton and Wood [2] for binary silicate solid solutions. An other important feature of melilites is the presence of an incommensurate modulated (IC) structure, especially for ak-rich compositions, which transforms into a normal (N) one upon heating [3,4,5]. The temperature of IC-N phase transition is 80 °C for pure akermanite and it is increased by Fe/Mg substitution and decreased by Al /(Mg+Si) exchange. We performed high temperature (HT) X-ray powder diffraction (XRPD) on terms of Ge-Ak-NaMel on the italian CRG beamline BM08 (GILDA) in order to measure reliable thermodynamical data (volume, thermal expansion) for several compositions and to investigate the IC-N phase transition for some terms near Ak end-member. The experiments were performed with monochromatic radiation; the samples were contained in quartz glass capillary, heated with a hot gas blower and data were collected with a translating image plate (T.I.P.) [6]. Special geometric corrections taking into account the small deviations of the detector from the ortogonality were applied to the collected data in order to achieve a reliable accuracy in lattice parameter determinations. IC and N phases are marked by a strong difference in thermal expansion along the main crystallographic directions. Thermal expansion measurements allowed to investigate the field stability of IC phase near ak composition. The phase transition is characterised by a contraction along *c* and also a slight negative volumetric expansion (fig. 2-3). The results obtained comprise also accurate thermal expansion measurements and crystal-structure Rietveld refinements for melilites in Ak-Ge and Ak-NaMel joins in the temperature range 270-1300 K.

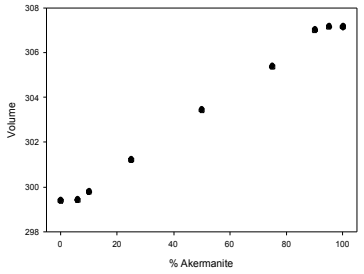	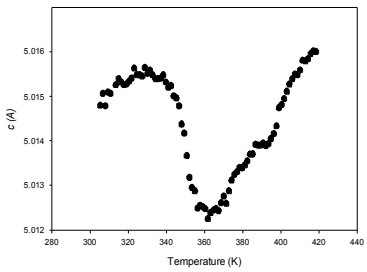	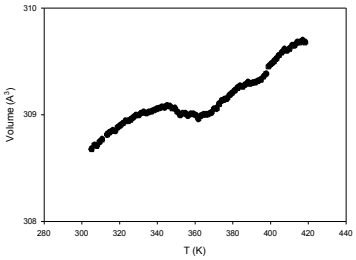
Fig. 1 - Volume ($Å^3$) in the join Ge-Ak at 300 K with the characteristic S-shaped form of the volume curve in binary silicate solid solutions.	Fig. 2- Variation of c lattice parameter value across the phase transition for akermanite measured with T.I.P. detector at GILDA beamline (ESRF)	Fig. 3- Thermal expansion of akermanite across the IC-N phase transition

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