ESRF	**Experiment title:** High pressure investigation on C2/c clinopyroxenes along the join diopside-enstatite ($CaMgSi_2O_6$-$Mg_2Si_2O_6$)	**Experiment number**: HS817
Beamline:	**Date of experiment**: from: 23/4/1999 to: 27/4/1999	**Date of report**: 12/7/1999
Shifts:	**Local contact(s)**: Davide Levy	*Received at ESRF:*

Names and affiliations of applicants (* indicates experimentalists):

Mario Tribaudino*, Mauro Prencipe*, Marco Bruno*
Dipartimento di Scienze Mineralogiche e Petrologiche, Università di Torino, Via Valperga Caluso, 35 - 10125 TORINO Italy

Davide Levy*
ESRF - Grenoble, France

Report:

Clinopyroxenes are among the main constituents of the upper mantle; their composition at extreme pressures can be well approximated (Gasparik 1989) along the join diopside-enstatite (Di-En, $CaMgSi_2O_6$-$Mg_2Si_2O_6$). As for the Ca-richer side of the join limited compressional data exist (up to 10 GPa, Zhang et al. 1997) only for the end member diopside and none solid solutions, a high pressure in situ investigation was performed.

In the reported experiment synthetic samples with three different compositions were examined, namely diopside and two solid solutions with compositions $Ca_{0.8}Mg_{1.2}Si_2O_6$ and $Ca_{0.5}Mg_{1.5}Si_2O_6$. The samples were chosen so to span the range for Ca-richer clinopyroxenes and loaded in a diamond anvil cell, with N_2 as pressure medium. The powder spectra were recorded in the line ID09, using monochromatized radiation (λ = 0.4526 Å); an image plate was used for the detection of the spectrum. The diopside was compressed up to 40 GPa, while the two solid solutions up to 15 GPa; a total of 87 spectra was collected.

The data on the image plate were integrated by means of the fit2d program, obtaining a one dimensional 2θ vs intensity array.

Rietveld analysis of the collected spectra was done in order to determine the precise cell parameter at the different conditions. In all the samples the pattern could be indexed in the

clinopyroxene cell; however it was observed a significant step in cell parameters, mainly in β, at a pressure between 3 and 5 GPa for the sample $Ca_{0.5}Mg_{1.5}Si_2O_6$ (Figure 1). This was interpreted as an evidence of the $P2_1/c$-C2/c phase transition, which was previously observed in Ca-free clinopyroxenes (Angel et al. 1992). Respect to previous works this does not occur with a sharp discontinuity in cell parameters at the transiton, but in a range of pressure, possibly as a consequence of compositional inhomogeneities.

Full amorphization at extreme pressure of the samples was not observed; in diopside however, significant peak broadening and decrease in intensity was observed at P higher than 35 GPa. After decompression the same sample recovered the previous intensity.

The bulk moduli ($K_{0,T}$) and their pressure derivatives (K_0') are respectively 105.0(9) GPa and 6.9(1) for pure diopside and 109(2) GPa and 5.5(5) for $Ca_{0.8}Mg_{1.2}Si_2O_6$.

The axial compressibilities follow the pattern commonly found in clinopyroxenes, with $\beta_b > \beta_c > \beta_a$; the compressibility for all directions decreases with increasing pressure. An analysis of the strain ellipsoid shows that the main compression occurs along the *b* axis and with an orientation of about 140° from the *a* axis onto the (010) plane. This orientation corresponds to previous findings in clinopyroxenes (Levien and Prewitt 1980, Comodi et al. 1995), and to that of the thermal expansion ellipsoid (Benna et al.1990). The deformation on the (010) plane becomes higher with increasing Mg content and in $Ca_{0.5}Mg_{1.5}Si_2O_6$ is the direction of the main deformation, both in the low and high pressure phases.

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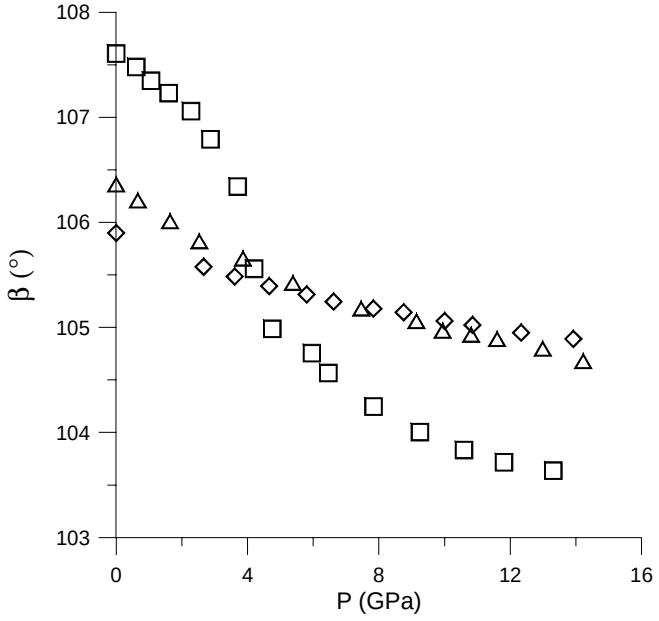

Figure 1: the behaviour of the β angle with pressure. Diamonds: diopside; triangles $Ca_{0.8}Mg_{1.2}Si_2O_6$; squares: $Ca_{0.5}Mg_{1.5}Si_2O_6$