

EIGHTH
SHHC
1995 HUNGARY

EIGHT INTERNATIONAL SYMPOSIUM
ON RELATIONS BETWEEN HOMOGENEOUS
AND
HETEROGENEOUS CATALYSIS

8th SHHC



*Book of Abstracts
Final Program*

HOTEL FÜRED
BALATONFÜRED, HUNGARY
SEPTEMBER 10-14, 1995

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SYMPOSIUM SITE

The 8th International Symposium on Relations Between Homogeneous and Heterogeneous Catalysis will be held in Hotel Füred, Balatonfüred, Hungary.

Address

Hotel Füred
Széchenyi út 20.
H-8230 Balatonfüred
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National Committee for Technological Development, Budapest, Hungary
Southern Hungarian Gas Company, Szeged, Hungary
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European Commission, Brussels, Belgium
Hungarian Oil Corporation, Budapest, Hungary
EGIS Pharmaceuticals Ltd, Budapest, Hungary

REGISTRATION DESK - OPENING HOURS

The Registration Desk will be located in the Main Lobby of Hotel Fűred.

September 09, 1995,	Saturday,	10:00 - 18:00
September 10, 1995,	Sunday,	10:00 - 20:00
September 11, 1995,	Monday,	08:00 - 18:00
September 12, 1995,	Tuesday,	08:00 - 18:00
September 13, 1995,	Wednesday,	08:00 - 18:00
September 14, 1995,	Thursday,	08:00 - 14:00

Registration Fee (in US \$)

Participant	440.00
Student (no Proceedings)	170.00
Accompanying person	100.00

Registration fee includes:

- participant
 - Welcoming reception, excursion to Tihany, Banquet, coffees, badge, conference bag, participation at the Symposium, Book of Abstracts, Proceedings
- student
 - Welcoming reception, excursion to Tihany, Banquet, badge, participation at the Symposium, Book of Abstracts
- accompanying person
 - Welcoming reception, excursion to Tihany, Banquet, badge

3. Lake Cruise on the Balaton

Balatonfüred - Balatonfüred
September 12, 1995, Tuesday
Departure: 19:30
Duration: about 2 hours
Minimum number of persons: 20
Price: USD 15.00 per person

Lake Balaton

Lake Balaton is a long, narrow sheet of water. At its longest point the lake stretches for 77 km, its coastline is 197 km long. The lake is 14 km wide at its widest point and 1.5 km at its narrowest point. The average depth is 2-3 m, though at Tihany it is 14 m deep. Since the water of the lake warms up rapidly it is pleasant to swim there from spring to late fall. The origin of the lake goes back to the time when the area of the present Hungary was covered by sea. The residue of this sea, the Lake Pannon, gradually became filled with silt. Hot spa gushed out to form the warm-water lake of Héviz. Lake Balaton is a relatively newly formed lake being about 22.000 years old.

SCIENTIFIC PROGRAM

Plenary and invited lectures as well as oral presentations will be held in the Conference Room located on the first floor. Overhead and slide projections will be available in the lecture hall. Slide check room is available at the Secretariat located on the first floor.

Poster presentation will be at the foyer located on the first floor.

International Advisory Board Meeting on September 10, 1995 at 15:00 will be arranged in a small meeting room located on the 3rd floor.

Registration is at the ground floor in the main lobby.

Notes

PL : plenary lecture
I : invited lecture
O : oral contribution
P : poster presentation

Morning, Monday, September 11, 1995

- 08¹⁵ Opening Ceremony
- Session: *Topic No. 7, Computer Modelling, Novel Instrumental Techniques*
- Chairmen: *G. A. Somorjai (USA), L. Guzzi (Hungary)*
- 08³⁰ PL 1 Computational-Chemical Advances in Heterogeneous Catalysis
R. A. van Santen (The Netherlands)
- 09³⁰ I 1 PTRF X-ray Absorption Fine Structure as a New Technique for Catalyst Characterization
O. Chung, M. Shirai, K. Tomishige, K. Asakura, Y. Iwasawa (Japan)
- 10⁰⁰ Coffee
- Chairmen: *J. Evans (UK), J. Raskó (Hungary)*
- 10³⁰ O 1 A Computer Modelling Study of Silica and NaY Zeolite
P. Fantucci, M. Bienati, C. Dossi, R. Psaro, L. Sordelli, F. Trabujo (Italy)
- 10⁵⁰ O 2 Modelling of Silica-Supported Ni(I)-Dihapto-Benzene Complexes
J. M. Garrot, C. Lepetit, M. Che (France)
- 11¹⁰ O 3 Mechanistic Studies of Methanol-to-Hydrocarbon Conversion by Polyphosphoric Acid: a Homogeneous Model for "Methanol-to-Gasoline" Chemistry
D. A. Hoover, M. Al-Azab, J. E. Jackson (USA)
- 11³⁰ O 4 Noble Metal Catalysed Homogeneous and Heterogeneous Processes in the Treatment of Simulated Nuclear Waste Media with Formic Acid
R. B. King, N. K. Bhattacharyya, H. D. Smith, K. D. Wiemers (USA)
- 11⁵⁰ O 5 Production of ¹¹C-Labelled n-Hexane for Use in Positron Emission Imaging
R. H. Cunningham, A. V. G. Mangnus, J. van Grondelle, R. A. van Santen (The Netherlands)
- 12¹⁰ O 6 The Secret of Catalytic Production and Purification of Buckytubes
A. Fonseca, K. Hernádi, J. B. Nagy, D. Bernaerts, (Belgium)
- 12³⁰ O 7 Metal Alkyl Complexes as Models for Catalytic Intermediates
J. R. Moss (South Africa)
- 12⁵⁰ Lunch

