ESRF	**Experiment title:** **High pressure X-ray diffraction study of the spinel $MgMn_2O_4$**	**Experiment number**: **HS 2372**
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ESRF

Report:

High pressure X-ray diffraction was carried out on 2 samples of the $MgMn_2O_4$ tetragonal spinel with different inversion degrees, namely about 20 and 40%, respectively. Measurements have been carried out up to 30 GPa for the first sample (20% inversion) and up to 22 GPa for the second one, as a consequence of a break in the metallic gasket.
The main results of this experiments are:

1. Both the $MgMn_2O_4$ spinels undergo a phase transition at HP towards an orthorhombic phase, as found for the Mn_3O_4 [1] and opposite to the $ZnMn_2O_4$ [2] spinel. This HP phase si of the $CaMn_2O_4$-type (marokite).
2. A correlation between the average ionic radius of the A site, $<r_A>$ (in 8-fold coordination, as for the A-ion in the marokite structure) and the pressure at which the transition from tetragonal to orthorhombic structure occurs has been established. See Figure 1.
3. The bulk moduli of the two samples have been derived by fitting the data according to the Birch-Murnagan EoS and by keeping the first derivative of the bulk modulus equal to 4.
4. We found that the more inverted sample has a lower transition pressure (P_T) with respect to the less inverted one. No other significant differences have been found in their

behaviors. The bulk modulus of the Low Pressure tetragonal structures are very close each other: 156±0.7 (20% inversion) and 155.1±1.2 (40% inversion). So, even within the limit of a relatively low estimated difference of the inversion degree between the two samples we can state that the overall compressibility behavior does not change significantly with the inversion. However, some differences can be observed in the relative compressibility of the crystal directions. Another meaningful difference between the two samples is the volume reduction at the phase transition. It has been seen that the more inverted sample contracts of nearly 1% less than the less inverted one. This can be mainly connected to the more "compacted" structure of the first due to an overall reduction of distortion as a consequence of a different ion distribution in the structure. Also the density tends to increase less for this sample with respect to the less inverted one.

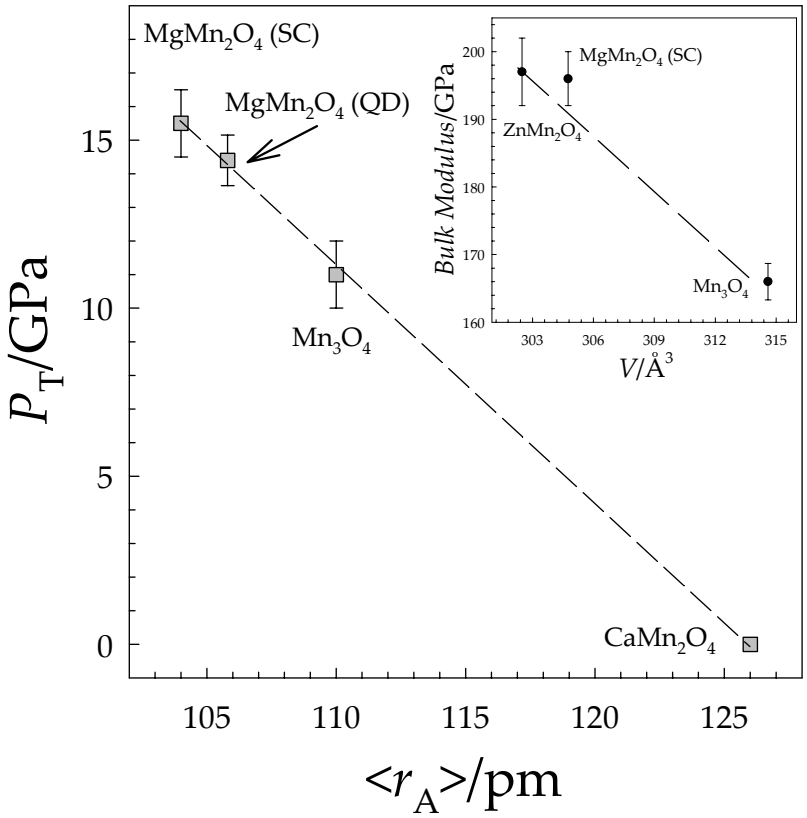

Fig. 1. – Transition pressures for various spinel manganites (see names in the plot) *vs*. the average ionic radius of the A-site. Inset: bulk modulus values *vs*. cell volumes.

1. E. Paris, C.R. Ross and H. Olijnyk, *Eur. J. Mineral*., **4,** 87 (1992).

2. S. Åsbrink, A. Waskowska, L. Gerward, J. Staun Olsen and E. Talik, *Phys. Rev. B,* **60,** 12 651 (1999).