



"GREEN CHEMISTRY: A SOLUTION FOR THE WORLD"
1st EVENT ON ECOBENIGN CHEMISTRY

2nd Workshop of the COST D29/0009/03 Working Group
Green Chemistry through Aqueous Organometallic Catalysis

AQUACHEM Midterm Review Meeting and Workshop
Transition Metal Chemistry and Catalysis in Aqueous Media
Project RIN n° MKTN-CT-2003-503864

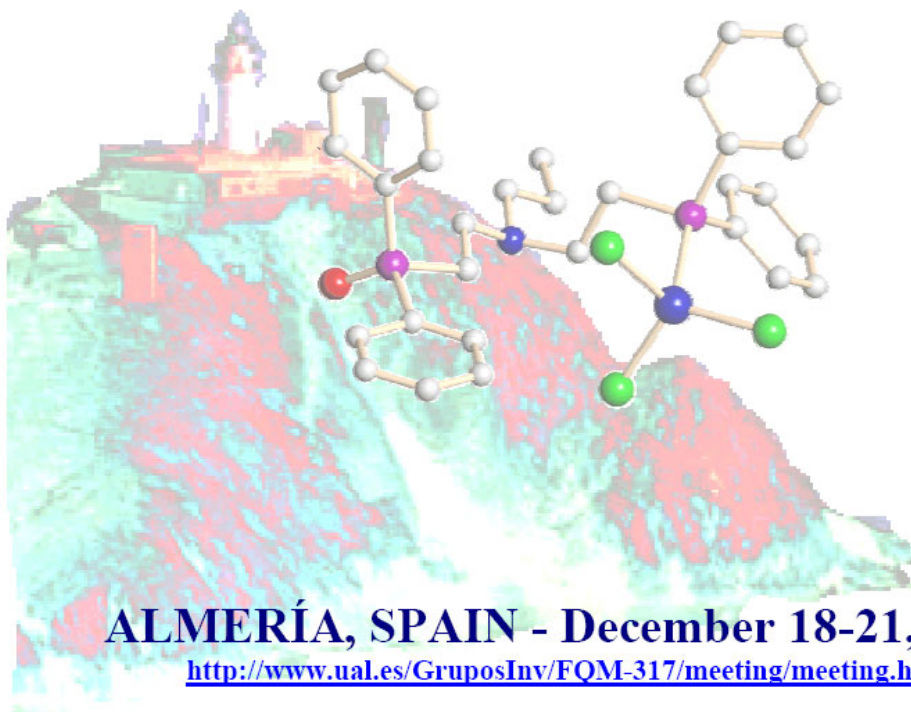


UNIVERSIDAD DE ALMERÍA
ALMERÍA, SPAIN
DECEMBER 18-21, 2005



GREEN CHEMISTRY: A SOLUTION FOR THE WORLD

"Andalusia meets Europe II"



ALMERÍA, SPAIN - December 18-21, 2005

<http://www.ual.es/GruposInv/FQM-317/meeting/meeting.htm>



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UNIVERSIDAD DE ALMERÍA





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“GREEN CHEMISTRY: A SOLUTION FOR THE WORLD”

“ANDALUSIA MEETS EUROPE II”

ALMERIA, SPAIN - DECEMBER 18-21, 2005

Location

*Dto. Química Física, Bioquímica y Química Inorgánica.
Facultad de Ciencias Experimentales, University of Almeria, Spain
La Cañada de San Urbano, s/n
04120 - Almería, Spain*

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1. Opening remarks

Prof. Antonio Manuel Romerosa Nievas, the Organizer, opened the Meeting addressing, on behalf of the President of the Inorganic Chemistry Section of the Royal Spanish Society of Chemistry, Prof. Jaume Casabó, a welcome speech to all the participants. He then acknowledged all those who have made possible this event. Then, the COST D29 Coordinator, **Prof. Ferenc Joo** expressed the welcome to the participants and introduced some aspects on the COST project. The Network Coordinator, **Dr. Maurizio Peruzzini**, presented the meeting and emphasized the close scientific links existing between the AQIACHEM network and the COST workshop. Finally **Dr. Juan José Jiménez** on behalf of the Rector of the University of Almería welcomed all the participants highlighting how this event was important for a young University as the University of Almeria is.

2. General discussion of the activity of the COST D29 consortium

In the first minutes of the meeting the participants remembered the late Prof. Birgit Driessen-Hölscher (University of Paderborn) whose untimely passing away is a great loss of the working group.