Afternoon, Monday, September 11, 1995

Session: *Topic No. 2, Catalytic Effects of Microporous Crystals*

- Chairmen: *P. Fantucci (Italy), P. Fejes (Hungary)*
- 14³⁰ I 2 Controlling the Chemistry of Micropore Volume in Pillared Clays and Micas
J. W. Johnson (USA)
- 15⁰⁰ O 8 Fe-Pillared Clays: a Combination of Zeolite Shape Selectivity and Iron Activity in the CO Hydrogenation Reaction
M. J. Pérez Zurita, G. Vitale, M. R. Goldwasser, D. Rojas, J. J. Garcia (Venezuela)
- 15²⁰ O 9 Selective Dehydration of 1-Phenylethanol to 3-Oxa-2,4-Diphenylpentane on Titanium Pillared Montmorillonite
A. Gil, H. del Castillo, J. Masson, J. Court, P. Grange (Belgium)
- 15⁴⁰ O 10 Heterogenation of Water Sensitive Organometallic Catalysts into Layered Aluminosilicates
C. S. Skordilis, P. J. Pomonis (Greece)
- 16⁰⁰ Coffee
- Chairmen: *J. S. Bradley (USA), J. L. Margitfalvi (Hungary)*
- 16²⁰ O 11 Studies on the Synthesis, Characterization and Catalytic Properties of the Large Pore Titanosilicate, ETS-10
T. Das, A. J. Chandwadkar, S. Sivasanker (India)
- 16⁴⁰ O 12 Radiation Enhancement of the Catalytic Properties of Three Dimensional Coordination Polymers of Ru(II) with Diisocyanide Ligands
R. Tannenbaum (USA)
- 17⁰⁰ O 13 Comparison between Homogeneous and Sol-Gel-Encapsulated Rhodium-Quaternary Ammonium Ion Pair Catalysts
J. Blum, A. Rosenfeld, N. Polak, O. Israelsohn, H. Schumann, D. Avnir (Israel)
- 17²⁰ Poster Session I. (*Gallery*)

Morning, Tuesday, September 12, 1995

Session: Topic No. 1, Molecular Design of Catalysts

Chairmen: *U. Schuchard (Brazil), G. Pályi (Hungary)*

- 09⁰⁰ PL 2 Molecular Metal Carbonyl Clusters and Volatile Organometallic Compounds for Tailored Mono and Bimetallic Heterogeneous Catalysts
R. Ugo, C. Dossi, R. Psaro (Italy)
- 10⁰⁰ I 3 The Role of Support in Formation and Stabilization of Cluster Metal Compounds
V. A. Likholobov (Russia)
- 10³⁰ Coffee
- Chairmen:** *Y. Iwasawa (Japan), D. Kalló (Hungary)*
- 10⁵⁰ O 14 Preparation of New Chiral Dioxo-Molybdenum Complexes Heterogenized on Silica and Modified USY-Zeolites. Efficient Catalysts for Selective Epoxidation of Allylic Alcohols
A. Corma, A. Fuerte, M. Iglesias, F. Sánchez (Spain)
- 11¹⁰ O 15 Macrocomplexes on the Basis of Functionalized Polyethylene Glycols and Copolymers of Ethylene Oxide and Propylene Oxide: Synthesis and Catalysis
E. A. Karakhanov (Russia)
- 11³⁰ O 16 Heteropoly Anion-on-Carbon: Characterization and Use in 2,3,6-Trimethylphenol Oxidation
R. J. J. Jansen, H. M. van Veldhuizen, H. van Bekkum (The Netherlands)
- 11⁵⁰ O 17 Palladium Salts of Heteropolyanions as Catalyst in Heterogeneous Wacker Oxidation of 1-Butene
A. W. Stobbe-Kreemers, M. van der Zon, M. Makkee, J. J. F. Scholten (The Netherlands)
- 12¹⁰ O 18 A Molecular Approach to Heterogeneous Catalysis. Ethylene Hydroformylation Catalyzed by Silica-Supported $[\text{Rh}_{12}(\text{CO})_{30}]^{2-}$ Cluster Anion: Influence of the Counteranions (Li^+ , Na^+ , K^+ , Zn^{2+})
R. Psaro, C. Dossi, A. Fusi, L. Garlaschelli, F. Cozzi (Italy)
- 12³⁰ O 19 Supramolecular Approach to Metal-Support Interaction: Reactivity of Silica Supported Bis(allyl) Rhodium(III) and the Influence of Surface Hydroxyl Groups
C. C. Santini, S. L. Scott, J.-M. Basset (France)
- 12⁵⁰ Lunch

