

Dedication

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This special issue of Theoretical Chemistry Accounts is dedicated by the scientific community to the memory of the late Professor Serafín Fraga.

Serafín Fraga was born in Madrid (Spain) in 1931. After getting a Ph.D. from the Universidad de Madrid, he joined the Department of Physics at the University of Chicago where he collaborated with Professor Robert S. Mulliken as a Research Associate (1958–1961). He was very proud of his stay at Mulliken's Laboratory of Molecular Structure and Spectra where fundamental contributions to Chemistry and Physics were being developed at that time. Whilst he was there he met, amongst others, Enrico Clementi, Sigeru Huzinaga, Gulzari Malli, Paul Bagus and Roberto Moccia, who have all contributed to the present special issue.

After a short stay in the Département de Physique at the Collège Militaire Royal, St. Jean, he joined the Department of Chemistry of the University of Alberta where he became a Professor in 1969 and Professor Emeritus in 1994.

Professor Fraga always remained in close contact with scientific developments in his home country, Spain. Apart from hosting a long list of visitors, he also welcomed a number of Spanish postdoctoral fellows who worked in his laboratory at the University of Alberta. These include Carmela Valdemoro (CSIC, Madrid), Ramón Carbó (Universitat de Girona), José Ángel Sordo (Universidad de Oviedo), Mercedes Campillo (Universitat Autònoma de Barcelona), and Emilio San Fabián (Universidad de Alicante), all currently professors at Spanish universities. After his retirement in 1994, he spent a lot of time at the Universidad Autònoma de Madrid, collaborating with Professors Jaime Fernández Rico and José Manuel García de la Vega.

Serafín Fraga was honoured with the degree of Doctor Honoris Causa by Universitat Autònoma de Barcelona (1984) and Universidad Autònoma de Madrid (2006). He contributed more than 130 articles and nine books in a number of fields, ranging from Atomic Structure to Protein Structure. Special mention should be made of his series of papers in *Theoretica Chimica Acta* during 1964–1974 on the calculation of atomic properties, as well as his celebrated *Handbook of Atomic Data* (Elsevier, Amsterdam, 1976), co-authored with Dr. K. M. S. Saxena and Professor Jacek Karwowski. This book was considered the 'bible' for atomic physicists and theoretical chemists for more than a decade and is on the shelves of most scientific libraries around the world.

Serafín married Ester who had been carrying out research in Biochemistry at the University of Alberta, and they have three sons, Eric, Erwin, and Werner. Ester and Serafín co-authored a number of papers and books on Quantum Biochemistry. Eric also collaborated with his father in the resolution of the Schrödinger–Riccati equation.

Serafín Fraga passed away suddenly in Edmonton on May 4th 2006, at the age of 75, soon after his return from Madrid where he had been working since January and had received the title of Doctor Honoris Causa.

The guest editors are very grateful to all the contributors in this issue. Their effort in preparing materials of great interest and high scientific value is, to be sure, the best homage Professor Fraga would ever have wished. We also are indebted to the referees whose suggestions and comments have contributed to enriching the submitted manuscripts.

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