ESRF	**Experiment title:** **Large orbital moment in α-Fe phthalocyanine.**	**Experiment number:** **HE2486**
Beamline:	**Date of experiment:** from: 26th Sept 2007 to:29th Sept 2007	**Date of report:**
Shifts:	**Local contact(s):** Dr. Julio Criginski CEZAR	*Received at ESRF:*

Names and affiliations of applicants (* indicates experimentalists):

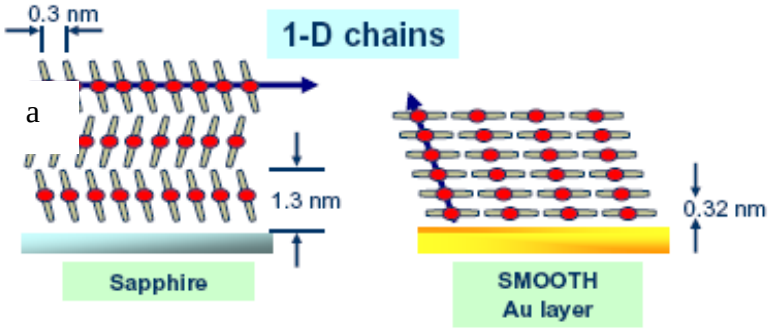
Dr. Juan Bartolomé Sanjoaquín*, ICMA, CSIC- Universidad de Zaragoza. Spain

Dr. Fernando Bartolomé*. ICMA, CSIC-Universidad de Zaragoza. Spain

Dr. Luis Miguel García*. ICMA, CSIC-Universidad de Zaragoza. Spain

Dr. George Filoti. National Institute for Research and Development. Magurele. Bucharest. Romania

Report:



In metal Phthalocyanines (MPc), the M atom has square-planar coordination with four pyrrolic N atoms. These molecules may be deposited on a substrate forming a well defined film.In case of depositing on sapphire the MPc molecules stack in a herringbone structure forming long needles parallel to the substrate Fig. 1a. In contrast, when deposited on Au substrate the molecule plane is parallel to the substrate Fig. 1b.

Fig.1. Sketch of the FePc thin films.

From Mössbauer experiment it was conjectured that in FePc alfa-phase the record highest hyperfine field ever measured on an Fe(II) ion (B_{hf}=66.2 T) could be related to the electronic configuration $d_{xy}^2(d_{xz},d_{yz})^3d_z^2$, which has an **orbitally degenerate** ground state, and as a consequence, **an expectation value of** $\langle L_z \rangle \approx 1$. [2]. In experiment HE2486. we have measured the Fe $L_{2,3}$ edges XMCD of the two samples, at 5 K and H=6 T in the TEY mode, as a function of incidence angle. We could prove the following facts:

a) The samples do not show any radiation damage decay.
The XMCD spectra show a rich structure of peaks at L_3 and L_2 edges, from which information about the 3d states can be obtained. Noteworthy is the fact that for sample b, the L_2 spectra is small compared with the L_3 component, and changes sign as a function of angle, Fig.2.

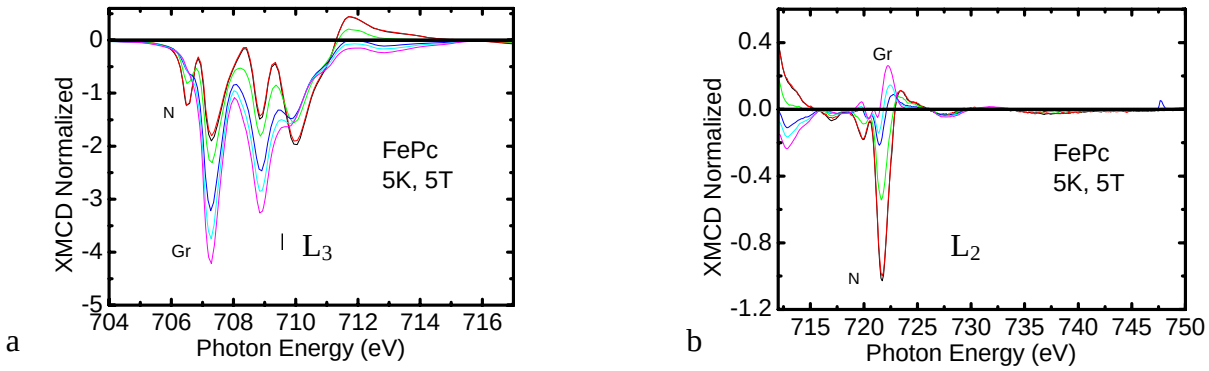


Fig. 2. XMCD spectra of the Fe L_3 (a) and L_2 edges (b) of FePc, as a function of incident angle. N) normal incidence, Gr) grazing angle 75°.

b) From the analysis of the sum rules, the orbital and spin moments could be derived. Scaling the total moment to the saturation magnetization measured by SQUID, (Ms=1.6 μ_B), one deduces a maximum orbital moment in m_L=0.67(1) μ_B, contained in the molecule plane. To our knowledge, this is the highest orbital moment measured on an Fe(II) molecule.

c) From the analysis of the angle dependent XMCD the anisotropy ratio $m_l^{xy} / m_L^z \approx 2$ was derived, implying that the local easy axis of magnetization is contained in the molecule plane. The values of the deduced moments after scaling to Ms=1.6 μ_B, as deduced from the M(H) experiments [1], was done.This scaling is necessary since we have no theoretical prediction of the effective number of holes, or any theoretical prediction for the scaling factor. The values obtained are
m_L^z=0.37 μ_B, m_L^{xy}=0.67 μ_B, m_S^z=0.13 μ_B, m_S^{xy}=1.08 μ_B

d) The X-ray Natural Linear Dichroism, XNLD, at the N-K edge was also performed. The results are similar to those reported for NiPc molecules also deposited flat on a substrate. The result implies that the molecular orbital highest density of holes in the π orbital is perpendicular to the molecule. The actual resonance energies can be derived.

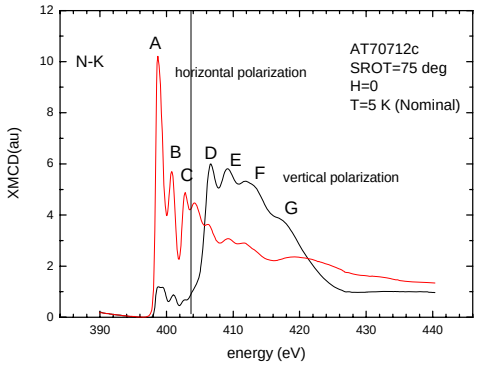


Fig. 3. XNLD of sample b) in grazing angle θ=75°, in the two polarizations, horizontal and vertical to the beam polarization plane. The vertical line indicates the K edge energy.

Therefore, that experiment has been very successful in proving not only the high value of the orbital moment, but also determining the component, albeit, of only the contribution due to the d states.

[1] M. Evangelisti, J. Bartolomé, L.J. de Jongh and G. Filoti. Phys. Rev. B 66, 144410 (2002)
[2] G. Filoti, M.D. Kuz'min and J. Bartolomé. Phys. Rev. B 74, 134420 (2006)
[3] Rocco et al. J. Chem. Phys. 93, 6859 (1990)