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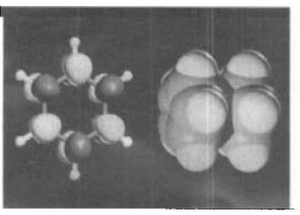

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Presentation of the Research Activities Carried out in the Framework of COST Action D3: *Theory and Modelling of Chemical Systems and Processes*

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Introduction

In this Column, we would like to present the various research projects which are currently carried out in the framework of the COST Action D3 dedicated to computational chemistry under the following title: *Theory and Modelling of Chemical Systems and Processes.*

As summarized by its acronym, COST (Coopération Européenne dans le domaine de la recherche Scientifique et Technique) is a framework for scientific and technical cooperation, allowing the coordination of national research at a European level. COST Actions consist of basic and precompetitive research as well as activities of public utility. There are 25 COST member countries: the fifteen EU member states, Iceland, Norway, Switzerland, the Czech Republic, Slovakia, Hungary, Poland, Turkey, Slovenia and Croatia.

COST cooperation, which was set up in 1971, is based upon a flexible set of arrangements enabling different national organisations, institutes, universities and industries to join forces and make concerted efforts in a broad range of scientific and technical areas. From the beginning, the European institutions (Commission and Council Secretariats) have played a particularly important role in the COST framework.

Since 1989, organisations and institutes from non-COST countries, and especially from other Central and Eastern European countries, may also participate in individual COST Actions, if there is a justified mutual interest.

Four basic principles underlie COST mechanisms:

1. All COST member countries, as well as the European Commission, can propose COST Actions.
2. Participation in these Actions is voluntary and *à la carte* (variable geometry), associating only interested countries.
3. The research to be coordinated is funded nationally. The coordination costs are funded both by the participating countries and by the European Commission.
4. A COST Action aims to coordinate national research at a European level (concerted action). The work undertaken by each Action is administered by a Management Committee.

In contrast to Community research programmes, this form of collaboration does not require an agreed overall research policy. It focuses on specific themes for which there is particular interest in the COST countries.

From an initial 7 Actions in 1971, COST has grown to 115 Actions in 1995, covering the following areas:

- informatics
- telecommunications
- transport
- oceanography
- materials
- environment
- meteorology
- agriculture and biotechnology
- food technology
- social sciences
- medical research
- civil engineering
- chemistry
- forests and forestry products
- fluid dynamics.

Surprisingly, it is only in 1992 that COST decided to launch seven Actions in the field of chemistry. The COST CHEMISTRY activities within these seven Actions correspond to 86 collaborative projects in which 391 European groups (among them, 38 Swiss groups) are involved. As mentioned above, the basic principles and main characteristics of the COST Actions are: the bottom-up approach (the initiative comes from the researcher) and the funding of the research which is national. In Switzerland the main sources of funding for COST CHEMISTRY arise from the Federal Office of Education and Science, and partially from the Swiss National Science Foundation.

The seven existing COST CHEMISTRY Actions are the following ones:

- D1 Coordination Chemistry in the Context of Biological and Environmental Studies.

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- D2 Selective Synthesis.
- D3 Theory and Modelling of Chemical Systems and Processes.
- D4 Design and Preparation of new Molecular Systems with Unconventional Electrical, Optical and Magnetic Properties.
- D5 Chemistry at Surfaces and Interfaces.
- D6 Chemical Processes and Reactions under Extreme or Non-Classical Conditions.
- D7 Molecular Recognition Chemistry.

This Column is concerned with a presentation of *i*) the objective of the D3 Action, *ii*) the research projects which have been formally accepted by the Management Committee of the D3 Actions and *iii*) the conclusions of a brainstorming workshop organized by the D3 Action to discuss the most important issues concerned with European research in theoretical chemistry and modelling.

Objectives of the COST Action D3

The Action aims at encouraging *i*) collaboration between theoreticians and experimentalists, *ii*) suggestions for the development of new experimental techniques and *iii*) enhancement of theoretical contributions in the laboratory (*e.g.* molecular modelling, *etc.*) [1]. Its purpose is also to develop an improved collaboration between theoretical chemists and industry, as well as a more rapid penetration of theoretical methods and concepts into the laboratories. Particular attention is devoted to the promotion of computer network communications, software exchange and network access to large instrumentations among European laboratories.