Prof. Ferenc Joó gave an overview of the scientific activity of the COST D29 WG 0009/03 consortium mostly based on the mid-term report of the working group presented at the mid-term review meeting of the D29 Action in Tallinn, Estonia, in June 2006. It was agreed upon that since its formation the working group made impressive achievements in aqueous organometallic catalysis. A very severe debate arose on the questions of financing the working group activities. The lack of COST funds available for the Almeria meeting made it impossible for two new members (A. Whiting and G. Papadogianakis) to participate. Similarly, the lack of STSM funds severely hampers the core activity of the working groups, i.e. the exchange of young researchers to carry out experiments in other laboratories of the WG (or the Action).

In spite of these difficulties, the members of the working group agreed to carry on their joint research but expressed their strong opinion that STSM-s are vital to the successful research activity of a working group.

3. General discussion of the activity of the AQUACHEM consortium

Dr. Peruzzini welcomes all meeting participants and reports on the status of the AQUACHEM network. In particular he brings to the attention of the participants the rules and obligations for all the partners. The discussion was then organised by conferences and round tables (see the Programme), and the Midterm session.

The following topics were put on the agenda:

- The budget distribution and problems.
- The second and third year allocation for each partner laboratory.
- The first and second year experience for hiring ESR and ER researchers. A special mention to the rules to be followed to hire ESR/ER researchers is done and emphasis is put to recall the equal gender opportunities inspiring the project and the rules governing the possibility within the 6th RFP MC-RTN programs to recruit non-EC ESR/ER researchers. Peruzzini points out that only few secondments ESR/ER stays were made and encourage to granted researches to go to other partner's laboratories.
- Peruzzini show a overview of the success obtained and of the project subjects to be developed.

4. Future meetings.

It was agreed that the next annual meeting will be held in Debrecen or in another location in Hungary (likely, Budapest), to be organized by Prof. Ferenc Joo, in a period between the end of November 2006 and the end of January 2007. During the meeting, or even before, the Coordinator and the Network Manager will take care to collect the scientific and the financial reports from each team leader.

This second annual meeting, as well as the fourth one (at the end of 2007/beginning of 2008, to be organized by Prof. R. Poli and Dr. A.-M. Caminade in Toulouse, France), should take the layout of enlarged meetings corresponding to the first two AQUACHEM workshops as indicated in the Annex. As previously agreed, these should represent small conferences (< 100 participants) in the area of Green Chemistry through Aqueous Organometallic Chemistry and Catalysis and should be extended to both expert scientists and interested young researchers in this emerging area of chemical science.

5. Scientific presentations.

The scientific presentations, attended by 71 active participants (see above), closely, followed the Programme given below. Usually each team leader gave an overall presentation of the research undertaken in his/her laboratory within the AQUACHEM project, and highlighted the topics capable of fostering possible collaborations. The group leader's presentation was followed by others delivered by the recruited ESR/ER AQUACHEM researchers and other researchers of the team.

The scientific presentations were all of high level and attracted a large interest. Remarkably, all the ESR/ER researchers gave a short oral presentation of the work accomplished under the AQUACHEM contract and illustrated the future development of the running projects. The Chairman in charge of the Scientific Sessions stimulated discussions and questions at the end of each scientific presentation, particularly of those presented by the young researchers.

Participants interested in the research subjects of the COST and AQUACHEM projects were invited to give conferences on aspects interesting for the project teams. Two plenary sessions were opened by lectures delivered by Prof. Christian Bruneau from CNRS unit associated to the University of Rennes (France) and Prof. Jose Gimeno from the University of Oviedo (Spain) on relevant topics of organometallic chemistry and catalysis.

5. Adjournment.

Thanks were warmly expressed by all the participants to the meeting organization, for the friendly atmosphere provided by the hosting team of the university of Almeria and for their kind hospitality in Almería. Antonio Romerosa acknowledged the presence and active participation of all the other attendants and expressed his believe that the meeting had contributed to the establishment of closer scientific and friendly ties towards the development of fruitful collaborations. On request of Dr Peruzzini, the host of the meeting was invited to prepare the minute of the meeting.

Program of the meeting

COST D29

SUNDAY DECEMBER 18th, *Vincci Mediterraneo Hotel, Almería, Spain*

Arrival at Almería.

