ESRF	**Experiment title:** EXAFS study of local order and structure related to a potential spin-lattice coupling in $RE_2Mo_2O_7$ pyrochlores	**Experiment number**: HC-2414
Beamline: BM25A	**Date of experiment**: from: 7 April 2016 to: 12 April 2016	**Date of report**: 12 July 2016
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Report:

Extended X-ray absorption fine structure spectroscopy (EXAFS) measurements were performed at beamline BM25A in transmission geometry on $RE_2Mo_2O_7$ pyrochlores (with RE = Gd, Sm, Dy, Ho, or Er) at the Mo K edge. We acquired spectra at about 30 different temperatures in the range 8-300 K for Sm and Gd samples, and between 6.5 and 320 K for the Ho, Dy, and Er samples. The Debye-Waller factor $\sigma^2(Å^2)$ as a function of temperature is reported in Figure 1 for all the five analyzed samples. The RE = Gd and Sm samples exhibit a ferromagnetic transition temperature at about 100 K while the other three samples have a spin-glass behaviour at the lower limit of our temperature range of analysis. Nevertheless, it would be possible to investigate any magneto-elastic coupling by looking at the Debye-Waller factor behavior at higher temperatures: if this is in some way affected, one could in principle observe some feature, a plateau or a flatter curve than expected in the ideal case. Here, just the Gd sample shows the typical correlated Debye-Waller curve (with possibly some anomaly arising around 50-

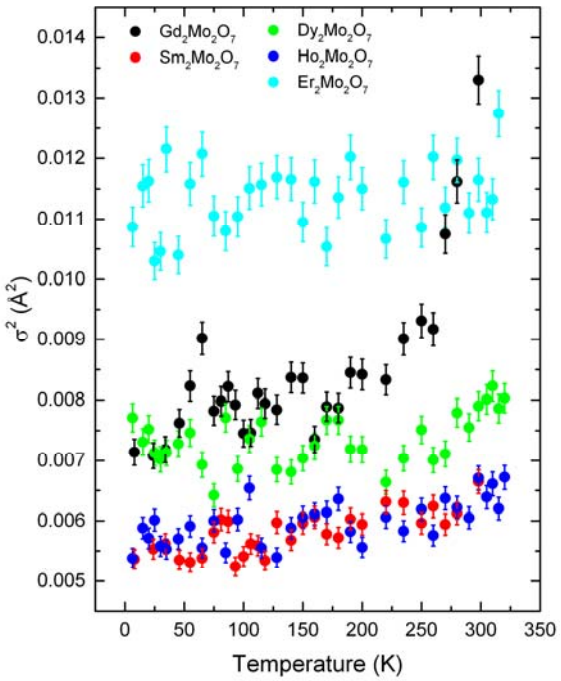

Figure 1: Debye-Waller factor as a function of temperature for all the analyzed samples

60 K), while the other ones are all flatter. The possible presence of local disorder in these compounds has been taken into account by modifying the fitting model of experimental data. The first coordination shell, made of MoO_6 octahedra, was fitted with a bimodal distribution of distances (see Figure 2): best fits were obtained with decreased apical distances (between 1.8 and 1.9 Å), while the basal plane ones appear to be always more or less equal to the values retrieved by long-range-sensitive techniques (e.g. diffraction, between 2.00 and 2.04 Å for our set of samples). We should note here that, while basal distances are affected by very little noise (at least, within the experimental error), the two apical shorter distances are, in all cases, much more scattered. In Figure 3, the second shell distances are reported for the same samples. The dashed lines represent the values retrieved from diffraction experiments for Gd, Sm, and Dy samples (3.65 Å, 3.68 Å, and 3.63 Å, respectively). Also in this case there is a splitting between Mo-Mo distances, which remain little affected by noise and always slightly higher than expected, and Mo-Rare earth ones, much more scattered with respect to the temperature and, at least in the case of Gd and Dy, with a smaller mean value.