Afternoon, Tuesday, September 12, 1995

Session: Topic No. 5, Selective Synthesis of Fine Chemicals

Chairmen: *J.-M. Basset (France), A. Tungler (Hungary)*

- 14³⁰ I 4 Selective Catalytic Synthesis of Fine Chemicals: Opportunities and Future Prospects
R. A. Sheldon (The Netherlands)
- 15⁰⁰ I 5 Enantioselective Hydrogenation of α -Ketoesters: Comparison of Homogeneous and Heterogeneous Catalysts
H.-U. Blaser, H.-P. Jalett, F. Spindler (Switzerland)
- 15³⁰ O 20 Immobilized Catalysts for Enantioselective Hydrogenation: the Effect of Site Isolation
B. Pugin (Switzerland)
- 15⁵⁰ Coffee
- Chairmen:** *M. Hidai (Japan), J. Petró (Hungary)*
- 16¹⁰ O 21 Enantioselective Hydrogenation of α -Keto Esters over Cinchona- $\text{Pt}/\text{Al}_2\text{O}_3$ Catalysts. New Interpretation of the Rate Acceleration and the Induction of Enantio-Differentiation
J. L. Margitfalvi, M. Hegedüs (Hungary)
- 16³⁰ O 22 Asymmetric Resolution Using Modified Zeolite Catalyst
S. Feast, D. Bethell, P. C. Bulman Page, F. King, C. H. Rochester, M. Rafiq H. Siddiqui, D. J. Willock, G. J. Hutchings, (UK)
- 16⁵⁰ O 23 Asymmetric Hydrogenation of α,β -Unsaturated Carboxylic Acid Esters by Rhodium(I)-Phosphine Complex Supported Smectites
S. Shimazu, K. Ro, N. Ichikuni, T. Uematsu (Japan)
- 17¹⁰ O 24 Transformation of Diols in the Presence of Heteropoly Acids under Homogeneous and Heterogeneous Conditions
B. Török, I. Bucsi, T. Beregszászi, I. Kapocsi, Á. Molnár (Hungary)
- 17³⁰ Poster Session II. (*Gallery*)

Morning, Wednesday, September 13, 1995

Session: Topic No. 3, Transition Metal Clusters

Chairmen: *R. Psaro (Italy), Á. Molnár (Hungary)*

- 08³⁰ **PL 3** Catalysis by Metal Clusters on Surface and in Microporous Space: Molecular Approaches in Heterogeneous Catalysis
M. Ichikawa (Japan)
- 09³⁰ **I 6** Synthesis and Catalytic Properties of Large Ligand Stabilized Palladium Clusters
G. Schmid, S. Emde, V. Maihack, W. Meyer-Zaika, S. S. Peschel (Germany)
- 10⁰⁰ **O 25** Cyclosiloxanolate Sandwich Cluster Complexes of High Valent Transition Metals
C. Zucchi, A. Cornia, M. Borsari, G. Gavioli, A. C. Fabretti, G. Pályi, R. Psaro, R. Ugo, O. I. Shchegolikhina, A. A. Zhdanov, S. V. Lindeman (Italy, Russia, Hungary)
- 10²⁰ Coffee
- Chairmen:** *G. Schmid (Germany), A. Sárkány (Hungary)*
- 10⁴⁰ **O 26** Synthesis and Reactivity of Organoplatinum-Rhenium Clusters Having Sulfur Ligands
A. Fukuoka, Y. Minami, N. Nakajima, M. Hirano, S. Komiya (Japan)
- 11⁰⁰ **O 27** Mixed Iron-Rhodium Carbidocarbonyl Clusters on Oxide Supports: Chemistry and Catalysis of Syngas Reactions
V. I. Kovalchuk, N. M. Mikova, N. V. Chesnokov, L. V. Naimushina, B. N. Kuznetsov (Russia)
- 11²⁰ **O 28** Soluble and Supported Carbonylation Catalysts Derived from Rhodium-Phosphonate-Phosphane Complexes
S. Bischoff, A. Weigt, H. Miessner, B. Lücke (Germany)
- 11⁴⁰ **O 29** Catalytic Activity of Pd(II) Sorbed on an Inorganic Ion Exchanger - Zirconium Molybdate
B. Beena, A. Shivaneekar, U. Chudasama (India)
- 12⁰⁰ **O 30** The Influence of Water on Cyanide Displacement of 1-Halobutanes Using 18-6 Crown Ether as Phase Transfer Catalyst
A. Baudoul, A. Borcy, S. Mommerency, P. Vanderwegen, G. Jannes (Belgium)
- 12⁴⁰ Lunch