- | | |
|------------------------|---|
| h 15:30 | Registration. <i>Vincci Mediterraneo Hotel</i> |
| h 16:30 | <i>Meeting of the participants and informal discussion</i> |
| h 16:45 | Welcome speech from the Chairman ANTONIO ROMEROSA |
| h 16:55 | Welcome speech by:
Rector (Universidad de Almería).
Jaume Casabó (Presidente del Grupo Especializado de Química Inorgánica. Real Sociedad Española de Química). |
| h 17:20 | Opening remarks by the COST D29 WG009/003 coordinator FERENC JOO |
| |
<i>First scientific session</i> |
| h 17:50 – 19:00 | General discussion of the activity of the Working Group and information concerning the situation of COST Action D29
F. Joó (University of Debrecen, Hungary) |
| h 20:00 | Reception. <i>Vincci Mediterraneo Hotel.</i> |

MONDAY DECEMBER 19th, University of Almería, Spain
COST D29 MEETING & AQUACHEM 2nd YEAR MEETING

Second scientific session

- h 9:00 – 9:50** **José Gimeno.** (University of Oviedo, Spain)
“New ruthenium catalysts in aqueous media: competitive applications in organic synthesis”
- h 9:50 – 10:15** **Antonio Romerosa.** (Team UAL, (AQUACHEM + COST) Almería, Spain)
“New non classical water soluble vinylidene ruthenium complexe: reactivity and catalytic properties”
- h 10:15 – 10:40** **Rinaldo Poli.** (Team LCC CNRSb, (AQUACHEM + COST) Toulouse, France)
“Aqueous reduction chemistry of compound $\text{Cp}^*_2\text{Mo}_2\text{O}_5$: generation and characterization of a mixed oxo-hydroxo triangular cluster with an unusual electronic structure”
- h 10:40 – 11:05** **Alexander M. Kirillov.** (Team IST; AQUACHEM, Lisbona, Portugal)
“New water-soluble multinuclear copper triethanolamine complexes as efficient catalysts for mild peroxidative oxidation of alkanes in aqueous biphasic liquid medium”
- h 11:05 – 11:30** *Coffee break*

Third scientific session

- h 11:30 – 11:55** **Antonio Fernández Barbero.** (Univesidad de Almería, Spain).
“Discontinuous phase transition of thermosensitive microgel particles”

- h 11:55 – 12:20** **Ovadia Lev.** (Team HUJI; AQUACHEM, Jerusalem, Israel).
“Distribution of Polysulfides in aqueous solutions”
- h 12:20 – 12:45** **Ferenc Joó.** (Team UD; (AQUACHEM + COST) Debrecen, Hungary).
“Recent results of the UD team in aqueous organometallic catalysis”

h 13:00 – 15:00 Lunch

Fourth scientific session

- h 15:00 – 15:25** **Chiara Ciardi** (Team UAL, (AQUACHEM + COST) Almería, Spain)
“Synthesis of New Chiral Water soluble Phosphines from Naturally Occurring Amino Acids”
- h 15:25– 15:50** **Abel Moreno.** (Instituto de Químicas, UNAM; México)
"The effects of electric and magnetic fields on the 3D structure of biological systems in aqueous/gel solutions"
- h 15:50 – 16:15** **Luca Gonsalvi.** (Team CNR; (AQUACHEM + COST) Florence, Italy).
“Water soluble Ru and Rh complexes for selective oxidations and hydrogenations”

h 16:15 – 16:45 *Coffee break*

Fifth scientific session

- h 16:45 – 17:10** (a) **Luisa Martins.** (Team IST; AQUACHEM, Lisbona, Portugal).

"Synthesis of new tris(pyrazolyl)methanesulfonate complexes in aqueous medium"

Elisabete C.B.A. Alegria, Luísa M.D.R.S. Martins, Telma F.S. Silva and Armando J.L. Pombeiro.

(b) **Elisabete Alegria.** (Team IST; AQUACHEM, Lisbona, Portugal).

"Peroxidative oxidation of cyclohexane in aqueous medium by rhenium and iron complexes".