More specifically, the Action focuses on the following objectives:

- Development of methods and software with emphasis on vector and parallel processing and cost efficiency: use of modern fast low price hardware (*e.g.* workstations). Development of graphics and visualising techniques.
- Development of methods for the study of large molecules (*e.g.* polymers, biopolymes, clusters) and molecular materials.
- Design of pharmaceutical products and of synthetic enzymes for technical catalysis.
- Information on the activation of N_2, CO_2, hydrocarbons, and other inert substances by metal centers and surfaces.
- Information on the reversible transfer of electrons for the purpose of energy accumulation and other applications (molecular energy storage).
- Improvement in the methods of studying highly reactive or short-lived species in gas and liquid phases.
- Model and experimental studies of energetic and entropic control of covalent and noncovalent single and multisite molecular interactions.
- Improvement of methods for treating complex reactions systems (*e.g.* combustion and atmospheric chemistry).
- Improvement in the theoretical approaches and beam experiments for the investigation of state specific processes.
- Improvement in *ab initio* methods to handle electronic correlation in arbitrary electronic states and in efficient calculations of potential-energy surfaces.
- Development of new techniques for the modelling of molecular aggregates (*e.g.* polycyclic aromatic hydrocarbons, *etc.*), coordination compounds and organometallic systems.

Research Projects Currently in Progress in the Context of COST Action D3

Since the beginning of the D3 Action, 14 research projects have been accepted, after a strict refereeing procedure, by the European Management Committee [1] :

1. *Computer Modelling of Coordination Compounds, Organometallic and Inorganic Systems: Structure, Spectroscopy and Reactivity*
   Applicants: *J. Weber* (Geneva), *C. Daul* (Fribourg), *A. Gamba* (Milano), *A. Goursot* (Montpellier), *L. Helm* (Lausanne).
2. *Molecular Modelling to Target Specific Functions: Ground and Ionized States*
   Applicants: *A. Sgamellotti* (Perugia), *C. Floriani* (Lausanne), *L.S. Cederbaum* (Heidelberg), *M.F. Guest* (Daresbury).
3. *Structure, Rearrangements and Fragmentation of Organic Ion-Molecule Complexes*
   Applicants: *T. Bally* (Fribourg), *Z. Herman* (Praha), *P. Carsky* (Praha).
4. *Accurate Calculations of the Reactive Properties of Small Molecules for the Purpose of Modelling Gas-Phase Systems*
   Applicants: *A. Lagana* (Perugia), *A. Aguilar* (Barcelona), *J.M. Alvarino* (Salamanca), *D. Clary* (Cambridge), *G. Lendvay* (Budapest), *C. Leforestier* (Paris), *G.G. Balint Kurti* (Bristol), *R. Schinke* (Göttingen), *J. Linderberg* (Aarhus).
5. *Charge Sensitivity Concepts for Molecular Structure and Chemical Reactivity: Theory Development and Applications to Catalytic and Biological Systems*
   Applicants: *R.F. Nalewajski* (Krakow), *E. Broclawik* (Krakow), *K. Jug* (Hannover), *W. Mortier* (Machelen), *R. Schoonheydt* (Leuven), *P. Geerlings* (Brussel), *S.J. Formosinho* (Coimbra).
6. *Quantum and Stochastic Density Approaches to the Structure and Dynamics of Atoms, Molecules and Crystals*
   Applicants: *J. Maruani* (Paris), *S. Christov* (Sofia), *R. McWeeny* (Pisa), *S. Wilson* (Rutherford), *Y. Smeyers* (Madrid).
7. *Development of New Quantum Chemical Methods and the Accurate Calculation of Molecular Properties of Small- and Medium-sized Molecules*
   Applicants: *H. Lischka* (Wien), *I. Hubac* (Bratislava), *I. Cernusak* (Bratislava), *P. Carsky* (Praha).
8. *Intelligent Software in Computational Chemistry: The OpenMol Project*
   Applicants: *G. Diercksen* (Garching), *N. Drakos* (Leeds), *L. Laaksonen* (Espoo), *W.C. Nieuwpoort* (Groningen), *N.S. Scott* (Belfast), *M. Urban* (Bratislava), *W. Duch* (Torun).
9. *Dynamical Modelling of Stability and Fragmentation in Large Ionic Clusters*
   Applicants: *F.A. Gianturco* (Roma), *P.J. Toennies* (Göttingen), *G. Delgado-Barrio* (Madrid).
10. *Structural and Dynamical Properties of Liquid Crystalline Materials*
    Applicants: *P.L. Nordio* (Padova), *C. Zannoni* (Bologna), *R. Righini* (Firenze), *G. Luckhurst* (Southampton), *R. Richardson* (Bristol), *G. Kothe* (Stuttgart), *Y.K. Levine* (Utrecht), *L.F. Rull* (Sevilla), *F.M. Assis* (Lisboa).