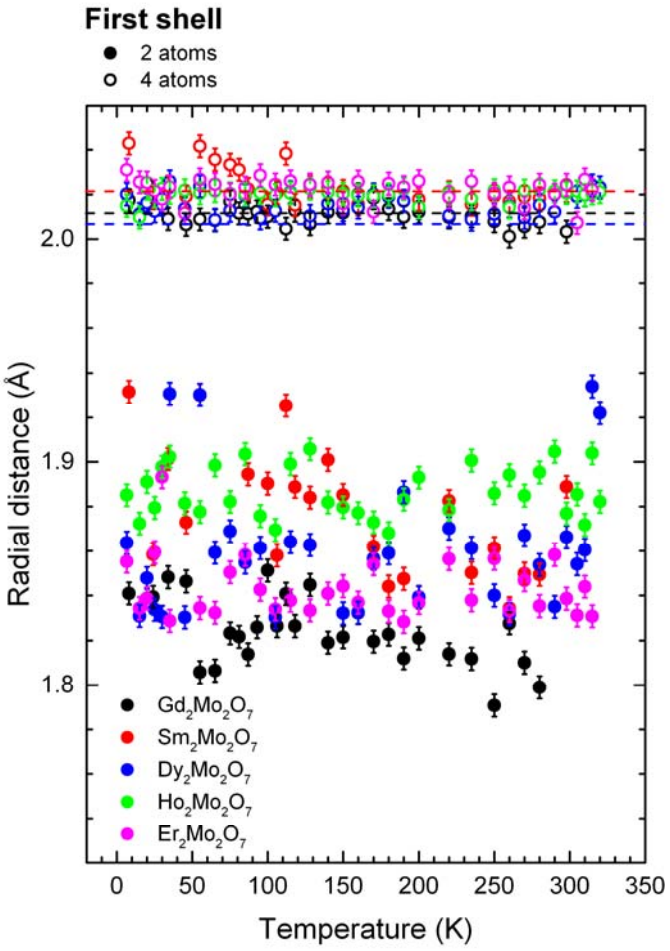

Figure 2: Mo-O interatomic first shell distances

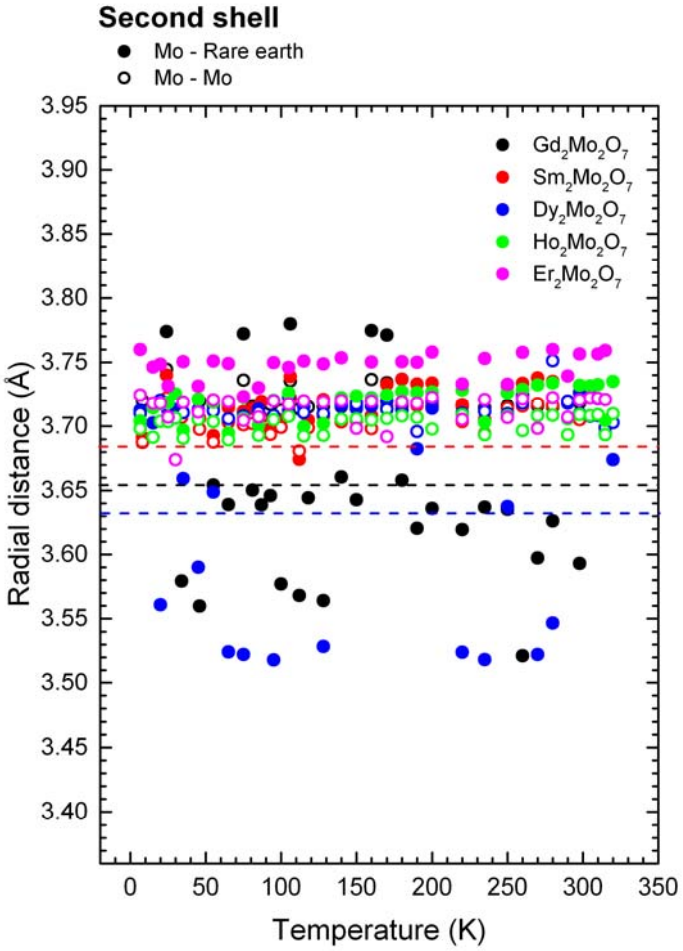

Figure 3: Mo-RE and Mo-Mo interatomic second shell distances

The observed local lattice distortion and related higher static component of σ^2 disorder are in agreement with the occurrence of short-range ordered phases such as spin glasses in several geometrically frustrated pyrochlores. In fact, it is well known the tendency of these systems to relieve magnetic frustration through a lower symmetry phase [1].

[1] C. Castellano, G. Berti, S. Sanna, R. Ruiz-Bustos, J. van Duijn, A. Brambilla, A. Muñoz-Noval, P. Carretta, L. Duò, F. Demartin, *Phys. Rev. B* **91** (2015) 224101