Elisabete C.B.A. Alegria, Luísa M.D.R.S. Martins and Armando J.L. Pombeiro.

h 17:10 – 18:00 **POSTERS SESSION.**

h 18:00 – 19:00 **Round table** with flash presentations of the young participants (10 min each) from the different groups and discussion of the scientific results.
Chairman M. Peruzzini

h 20:00 Reception by City Hall at “Baños Árabes” (IX century monument)

TUESDAY DECEMBER 20th, University of Almería, Spain
COST D29 MEETING & AQUACHEM 2nd YEAR MEETING

Sixth scientific session

- h 9:00 – 9:50** **Christian Bruneau.** (University of Rennes. Rennes, France)
“Rhodium and ruthenium precursors For selective catalytic transformations”
- h 9:50 – 10:15** **Maurizio Peruzzini.** (ICCOM CNR, Florence, Italy)
Introductory remarks concerning the AQUACHEM consortium
- h 10:15 – 10:40** **Anne Marie Caminade.** (Team LCC CNRSa ; AQUACHEM, Toulouse, France)
"Organometallic derivatives of phosphorus dendrimers"
A.M. Caminade, R. Laurent, P. Servin, J.P. Majoral
- h 10:40 – 11:05** **Jenny Gun.** (Team HUJI; AQUACHEM, Jerusalem, Israel)
"Analytical and electroanalytical applications of siderophores"
- h 11:05 – 11:30** *Coffee break*

Seventh scientific session

- h 11:30 – 11:55** **Agustí Lledós.** (Team UAB. AQUACHEM, Barcelona, Spain)
"Computational modelling of reaction mechanisms in aqueous media"
- h 11:55 – 12:20** **Zeric Snezana.** (University of Belgrade, Serbia)
“Study of CH/ π interactions in acetylacetonato complexes”
- h 12:20 – 12:45** **Joo Eu Jeon.** (Team UEN, AQUACHEM, Erlangen, Germany)
“Activation of peroxides by heme and non-heme Fe(III) complexes”

h 13:00 – 15:00 Lunch

Eighth scientific session

h 15:00 – 15:25 **a) Mathew Herbert.** (University of Sevilla, Spain)
"Poly(dimethylsiloxane) chains as solubilisers of Cu Complexes in supercritical carbon dioxide"
b) Gabor Papp (Team UD; (AQUACHEM + COST) Debrecen, Hungary)
"New Classical and Non-Classical Hydrides of Ru(II) in Aqueous Solutions"

h 15:25– 15:50 **Armando J. L. Pombeiro.** (Team IST; AQUACHEM, Lisbon, Portugal).
"Chemistry in Aqueous medium at the IST Group: Overall View"

h 15:50 – 16:15 **Natalia Belkova.** (Team INEOS; AQUACHEM, Moscow, Russian).
"Spectroscopic and theoretical studies of the solvent influence on the proton transfer to transition metal hydrides"
E. Shubina, N. Belkova.

h 16:15 – 16:25 *Coffee break*

Ninth scientific session

h 16:45 – 17:20 **Dr. Eric Manoury and Dr. Agnes Labande.** (Team LCC CNRSb, Toulouse, France).
"New ferrocenyl ligands for (asymmetric) catalysis: candidates for catalysis in aqueous media?"

- h 17:20 – 17:40** **Amadeo Rodríguez.** (Universidad de Almería, Almería, Spain).
Responsible of CIESOL (Solar Institute).
“The CIESOL a research centre to find new applications for the sun”
- h 17:40 – 19:00** Visit to CIESOL institute.
- h 21:30** Social Dinner in a typical Andalusia Restaurant

WEDNESDAY DECEMBER 21st, University of Almería, Spain

AQUACHEM MIDTERM REVIEW MEEETING

**Program defined in collaboration with
the EC Scientific Officer in charge of the RTN Network**

- | | |
|-------------------------|--|
| h 9:00 – 9:15 | Dr. Sergio di Virgilio (Scientific Officer, European Commission, Brussels, Belgium)
General introduction |
| h 9:15 – 9:45 | Dr. Maurizio Peruzzini (ICCOM CNR, Florence, Italy)
Activity and perspectives of the AQUACHEM network |
| h 9:45 – 10:00 | Team ICCOM CNR (Florence, Italy). Dr Maurizio Peruzzini
“An overview of the work done in Florence within the AQUACHEM project. Chemistry and catalysis in water”
<i>V. Landaeta, L. Gonsalvi, M. Peruzzini</i>
Presentation of ICCOM CNR team (expertise and activity) |
| h. 10:00 – 10:25 | Team LCC CNRS (Toulouse, France) Mr Paul Servin ,
“Organometallic catalysts in aqueous media. The use of dendritic PTA ligands”
<i>P. Servin, R. Laurent, A.M. Caminade, J.P. Majoral</i> |
| h. 10:25 – 10:30 | Team LCC CNRS (Toulouse, France) Dr Anne Marie Caminade ,
Presentation of LCC/a team (expertise and activity) |
| h 10:30 – 11:00 | <i>Coffee break</i> |
| h. 11:00 – 11:25 | Team LCC CNRS (Toulouse, France) Ms Chiara Dinoi ,
“Reactions of hemimetallocenic molybdenum (VI) complexes with Sulfur Compounds”
<i>C. Dinoi, R. Poli, J.-C. Daran, M. Baya, F. Demirhan, G. Taban</i> |