11. *Modelling of Selective Energy Transfer, Spatial and Time Coherence in Catalytic Reactions, Tested on Carbon Dioxide Reactions*
Applicants: *R. Larsson* (Lund), *M. Borowiak* (Warszawa), *M. Jamroz* (Warszawa), *M. Aresta* (Bari), *J. Mascetti* (Bordeaux).
12. *A Novel Approach to Chemical Structures – Quantum Mechanical and Algebraic Treatment*
Applicants: *H. Chojnacki* (Wroclaw), *F. Cramer* (Göttingen), *J. Ladik* (Erlangen-Nürnberg), *J. Rychlewski* (Poznan).
13. *Theoretical Modelling of Bioreceptor-Ligand Systems and Development of New QSAR-Methods*
Applicants: *T. Pakkanen* (Joensuu), *M. Karelson* (Tartu), *W.G. Richards* (Oxford), *F. Gago* (Alcala de Henares), *C. Menziani* (Modena), *O. Tapia* (Uppsala).
14. *Coordinate Systems for Molecular Reaction Dynamics and Large Amplitude Motion*
Applicants: *G.D. Billing* (Copenhagen), *V. Aquilanti* (Perugia), *J. Brickmann* (Darmstadt).

The European Workshop of COST Action D3

To promote new activities in the frame of the COST CHEMISTRY D3 Action and to help the Management Committee in determining future trends in theory and modelling of chemical systems and processes, a European Workshop was held in Como, Villa Olmo, 25–26 March 1994 [2].

The Workshop had a brainstorming nature and was focused on the future of the theoretical approaches to the calculation of the electronic structure of small and large molecules, on the techniques for calculating properties of elementary gas-phase processes, on the computer tools for the design of complex molecules and condensed phase systems, as well as on the emerging innovative computational techniques. In the discussion of these items, the comparison with experimental results was always emphasised. The Workshop has succeeded in bringing together the leading European scientists in the field of theory and modelling on chemical systems and processes and in promoting lively discussions among the participants.

All the participants have emphasised the role that the COST Action D3 has to play in:

- favouring the development of research networks on a true European scale by selectively supporting short and planning visits;
- singling outmost promising and productive research lines by promoting meetings in hot topics and future trends analysis;
- advising national and community research fund administrators in channelling resources.

Specific trends in European research were agreed to be:

- Find synergism between different theoretical methods.
- Understand reaction mechanisms at a microscopic level by developing techniques aimed at determining realistic potential-energy surfaces and performing accurate dynamical calculations.
- Extend the theoretical work from gas phase to include solvent effects, surface phenomena, catalytic actions, condensed phase properties.

Suitable tools for facilitating the evolution along the above mentioned trend lines are:

- Establish robust European teams of researchers to work in the same area in a synergic way.
- Favour young scientists (postdocs) and Ph.D. students exchange to spread new technologies and to increase scientific expertise.
- Protect scientific software and create a parallel market (separate from commercial one) to encourage development, integration and circulation of scientific software among European scientists.
- Organize brainstorming workshops bringing together experts from a given field to promote scientific progress.

The participants unanimously urged the European Community to adopt the recommendations of this Workshop as guidelines of its scientific action in this field.

Conclusions

Undoubtedly, the COST Action D3 has succeeded in setting up networks enabling European computational chemists to collaborate on challenging topics centered on theory and modelling in chemistry. The developments achieved in the framework of this collaboration are impressive and will benefit the entire European scientific community. As the D3 Action terminates in September 1997, it is anticipated that a new Action devoted to computational chemistry will be proposed under the title *Advanced Computational Chemistry of Increasingly Complex Systems*, with the main objective of extending the range of theoretical investigations to a realistic modelling of many-particle phases in which chemistry takes place, such as solute/solvent, liquids, solid materials and biological macromolecules.

The readers interested in the COST Action D3 will have a chance of learning more about its achievements and recent progresses by attending the *First Swiss COST CHEMISTRY Symposium* which will take place on 20th November 1996 at the ILMAC in Basel. During this Symposium, the major activities of the Swiss Groups involved in the seven COST CHEMISTRY Actions will be presented as posters, and prominent European scientists will lecture on important topics addressed by these Actions. This Symposium will therefore provide a unique opportunity to get a valuable information on the developments carried out in the framework of COST CHEMISTRY.

Informations

General informations on COST CHEMISTRY Actions may be obtained from the Chairman of the Swiss COST CHEMISTRY Committee, Prof. *A.E. Merbach*, Institut de Chimie Minérale Analytique, Université de Lausanne, CH–1015 Lausanne-Dorigny, fax +41 21 692 38 75.

More specific questions concerning the COST Action D3 should be addressed to the author of this article.

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[1] Activity Report 1994 of the COST CHEMISTRY Actions D1-D7, Eds. S. Bénéfice-Malouet and B. Reichert, COST CHEMISTRY Secretariat, Brussels.
[2] Report of the European Workshop of the COST CHEMISTRY Action D3 held in Como, 25–26 March 1994, Eds. A. Sgamellotti, J. Brickmann, A. Lagana, T. Pakkanen, S.D. Peyerimhoff, J. Weber, P. Fantucci, and B. Reichert, COST CHEMISTRY Secretariat, Brussels.