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biography and bibliography

Professor ENRIC CASASSAS (1920 – 2000)*

Enric Casassas i Simó, whose scientific, cultural, and civic activities had earned him great respect in both the scientific and the nonscientific communities, died in Barcelona on February 16, 2000. Through his scientific, cultural and civic activities Prof. Casassas became a recognised authority in Chemistry and a very relevant personality in Catalonia.

The information given below deals with some of the several aspects of his university career, research activities, and civic and humanistic interests. A more detailed biography of Dr Casassas can be obtained from the Biographical Notes written by Prof. Salvador Alegret for the *Miscel·lània Enric Casassas*, co-edited by S. Alegret, J.J. Arias, D. Barceló, J. Casal and G. Rauret (Publicacions de la Universitat Autònoma de Barcelona, Bellaterra, 1991).

University career

Enric Casassas immediately began to work as a university teacher on completion of his undergraduate studies in chemistry at the University of Barcelona (UB). His doctoral dissertation (1962) was done at the Faculty of Sciences of the UB under the direction of Prof. Francisco Buscarons. This work, an examination of the behaviour of some aliphatic mercaptans, with –OH or –COOH groups contiguous to –SH groups, towards inorganic ions and of their analytical applications, was awarded the Martí d'Ardenya Prize by the Institute for Catalan Studies.

Prof. Casassas spent two years (1954-55) at the laboratory of Prof. I. M. Kolthoff, at the University of Minnesota at Minneapolis, USA.

Prof. Casassas worked as assistant university professor at the UB from 1949 until 1967, when he became holder of the Chair of Analytical Chemistry at the University of La Laguna (ULL) in the Canary Islands. Two years later, he acceded to the Chair of Chemistry II (in charge of Inorganic and Analytical Chemistry) at the Higher School of Industrial Engineers of Barcelona at the Polytechnic University of Catalonia (UPC). Upon returning to Barcelona he was put in charge of organising the teaching of Analytical and Inorganic Chemistry at the Autonomous University of Barcelona (UAB), which had just been created (1969). He was also charged by the UAB with organising and initiating the teaching of university level science in Girona. Some years later, this programme became the Faculty of Sciences of the University of Girona.

In 1976, Prof. Casassas occupied the Chair of Analytical Chemistry of the Faculty of Chemistry of the UB, a position he continued to hold until his compulsory retirement in 1987. He then became Professor Emeritus of the UB, a position whose tasks he performed very actively until only a few months before his death.

Prof. Casassas' proven capacity in his field and his personal qualifications as an outgoing organiser made him an obvious choice for many different tasks of academic responsibility. He served as Head of Department, Vice-Chancellor for

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Research at the UAB (1976), Vice-Chancellor for Academic Affairs at the UB (1978 – 82), and as a member of the Academic Committee of the UB (1986-1987). In 1999, he was elected Protector of the University Community at the UAB .

Prof. Casassas was a great communicator of ideas and of his passion for science and knowledge. His brilliant, open and young mind charmed students, co-workers and colleagues throughout his academic career.

Civic and humanistic interests

The parents of Enric Casassas were both schoolteachers who were trained in the new pedagogical tendencies promoted in Catalonia at that time. He attended the Institut-Escola, a pedagogical institution promoted by the Autonomous Government of Catalonia (the Generalitat) for the renovation of secondary education. Unfortunately, he finished secondary school (1937) in the middle of the Spanish Civil War and was called up for service in the armed forces. At the end of the war, he was obliged to do further military service by the Francoist dictatorship and suffered a serious illness. Following this, he attended the Industrial School of Terrassa, where he studied Mechanical Industrial Technology (1943) and Chemical Industrial Technology (1944). Finally, he studied at the University of Barcelona, an institution which had been devastated by the Civil War, with most of its original professors having either gone into exile or been dismissed.