- h. 11:25 – 11:30** Team **LCC CNRS** (Toulouse, France) Prof **Rinaldo Poli**,
Presentation of LCC/b team (expertise and activity)
- h 11:30 – 11:55** Team **UD** (Debrecen, Hungary) Dr **W. Wojtków**
“Reactions of alkynes in formic acid”
F. Joó, W. Wojtkov
- h. 11:55 – 12:00** Team **UD** (Debrecen, Hungary) Prof **Ferenc Joó**,
Presentation of UD team (expertise and activity)
- h 12:00 – 12:25** Team **HUJI** (Jerusalem, Israel). Dr **Petr Prikhodchenko**,
“EC/ESI-MS studies of transition metal complexes”
P. Prikhodchenko, J. Gun, V. Gutkin
- h. 12:25 – 12:30** Team **HUJI** (Jerusalem, Israel) Prof **Ovadia Lev**,
Presentation of HUJI team (expertise and activity)
- h 12:30 – 12:55** Team **UAB** (Barcelona, Spain). Dr **Andrea Rossin**
“Selectivity of C=O hydrogenation in alpha,beta-unsaturated aldehydes with Ru(I) water-soluble complexes: A computational analysis”
A. Rossin, G. Kovács, G. Ujaque, A. Lledós, F. Joó
- h. 12:55 – 13:00** Team **UAB** (Barcelona, Spain) Prof **Agusti Lledos**,
Presentation of UAB team (expertise and activity)
- h 13:00 – 13:25** Team **YoK** (York, UK) Dr **Nicole Reddig**
“The excited dynamics of molybdate sensors and the structure of the molybdate-rhenium sensor complex”
- h. 13:25 – 13:30** Team **YoK** (York, UK) Prof **Robin Perutz**,
Presentation of YORK team (expertise and activity)
- h 13:30 – 13:55** Team **UEN** (Erlangen, Germany) **Ms. Joo-Eun Jee**.
Comparative Study of the Interaction of NO with Water Soluble Cationic- and Anionic FeIII Porphyrins
Joo-Eun Jee, Maria Wolak, Achim Zahl and Rudi van Eldik

h. 13:55 – 14:00	Team UEN (Erlangen, Germany) Ms. Ariane Brausam , Presentation of UEN team (expertise and activity)
h 14:00 – 15:30	Lunch
h 15:30 – 15:55	Team IST (Lisbon, Portugal) Mr Yahuen Karabach "New 1D and 2D water-soluble Cu(II) polymers derived from pyromellitic acid" <i>E.Yu. Karabach, M.F.C. Guedes da Silva, M. Haukka, A.M. Kirillov, M.N. Kopylovich and A.J.L. Pombeiro</i>
h. 15:55 – 16:00	Team IST (Lisbon, Portugal) Prof. Armando Pombeiro , Presentation of IST team (expertise and activity)
h 16:00 – 16:25	Team UAL (Almeria, Spain). Ms Inocenta Mery Mallqui Ayala "New water soluble allenylidene ruthenium complexes including the Cp(CONC(CH ₃) ₃) ₂ ligand" <i>A. Romerosa, I. M. Mallqui Ayala, M. Serrano-Ruiz</i>
h. 16:25 – 16:30	Team UAL (Almeria, Spain) Prof. Antonio Romerosa , Presentation of UAL team (expertise and activity)
h 16:30 – 16:55	Team INEOS (Moscow, Russia). Dr Natalia Belkova . "Intermolecular Hydrogen Bonding Between Neutral Transition Metal Hydrides (CpM(CO) ₃ H, M = Mo, W) and Bases" N. Belkova, O. Filippov, V. Levina, E. Gutsul, L. Epstein, E. Shubina
h. 16:55 – 17:00	Team INEOS (Moscow, Russia) Prof. Elena Shubina , Presentation of INEOS team (expertise and activity)

h 17:00 – 17:30	<i>Coffee break</i>
h 17:30 – 18:00	Meeting of the EC Officer with Young Scientists of the AQUACHEM network (Restricted participation)
h 18:00 - ...	Conclusions from the EC Officer and the AQUACHEM Coordinator Round table about the perspectives and ideas for future collaborations and future meetings. Closing notes.