

# GASTPROFESSUR

IM RAHMEN DES SONDERFORSCHUNGSBEREICHS 623  
DER UNIVERSITÄT HEIDELBERG  
MOLEKULARE KATALYSATOREN: STRUKTUR UND FUNKTIONSDESIGN

**15.-28. Juni 2003**

**Professor Brian T. Heaton**

University of Liverpool, UK

1. Vortrag: Dienstag, 17. Juni 2003, 10:15 Uhr

**“In situ Spectroscopic (IR and NMR) Measurements on  
Homogeneous Catalytic Reactions Under Pressures of Gas”**

2. Vortrag: Mittwoch, 18. Juni 2003, 10:15 Uhr

**“*In situ* NMR Measurements on the Pd-Catalysed  
Methoxycarbonylation of Ethene and Related CO/C<sub>2</sub>H<sub>4</sub>  
Copolymerisation Catalysts”**

3. Vortrag: Montag, 23. Juni 2003, 10:15 Uhr

**“Identification of Catalytic Intermediates in the CATIVA  
Reaction and Hydrogenation Reactions”**

Die Vorträge finden im OCI-Seminarraum, INF 270, EG statt.

Gäste sind herzlich willkommen.

## **“*In situ* Spectroscopic (IR and NMR) Measurements on Homogeneous Catalytic Reactions Under Pressures of Gas”**

This lecture will review the range of IR and NMR cells which have been used to measure spectra under high pressures of gas and, for reactions involving M-CO's, the advantages of having both IR and NMR measurements on the same reaction under the same conditions. Selected examples will illustrate:-

The spectroscopic identification of intermediates *in situ*.

The application of a variety of modern NMR techniques.

How meaningful kinetic data can be obtained; this is relatively straightforward from IR measurements but more difficult from NMR measurements when using a flow cell and a mixed gas feedstock eg. CO/H<sub>2</sub>.

## **“*In situ* NMR Measurements on the Pd-Catalysed Methoxycarbonylation of Ethene and Related CO/C<sub>2</sub>H<sub>4</sub> Copolymerisation Catalysts”**

*In situ* NMR measurements will be described which have enabled the identification of all the intermediates in the catalytic methoxycarbonylation of ethene to methyl propanoate; this route, *via* a Pd-H, is one of the few catalytic cycles where all the intermediates in the cycle have been spectroscopically characterised.

Related studies will be described aimed at providing a better understanding of the mechanism of related CO/C<sub>2</sub>H<sub>4</sub> copolymerisation catalysts; in this case, the cycle involves both Pd-H and Pd-OMe intermediates.

## **“Identification of Catalytic Intermediates in the CATIVA Reaction and Hydrogenation Reactions”**

BP have recently introduced the CATIVA process for the carbonylation of methanol to acetic acid; this involves an Ir/Ru catalyst and allows a 30% increase in throughput compared with the Monsanto/BP process based on Rh. The factors responsible for this increase together with the mechanism of this cycle, which has been deduced from both high pressure IR and NMR measurements, will be described.

The lecture will describe spectroscopic measurements on a variety of Rh- and Ru-catalysed hydrogenation reactions; the use of p-H<sub>2</sub> has been shown to be most useful in these studies and the lecture will describe how these and other measurements have allowed the identification of a variety of catalytic intermediates/mechanisms.