Prof. Casassas' childhood environment and the environment he encountered in his early schooling were based on social responsibility and the predominance of culture and justice. It was, thus, totally opposed to the sordid post-war military regime. In opposition to the situation, Prof. Casassas actively participated in the first student resistance organisations and in many scientific, cultural and civic resistance activities.

In 1959, he participated in the recuperation of the Catalan Society of Physics, Chemistry and Mathematics, being elected president of the Chemistry Section (1959-72) and later of the Society (1973-76).

With the transition to democracy, his activities became more official and took on even greater relevance than before. In 1977, he was named full member of the Institute for Catalan Studies (IEC). He was later the organisation's president (1982-86). He was also president of the Science & Technology Council of the Research & Technology Commission of the Catalan Government from 1981 until its dissolution. In 1989, the Generalitat of Catalonia awarded Enric Casassas the Narcís Monturiol Medal for his services to Catalonia in the field of scientific and technological progress, and in 1992 he received the Premi d'Honor Jaume I.

Research Activities

Solution chemistry

A significant part of Prof. Casassas' research work was devoted to the field of solution chemistry. His work in this area began during his PhD research at the University of Barcelona, where he investigated the formation of metal complexes in solution, especially with ligands having S-donor atom groups (i.e. mercaptoethanols and mercaptoacids). Already in these preliminary studies, he paid special attention to the accurate determination of equilibrium stability constants, considering both experimental and numerical aspects and using either potentiometric or voltammetric methods. It should be remembered here that he was using the numerical tools available at that time, the first primitive calculators and electronic computers. This research subject was of considerable and increasing interest from the 1960s to the 1980s, when many accurate stability constant determinations were compiled for common inorganic and organic ligands. In particular, Casassas paid special attention to the implementation of the solution chemistry research methods developed by the Scandinavian school of solution equilibria headed by Lars Gunnar Sillen from the Royal Institute of Technology of Stockholm, the main exponent of this school of thought. Several research co-workers of Professor Casassas were also engaged in this same type of research work at this Institute during these years.

While developing new voltammetric methods in the study of mercaptoethanols and mercaptoacid ligands, Prof. Casassas also focussed his attention on the study of mixed ligand complex formation using potentiometric and spectroscopic techniques. He studied the metal complexation properties of different ligands derived from aromatic o-hydroxycarboxylic acids (like salycylic, hydroxynaftoic and pamoic acids), nitrogen bases and aminoalcohols. These investigations were performed either in water media or in hydro-organic solvent mixtures. They led to the implementation of experimental methodologies for the establishment of the nature of the reactions and equilibria involved in these systems and hence for their chemical speciation. These metal complexation studies were later extended (see below, the list of references from approximately 1992) to the study of metal complexation with ligands of biological and environmental interest, including macromolecular ligands like humic and fulvic acids as well as nucleic acids and polynucleotides. The interest here was in the study of the solution chemistry of these complex macromolecular ligands. This includes their acid-base and metal complexation equilibria, their polyelectrolyte properties, and also their conformational equilibria. Work on these macromolecular ligands still comprises a subject of great research interest in biochemical and environmental analytical chemistry fields.

Chemometrics

Initial equilibrium and solution chemistry studies using data treatment methods based on univariate least squares curve-fitting methods were extended afterwards to multivariate spectral data treatment methods. These new methods involved the development and implementation of new algorithms and computer programs. In a few years, these new computational methods were first implemented for large mainframe computers and downsized afterwards to person-

