ESRF	**Experiment title:** Study of the Cu environment in Cu/ZrO2 systems for the selective catalytic reduction (SCR) of NO.	**Experiment number**: ME-66
Beamline:	**Date of experiment**: from: 22-juin-00 to: 27-juin-00	**Date of report**: 28-08-02
Shifts: 15	**Local contact(s)**: Stuart Ansell, Michael Borowski,	*Received at ESRF:*

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Report:

This was an in situ red experiment using a high temperature cell and a wafer sample of Cu/ZrO_2 in contact with a NO-oxygen-hydrocarbon atmosphere.

The XANES spectra of the CuOx/ZrO2were obtained after different treatments with CH4-C3H8/NO/O2 mixtures are presented in figure 1. As can be seen, the XANES spectra show features related with different chemical states of Cu. These features are more evident when the first derivative of these XANES spectra are analyzed (figure 2). Maximum for Cu^0 (8979eV), Cu^+ (8982eV) and Cu^{2+} (8984eV) can be identified. Without oxygen, Cu^+ species are dominant with methane, and Cu^0/Cu^{2+} with propane. Otherwise, in the presence of oxygen, the copper is fully oxidized in all conditions, regardless of the hydrocarbon.

The Fourier transform obtained from the EXAFS functions (figure 3) and the structural parameters obtained by fitting agree with the results by XANES. Cu^{2+} is the only specie when O_2 is present (SCR conditions). Cu in the 0, +1 and +2 oxidation state can be detected if no oxygen is present.

Surprisingly, by treatment at 573K, Cu is more effectively reduced by methane than by propane. This effect can be explained considering that, as shown by IR measurements (1), the CuO_x/ZrO_2 is covered by carboxilates species after contact with propane, remaining unable to adsorb NO.

The previous derivative XANES spectra have been studied by factor analysis (2), which have provided additional evidence about the presence of the cited oxidation states of copper under these gas mixtures. This treatment (figure 4) have supplied *factors* that are related with the different valence states. The percentage of these *factors* are showed in the bar graph (figure 5).

This results have been presented at the E-MRS 2002 Spring Meeting at Strasbourg (France) and a publication is actually in preparation.

References

1.- J.Morales, A.Caballero, J.P.Holgado, J.P.Espinos, A.R. González-Elipe; J.Phys.Chem. B, 2002, in press.

2.- J.P.Holgado, G.Munuera, J.P.Espinós, A.R.González-Elipe; Appl.Surf.Sci., 158 (2000) 164

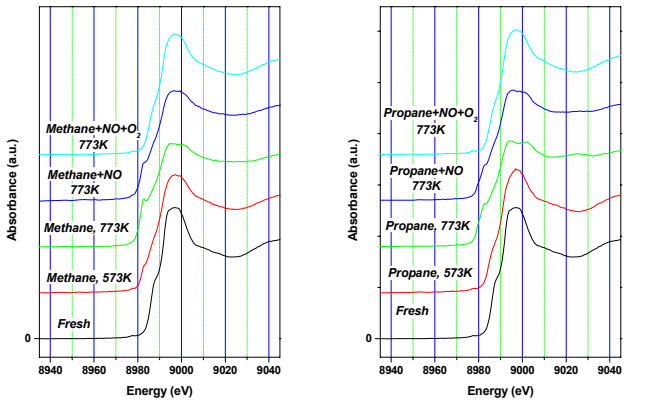

Figure 1

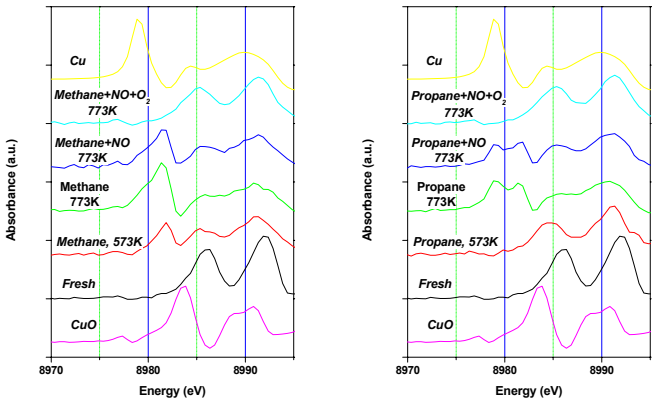

Figure 2

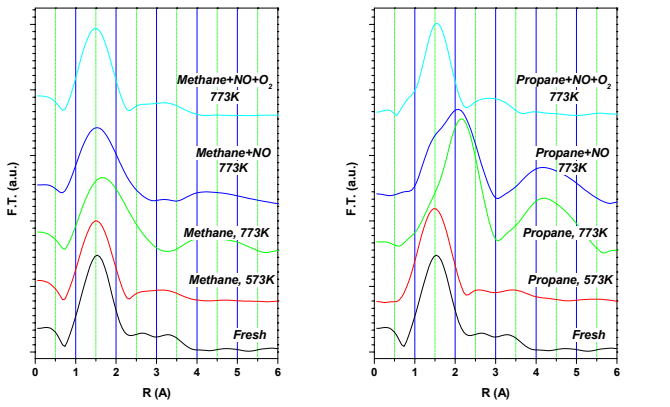

Figure 3

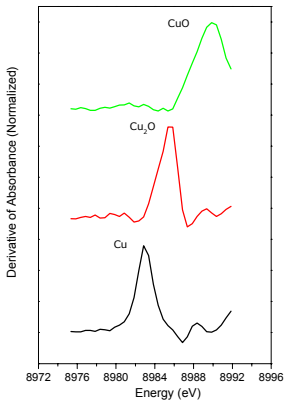

Figure 4

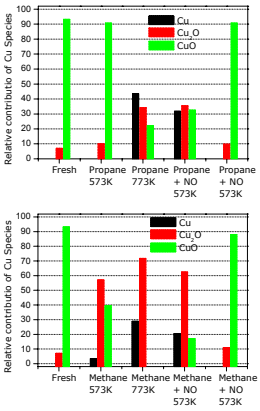

Figure 5