Dedication

Ramon Carbó-Dorca i Carré

1. The call of quantum

Ramon Carbó-Dorca i Carré was born in Girona in October 1940, on a wet, stormy day. The house of his birth, which still exists today, although much changed, stands on one of the city's most emblematic squares, Independence Square, and on the day of his birth there was serious flooding. He himself has always felt that this singular circumstance was to mark his life. It may have caused him to move towards Physical Chemistry—a cutting-edge discipline—within the avant-garde field of Quantum Chemistry.

He first studied in Girona; yet it can be said that his chemical training was gained at the Institut Quimic de Sarrià (IQS), between 1954 and 1964. It was at this prestigious center that he began his research work under Prof. J. Molina’s supervision. In 1968, he read his doctoral thesis in Chemical Engineering, entitled Estudi teòric de la quimsorció (Theoretical Study of Chemisorption) [1], which presented a model for heterogeneous catalysis. He then left for Alberta (Canada), where he continued his studies in Quantum Chemistry, a science that at least in Spain, was beginning to take off at that time (1960s). He had already worked at the CNRS Centre de Mécanique Ondulatoire Appliquée in Paris. His research concerned development of the foundations of quantum theory and he was interested in excited molecular states. He went on to obtain a degree in Chemical Sciences from the University of Barcelona (1970) and a doctorate in the same field from the Autonomous University of Barcelona (UAB), in 1974. This second PhD thesis was directed by Dr Serafin Fraga, whom he had known in Canada. A further stay in Canada (1977–1978), after a period of work at the University of Pisa’s Quantum Chemistry Laboratory, enabled him to work along with Dr Huzinaga.

2. The fortunate traveller

Ramon Carbó-Dorca has always fondly remembered these stays abroad, in addition to those in Tromsøe (Norway, 1978 and 1980), Minneapolis (USA, 1992), Saskatoon (Canada, 1994), Tokyo (Japan, 1995, 1997 and 2004), Hyderabad (India, 1998–1999) and Brussels (2004–2005). He also has fond memories of all those who worked with him and helped to deepen his knowledge of science. The result of his earlier trips was consolidation, under his leadership, of the Quantum Chemistry Section of the IQS Department of Organic Chemistry, while teaching at the IQS itself (from 1964) and at the UAB Faculty of Medicine. The outcome of his later trips was a scientific legacy which is the pride of our country.

In this later period, he laid the foundations for new approaches to perturbation theory, developed a general theory of the self-consistent field and began studies of structure–activity relationships. In the latter, he succeeded in establishing the vital theoretical foundations and contributed to establishment of the relationships underlying QSAR (Quantitative Structure–Activity Relationships). His first work in the discipline of Molecular Quantum Similarity dates from 1980. In fact, his article How similar is a molecule to another? [2] published in the International Journal of Quantum Chemistry in 1980, established him as one of the founders of modern molecular similarity. This article has been cited more than 300 times.

Since then, Carbó-Dorca has continued to work on mathematical aspects of Quantum Chemistry and has further explored perturbation theory [3] and configuration interaction methods. In recent times, his work has involved attempts to introduce a vector model of time, [4] which he has been considering for quite some time now. Non-stop research activity, as described above; a consistent flow of publications in the most prestigious journals; such high citation rates for all his work; all these factors have placed the name of Ramon Carbó-Dorca among the ‘Highly cited scientists’ on the Essential Science Indicators of the Institute for Scientific Information’s Web of Knowledge. Molecular similarity occupies a central position in much of this work [5]. It is not surprising that a similarity index bears his name [6].

3. Girona revisited

In the meantime, Prof. Carbó-Dorca returned to Girona as a teacher in 1985–1986. There, he completed his theories on the electronic density [7] and on the geometry of molecular similarity [8]. Finally, he joined the University of Girona as a full professor in 1992. Shortly
4. The legacy: research which sees clearly

All this has been possible because Ramon Carbó-Dorca succeeded in imbuing the University of Girona (UdG) with a sense of enthusiasm for promotion of Quantum Chemistry. His great work capacity, persuasive powers and self-confidence, all played an essential role in the establishment within the UdG of the Computational Chemistry Laboratory, which in 1993 became the Institute of Computational Chemistry (IQC). Not only has the IQC brought together scholars in this field, helped to find resources, made contributions to high-quality journals and led to numerous doctoral theses, it has also contributed to the University’s growing reputation and led to visits by many prestigious scientists from abroad, for example, K. Morokuma (USA), G. Frenking (Germany), J. Robles (Mexico), C. Bunge (Mexico), R. Ponec (Czech Republic) and P.G. Mezey (Canada), D.L. Cooper (UK), O. Gropen† (Norway), among others.

† Our friend unfortunately passed away in February 2005.

Ramon Carbó-Dorca was, until 2004, the director and driving force behind the Institute. Under his leadership, the IQC’s research has made it a point of reference in the world of Quantum Chemistry. Of course, the IQC has changed over the course of the years and its researchers have embarked on their own research paths; this only serves to highlight even further the value of the original founding spirit, which sought to establish collaborative work with other groups, at the national and international level and which achieved funding resources for cutting-edge projects in theoretical chemistry and its applications, projects which today lie in the realms of drug design, bioinorganic catalysis and nanoscience.

These areas are part of this great legacy: applications of ab initio and density-functional methods, [12] work on the topology of electronic density of macromolecules, [13] studies of metal–metal bonding, [14] numerous applications of QSAR to molecular properties (such as chirality), [15] to the solvation effect, [16] to biological activity (inhibitor character, toxicity, etc.) [17], accurate approximations to a full CI wave function [18], mathematical treatments [19] and programming [20], fuzzy sets [21], construction of fitted electronic density functions [22], theoretical paradoxes and conjectures [23], N-dimensional spaces [24] and so on. The articles cited merely provide a sample of the enormous productivity of Ramon Carbó-Dorca and the range of those who have worked with him.

References


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