al computers (PC). It is important to emphasise here the interest and effort of Prof. Casassas for the promotion and consolidation of chemometrics as an emerging field, closely related to the explosive incorporation and implementation of computer technologies in the laboratories and instrumentation. Chemometrics is defined as the scientific discipline that seeks the extraction of maximum valuable chemical information from experimental measurements using mathematical, statistical and computational means. Chemometrics can thus be considered a fundamental part of analytical chemistry, sharing its goals but focussing on mathematical, statistical and computational tools. In this sense, and especially during his last years, Prof. Casassas was a strong promoter of chemometrics in our universities. Since 1987, together with Prof. Forina of the University of Genova and Prof. Massart of the University of Brussels, he promoted the introduction of chemometrics in the Southern European Mediterranean countries. He led several international chemometrics conferences and schools, supported by the European Union. Significantly, his latest scientific publication had for title *Soft modelling of Analytical Data* (published by the Encyclopedia of Analytical Chemistry, John Wiley & Sons, 2000, Vol 11, 9800-9837). In this publication, emerging tools to analyse analytical data using multivariate data were reviewed and proposed as complementary tools for the investigation of chemical systems where physicochemical models are difficult or impossible to apply due to their complexity. Prof. Casassas was always a strong defender of the newest strategies and tendencies, but at the same time he was also a strong supporter of well-founded traditional approaches, trying to conserve and keep their positive aspects. In this sense, it is clear that the chemical knowledge provided by classical hard modelling methods, based on the postulation of physico-chemical models, is richer than the chemical knowledge provided by soft modelling methods. However, soft modelling methods are more flexible and do not require the experimental and highly demanding theoretical conditions associated with hard modelling assumptions. Soft modelling methods instead are more flexible and may be used directly to provide analytical information and more easily solve real life industrial and natural problems. Soft modelling methods can be used when hard modelling methods fail or as an independent validation tool to test hard modelling results. New approaches, mixing both soft and hard modelling strategies, have been shown to be optimal in the solution of many problems. Different research groups, including the research group of Solution Chemistry and Chemometrics at the University of Barcelona, the team that Prof. Casassas was leading, are developing such strategies at present.

Electroanalytical Chemistry

Since his stay at the laboratory of Prof. I. M. Kolthoff, at the University of Minnesota at Minneapolis, in the period 1954-55, Prof. Casassas further explored his initial interest for analytical chemistry in subjects more closely related to physical chemistry, in general, and electrochemistry, in particular. As mentioned above, a significant part of his research work was devoted to the study, by potentiometric, polarographic and voltammetric means, of the behaviour of many organic compounds, especially those with azo– and divalent sulphur–groups, and their metal complexes.

Prof. Casassas had a great interest not only in experimental electroanalytical studies but also in the development of voltammetric methods based on the postulation of physicochemical models and their further validation by experimental means.

In the first PhD thesis supervised by Casassas, he and Lluís Eek developed an original method for the polarographic determination of stability constants of metal complexes based on the ligand signal instead of the commonly used metal ion reduction signal (see *J. Chim. Phys.* 64, 1967, 971-977). This method has now been extensively described in specialised works (D.R. Crow, *Polarography of metal complexes*, Academic Press, London, 1969, pp. 80-84) and textbooks (J.A. Plambeck, *Electroanalytical Chemistry. Basic principles and Applications*, Wiley-Interscience, New York, 1982, p. 305). Some years later, in a miscellaneous collection of contributions in homage to the poet Gabriel Ferrater (see *Una lleu sorra* [37]), Casassas outlined the possibility of using the anodic oxidation signal of mercury (from the electrode) for the polarographic determination of stability constants of metal complexes other than mercury. This idea was then recovered and developed in detail, and an original method was described (*J. Electroanal. Chem. Interfacial. Electrochem,* 194, 1985, 11-25). The method is based on the use of the potential shifts of the anodic oxidation signal of the mercury (from the electrode). It was satisfactorily applied to sulphur-containing compounds, and this method has also been widely referenced in the literature. At that time, and in parallel to the above-mentioned item, the behaviour of anodic oxidation of mercury in the presence of many sulphur-containing compounds was exhaustively studied, by a variety of electrochemical techniques, in the lab of Prof. Casassas.

Prof. Casassas also attempt to understand and quantify the role played by ligand electrode adsorption on the determination of metal stability constants by polarographic means, a matter much discussed in the 1970s and 1980s. A variety of halide and pseudohalide metal complexes was systematically studied (*J. Electroanal. Chem. Interfacial. Electrochem, 2*13, 1986, 235 – 244), and these investigations led to wide further discussion in the literature.

