

**Experiment title:**

XAS of Ruthenium phthalocyanine: structural properties of the dimer and its dioxygen activation

Experiment number:

CH162

Beamline:GILDA
D8**Date of experiment:**

from: 27 Sept 95 to: 2 Oct 95

Date of report:

26 Feb 96

Shifts:

15

Local contact(s):

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28 FEB. 1997**Names and affiliations of applicants (* indicates experimentalists):**

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Report:

We measured on the Ruthenium K-edge Ru-Ru and Ru-N, structurally known systems. We studied the ruthenium dimeric compound, Ruthenium Phthalocyanine having two pyridines as adduct, that has been already structurally characterized (**1**), the monomeric specie of Ru phthalocyanine and a polymeric specie of Ru phthalocyanine in absorption mode, using pellets in BN and obtaining spectra of about 1000 eV above the edge, with a very good S/N. (**FIG.1a, 1b**)

Great care has been used in the choice of the Ruthenium complex compounds, structurally known, in order to use experimental phases to fit the data and to determine precisely the structure of the thin film that is presently under study showing some properties connected with oxygen activation and oxygen transfer. The "unknown" system, thin phthalocyanine film loaded by sublimation, the possible sensor, has been measured in fluorescence straight on the growth substrate (glass) with and without the filter, obtaining again good spectra.

In **FIG 2** are reported the Fourier transforms obtained for the dimer (a Ru-Ru bond is well defined) and the monomer (no Ru-Ru present) with the fit of the first neighbours, while in **FIG 3** the dimer is in comparison with the polymeric species, which shows a well defined Ru-O-Ru bondat ca. 4 Å. The Fourier transform of the thin film, reported in **FIG.4** shows not evidence for a Ru-O-Ru bond, and the superposition of the dimer parameters shows a perfect agreement within the first two shells .

This answers to one of the main questions, whether the film, which is produced using the dimer as starting material, retains or not the same primary structure: at the present we can already conclude that the structure of the dimer is retained, at least for the first surroundings, in the film.

A careful analysis of the data is still under way, but is very promising and, because the very good performance in reproducibility, in stability and in very high S/R of the beamline, we plan to take more measures, mainly in fluorescence on the thin film, to understand the actual behaviour of the film when it is acting as sensor.

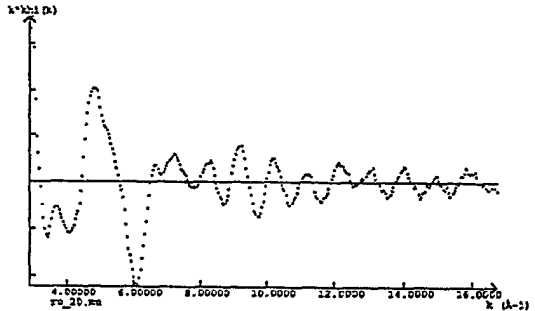
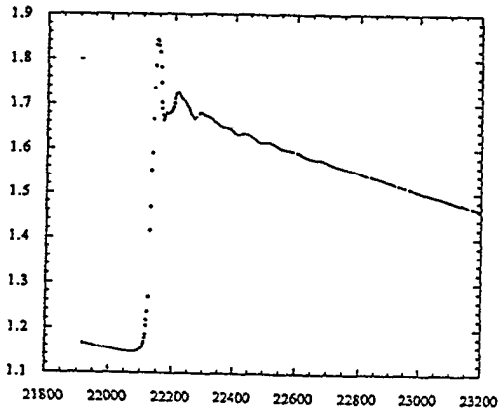


FIG. 1a

FIG. 1b

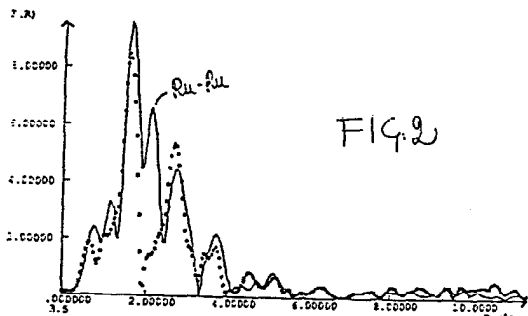


FIG. 2

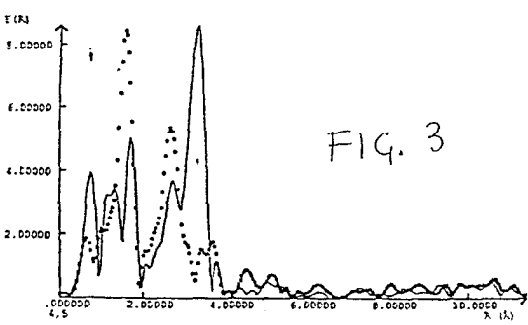


FIG. 3

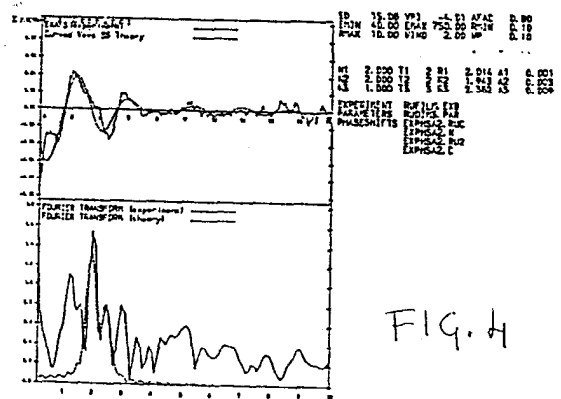


FIG. 4