## **EDITORIAL**

## The 65th birthday of Professor Santiago Olivella Nello

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Received: 11 February 2009/Accepted: 11 February 2009/Published online: 28 February 2009 © Springer-Verlag 2009



This special issue of Theoretical Chemistry Accounts is dedicated to Professor Santiago Olivella Nello on occasion of his 65th birthday. This event coincides with the 25th anniversary of the Catalonian Network on Theoretical and Computational Chemistry, one of the most important

Dedicated to Professor Santiago Olivella on the occasion of his 65th birthday and published as part of the Olivella Festschrift Issue.

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contributions that Professor Santiago Olivella has given to the progress of science in Catalonia. That Network was created in 1984 by Professors Joan Bertran, Ramon Carbó-Dorca and Santiago Olivella, and represents the general framework in which the theoretical and computational chemistry community of Catalonia has proved to be alive. From the very beginning, the three network founders and others who came later, have encouraged and introduced many young people to the research in theoretical and computational chemistry so that, along these years, this community has grown up to about 200 members of different research groups at the Universitat de Barcelona (UB), Universitat Autònoma de Barcelona (UAB), Universitat de Girona (UdG), Universitat Rovira i Virgili (URV), Universitat Politècnica de Catalunya (UPC), Universitat de Lleida (UdL), Consell Superior d'Investigacions Científiques (CSIC), Parc Científic de Barcelona (PB), Institut Català d'Investigació Química (ICIQ) and Universitat Pompeu Fabra (UPF). This is a story of success, especially if one takes into account the nowadays difficulties in doing fundamental research. Innovation, creativity and new scientific ideas have come from a multidisciplinary environment so that the different research groups have contributed in a relevant manner to the theoretical and computational chemistry with impact in different wide scientific areas as biochemistry, inorganic, organic and physical chemistry; from gas phase to biomolecules and solids.

It is a great pleasure for us to present here Professor Santiago Olivella and to dedicate him this special issue. Santiago Olivella was born on 14 October 1944 in Barcelona. He studied chemistry at the University of Barcelona achieving the degree in chemistry in 1968 and carried out his PhD studies under the supervision and the incitement of Professor Manuel Ballester, defending his



thesis in 1973 with full marks on radicals in organic chemistry. These PhD studies opened him the door to the quantum chemistry world and then he took a first post-doctoral position in the Laboratoire de Chimie Organique Physique du Centre d'Etudes Nucleaires in Grenoble, France, in 1973. A second postdoctoral position was spent in the University of Texas, Austin, from 1974 to 1976, in Dewar's group. It is at this period that he meets with Walter Thiel also a member of Dewar's group and since that time they keep a narrow relationship.

Professor Santiago Olivella has become Full Research Professor of Chemistry at the Barcelona Institute of Advanced Chemistry of the Spanish Research Council (CSIC) in 1988, and has been among the pioneers of the catalan Professors in Quantum Chemistry who have taught and promoted the concepts and tools of Quantum Chemistry in both the theoretical chemistry community and chemists of others areas as organic, inorganic and biochemistry, and his efforts and dedication has helped many young researches to overcome with success.

From 1981 to 2000, he was Invited Professor in the University of Barcelona where he as served as Director of the Research Center on Theoretical Chemistry of University of Barcelona between the years 1998 and 2000. Then he came back to the Spanish Research Council at this year where he leads the Theoretical and Computational Chemistry group, which is a productive group among those involved in the Catalonian Network on Theoretical and Computational Chemistry.

In addition, he has been honored and awarded by the prize medal Narcís Monturiol from Generalitat de Catalunya to scientific and technological merit, in 1999; the XVI Solvay Prize for the Research in Chemistry Sciences, in 2003 and he is also academic of the Reial Acadèmia de Ciències i Arts de Barcelona.

Professor Olivella is the author of many important contributions in the field of Quantum Chemistry, which range from theoretical models to structure and mechanisms of organic chemistry. He has successfully addressed many questions and problems in limitations of Woodward-Hoffman rules, organic photochemistry, reaction mechanisms and atmospheric chemistry. In addition, he has contributed to the development and implementation of the MOPAC code, one of the most widely used packages in computational chemistry. This program package opened the possibility to many young researchers to use this computational tool to treat different chemical problems from the early 1980s.

He has been also very active within the national context, with activities concerning the organization of meetings and congresses for the theoretical chemistry community of Catalonia, some of them focused to young researches.

Last but not less, we would like to stress here his human capabilities, which have been manifested in his availability to help others, his scientific rigor and his dedication, qualities that are recognized by most of the members of our Catalonian Network.

The papers collected in this issue cover many of the several topics of the theoretical and computational chemistry which are the focus of interest of the different groups of the network.

We would also like to specially thank Professor Walter Thiel for accepting to participate in this issue.

Finally, on behalf of all the contributors and the members of the groups represented by them, we want to emphasize here that this special issue is our sincere and modest way to say, with great pride, gratitude and emotion: Congratulations and thank you very much Santiago!