At the final stage of his academic career, as professor emeritus, he was actively involved in the voltammetric study of the interactions between metal ions and macromolecular polyelectrolytic ligands, of either environmental or biological interest, such as polysaccharides, humics and polycarboxylic acids. This is one of the subjects orienting the discussions of the research group of Electroanalytical Chemistry at the University of Barcelona founded by Prof. Casassas.

In this regard, it is worth remarking on the series of papers devoted to the development of a theoretical model for metal complex systems involving both species with very different

diffusion coefficients and adsorption phenomena because of the self-adsorption of the ligand and the induced adsorption of the metal. The theoretical model was developed for pulse polarography, checked by numerical simulation and experimentally tested with several metal-polycarboxylate systems. This model has been collected in recent reviews on Electroanalytical Chemistry in the literature. The research activity is one which was carried out in intimate collaboration with research groups of the Department of Physical Chemistry at the University of Barcelona and of the Department of Chemistry at the University of Lleida (ULL).

The aforementioned interest of Prof. Casassas on chemometrics is also reflected in his participation in a pioneering paper describing the use of several chemometric techniques to voltammetric data from metal-ligand equilibria systems (*J. Electroanal. Chem.* 393, 1995, 7 – 16).

Among the findings of Prof. Casassas we can also mention several new applications of voltammetric techniques to the determination of trace components in environmental samples and of compounds of pharmacological interest.

Other scientific activities

As a result of his research activity, Prof. Casassas kept up international relationships with different scientists and research groups all over the world. Already in the 1990s, Prof. Casassas was a strong supporter of cooperation between different research Institutes of the Russia Academy of Sciences and the Institut for Catalan Studies (IEC) (the national academy in Catalonia). He led fruitful cooperation projects between different scientists and research groups of Russia. Some of these cooperation projects were in the frame of international association research cooperation programs funded by the European Union (like the INTAS program).

Professor Casassas also excelled as a university professor. In the field of analytical chemistry, he promoted the curriculum reform of this discipline, arguing for a more rigorous and scientific treatment of the subject and specially emphasising the grounds of chemical methods of analysis, pushing for a deeper knowledge of solution chemistry and analytical applications of solution chemistry. At the same time, he urged the introduction and potentiation of modern instrumental methods of analysis, especially those based in electrochemistry and those related to environmental analysis. As we have already mentioned, he promoted the introduction of chemometrics at both undergraduate and postgraduate levels. This is now recognised and accepted as a normal thing in our analytical chemistry curricula. Indeed, it would be difficult to have achieved this without his significant contributions. Prof. Casassas supervised 26 doctoral dissertations (17 at the UB, 5 at the UAB, 2 at the UPC and 2 at the ULL).

In summary, we would like to point up two main features of the scientific personality of Prof. Casassas. First, we would like to mention his personality as an integral scientist. In our times, when scientists are becoming progressively restricted to their own narrow scientific specialities, Enric Casassas exercised a widespread scientific knowledge. He was always ready for a problem-solving approach and open to consultation on doubts, not only in his scientific speciality but also in many others. His extraordinary, profound, scientific knowledge went beyond chemistry into other fields, including the humanities and the arts. Second, we should underscore his great intelligence and his capacity to express scientific concepts in a clear, precise, and objective way. He had an enviable demanding attitude for describing and writing scientific concepts without ambiguities. This has been widely recognised by everybody who worked with him. His accurate opinions and corrections helped many of us in our research training and career development. In this sense, we want to express our admiration for his restless working capacity and his indefatigable efforts to improve our research work as well as his own. Finally, we simply wish to express our deep admiration for the strong personality of Prof. Casassas. He greatly influenced our generation, and his critical compromise and lucid opinions on old and new problems, like his dedication to science and to the university, as well as to his own country and society, have left their indelible mark and set very high standards.

Research papers

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