

**Experiment title:**

XANES and EXAFS at the K-Edge of Ni and Co in clay-like magnetic compounds.

**Experiment****number:**

HE-837

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67037 STRASBOURG cedex**Report:**

The principal aim in our proposal was to obtain information about the second coordination spheres of a series of layered metal-organic hybrid magnets belonging to the phyllosilicate family from a study of the K-edge EXAFS spectra of the transition metals (Ni and Co). It is hoped to shed some light on the structure and consequently on the long range magnetic orderings. The experiments were successful; we have collected data at low temperature of several compounds and some standards in the same conditions. Analysis of the data is progressing.

On figure 1 are depicted the Fourier transforms of nickel hydroxide ( $\text{Ni}(\text{OH})_2$ ), Ni talc ( $\text{Ni}_3\text{Si}_4\text{O}_{10}(\text{OH})_2$ ) and one of the new hybrid organic-inorganic Ni silicate of principal interest. The first two compounds are well known. In the former, Ni is surrounded by only 6 Ni at a distance of 3 Å whereas in the second one Ni is surrounded by 6 Ni at 3 Å and 4 Si at 3.2 Å. Using the FEFF6 package, the simulation for Ni talc indicates that multiple scattering

only occurs for distances longer than 3.5 Å. This distance is greater than the second coordination sphere, consequently our calculation may be conducted using only a single scattering approximation. The presence of additional silicon atoms in the out of plane of the layer modifies the intensity of the peak corresponding to the second sphere at 3 Å (see figure). It is clear in our analysis so far that the hybrid silicate contains, in addition, both Si and oxygen in its second coordination sphere.

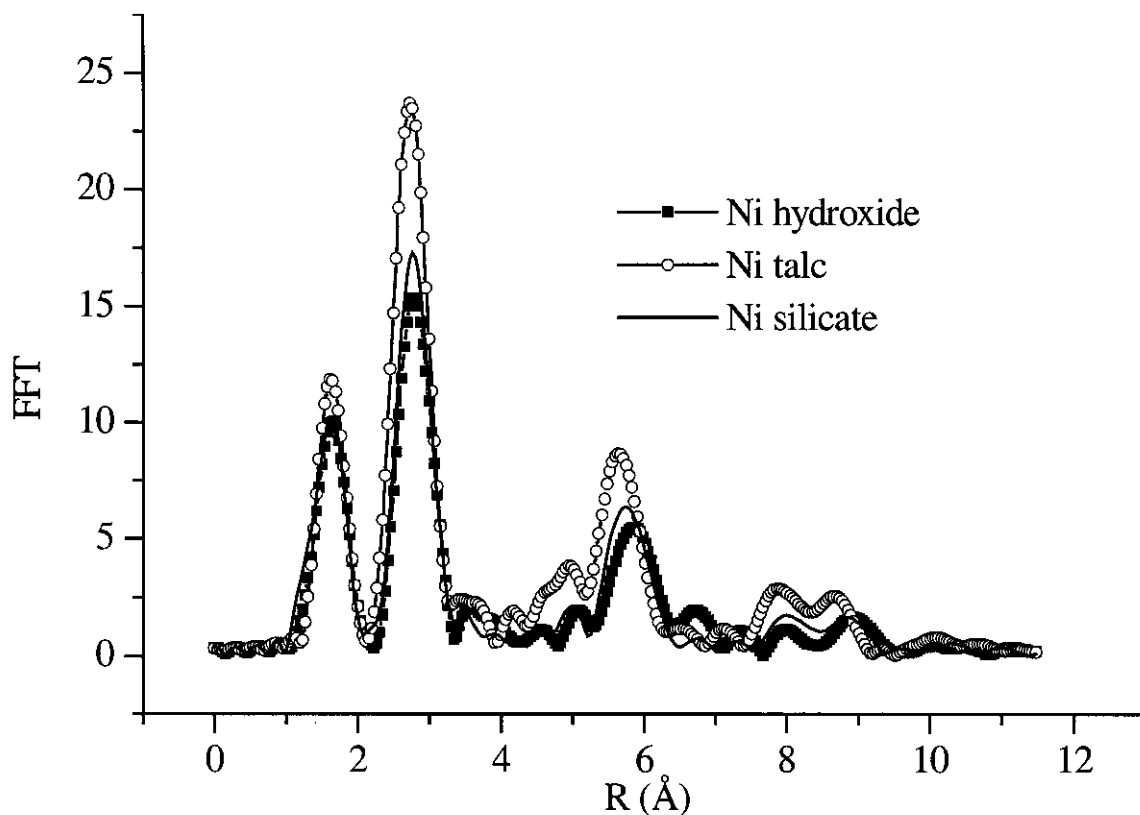


Figure 1 : Fourier transforms of the EXAFS spectra ( $k^3\chi(k)$ ) of nickel talc, Ni hydroxide and the organic-inorganic Ni silicate.

Further analyses and analogous calculations on the isostructural Co organic-inorganic silicate are in progress.

Another family of compounds studied is based on layered cobalt hydroxide separated by a range of carboxylates with varying lengths. Single crystal structure of one member of this family, performed after our visit to ESRF, shows that the octahedral cobalt ion is heavily distorted with six different Co-O distances ( $2.2\pm 0.3\text{Å}$ ). From our EXAFS data we can only show the structural similarities of this with the other members of the family.