Afternoon, Wednesday, September 13, 1995

14⁰⁰ - 15¹⁵

Round Table Discussion

Moderator: *Paul B. Weisz (USA)*

15³⁰

Excursion and Banquet

Morning, Thursday, September 14, 1995

Session: Topic No. 4, Molecular Aspects of Catalytic Reactions

Chairmen: M. Ichikawa (Japan), M. T. Beck (Hungary)

- 08³⁰ PL 4 The Flexible Surface. New Techniques for Molecular Level Studies of Time Dependent Changes in Metal Surface Structure and Adsorbate Structure during Catalytic Reactions
G. A. Somorjai (USA)
- 09³⁰ I 7 Toward Direct Synthesis of Organo-Nitrogen Compounds from Molecular Nitrogen
M. Hidai (Japan)
- 10⁰⁰ O 31 Mechanism of Surface Intermediate Formation During the Reactions between Adsorbed Molecules and Atoms: NO+H, NO+C, O₂+H, C₂+H, on Platinum
M. Y. Smirnov, V. V. Gorodetskii, J. H. Block (Russia-Germany)
- 10²⁰ Coffee
- Chairmen: H. van Bekkum (The Netherlands), F. Ungváry (Hungary)
- 10⁴⁰ O 32 On the Mechanism of Carbonylation in Acetic Acid and Higher Acid Synthesis from Methanol and Syngas Mixtures on Supported Rhodium Catalysts
L. Chateau, J. P. Hindermann, A. Kiennemann, E. Tempesti (France)
- 11⁰⁰ O 33 Dioxo-Molybdenum (VI) Complexes: Relation between Oxygen Transfer and ⁹⁵Mo NMR Chemical Shift
H. Teruel, A. Sicrralta (Venezuela)
- 11²⁰ O 34 Transfer of Concepts from Homogeneous to Heterogeneous Catalysis: Use of Hammett Relationships to Assess Reaction Mechanisms and Nature of Active Sites in Reactions Catalyzed by Sulfides, Metals, Clays and Zeolites
A. Finiels, P. Geneste, C. Moreau (France)
- 11⁴⁰ O 35 Homogeneous vs Heterogeneous Processes in Electrocatalysis. Different Types of Catalysis in Organic Electrooxidation
M. Michman (Israel)
- 12⁰⁰ O 36 Photocatalytic Decomposition of Nitric Oxide on the Ag⁺/ZSM-5 Catalyst Prepared by the Ion-Exchange Method
M. Matsuoka, E. Matsuda, K. Tsuji, H. Yamashita, M. Anpo (Japan)
- 12²⁰ I 8 Supported Transition Metal Complexes for Ethylene Polymerization
G. Braca, C. Sbrana, A. Raspolli-Galletti, A. Altomare, G. Arribas, M. Michelotti, F. Ciardelli (Italy)
- 12⁵⁰ Lunch

Afternoon, Thursday, September 14, 1995

Session: Topic No. 8, Application of Enzymes in Organic Synthesis

Chairmen: H. U. Blaser (Switzerland), J. Kosáry (Hungary)

- 14³⁰ I 9 Catalytic and Stoichiometric Multielectron Reduction of Hydrazine to Ammonia, Acetylene to Ethylene and Cyanide to Methane and Ammonia with Clusters that Contain the MFe₃S₄ Cores (M = Mo, V) Relevance to the Function of Nitrogenase
D. Coucouvanis, K. D. Demodis, S. M. Malinak, P. E. Mosier, M. A. Tyson, L. J. Laughlin (USA)
- 15⁰⁰ O 37 Microbial Synthesis of (+) and (-) Methyl-Chloro-4,4-Difluoro-3-Hydroxybutanoate
A. Forni, I. Moretti, F. Prati, G. Torre (Italy)
- 15²⁰ O 38 Enantioselective Hydrolysis of Racemic Esters Using Pig Liver Esterase
J.-M. Herdan, M. Balulescu, O. Cira (Romania)
- 15⁴⁰ Closing the Symposium