

Homage

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With great sorrow and pain I accept the fact that Professor Serafin Fraga is no more with us.

In the autumn of 1958 when I joined Mulliken's group in the Laboratory of Molecular Structure and Spectra (LMSS), University of Chicago, Fraga was already working with Mulliken, Roothaan and Ransil. Activities of the group are aptly described in THEO CHEM 537 (2001) by Garcia de la Vega, Sordo and Csizmadia. A bunch of people, including Bagus, Clementi, Fraga, Kolos, Mclean, Moccia, Ransil, Wahl, Weiss and Yoshimine, were flying back and forth between Chicago and Dayton, Ohio. They were frantically using the UNIVAC computers installed inside the Wright-Patterson Air Force Base in Dayton. The computational facility occupied a large separate building. The time was only 13 years after the end of the War. Still officially classified as an enemy alien (Japanese), I was treated differently from other members of the group at the gate of the American Air Force base. I was escorted by a Military Police jeep to the building where the UNIVAC facility was housed and at lunchtime I was not allowed to leave the building to go to a cafeteria situated in a different building. Very often I skipped eating proper lunch meal and kept working during lunch break, because I was a slow worker and I had a lot of work to do. Probably because of the stress, I developed symptoms of stomach ulcer. I remember with deepest gratitude the kindly concerns shown to me by Fraga and Clementi. Fraga's genuine concern of others' welfare was a clear signature of his warm personality. Friendship between us started early.

Those were feverish and hectic days. Roothaan was certainly a driving force of the molecular computation project but everyone in the bunch, sometimes called the Chicago

Gang, was driven by one's own passion to open a new chapter of the computational chemistry. As the published papers show, Fraga was among the first to report an early heavy crop by the Chicago Gang. The entire harvest reaped by UNIVAC was vast and extensive, including Kolos' historic work on the hydrogen molecule. The totality of their achievement was truly amazing if one ponders the fact that computers available to them were incomparably inferior to today's personal computers any school kid can lay his/her hands on, both in terms of speed and in terms of memory.

In Chicago, Fraga's small apartment was a hub of evening gatherings of the bunch, hosted by young Mrs. Fraga, Ester. The place was filled with laughter and spirited debates. The atmosphere was always merry and buoyant.

I worked there as a research associate for two years and went back to Japan. Soon after, Fraga moved to Canada. In 1968 he invited me to join him in the Department of Chemistry, University of Alberta. Fraga and Birss were successfully starting up a new quantum chemistry group in Western Canada with privileged access to the excellent University computing facility and I was more than happy to seize the opportunity given to me by Fraga. As would be seen from his fecund publication listing for the period from 1963 through 1967, his papers on the Self-Consistent-Field theory gave me strong stimuli to develop my own formulation of the open-shell SCF theory. About the same time Fraga was performing extensive numerical Hartree-Fock calculation of atomic data, including various relativity-related quantities. The result was his celebrated Handbook of Atomic Data (Elsevier, 1976) co-authored with Karwowski and Saxena, well known and utilized all over the world.

His adoption of the numerical Hartree-Fock approach and his emphasis on relativistic effects in the electronic structure of atoms (and therefore also of molecules), these two clearly attest Fraga's far-sightedness at that time. In fact, Roothaan

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himself later recognized the merit of the numerical Hartree-Fock approach, vis-à-vis his finite expansion method, and developed his own computer program. As for the relativity, Fraga's Handbook contains a thought-provoking figure that graphically demonstrates that the relativistic energy correction far exceeds the electron correlation energy already at atoms as light as P and S. Since then, relevance of the relativistic effects in chemistry has been increasingly recognized. To mention just one example, chemists now realize that the relativistic effect plays a vital role in the catalytic power of various metal surfaces. In this regard, I fancy that the excellent works on the relativistic molecular calculation done by Seijo and Barandiarán might have received a cue from Fraga's work: they are among Fraga's former collaborators.

Fraga was never trapped by the lure of the so-called *ab initio* molecular calculation, adherence to that may have been detrimental to healthy development of computational methods for chemically interesting molecular systems. Fraga later expanded his computational activity into the field of molecular mechanics. It is to be noted, however, that his real interest was not in the invention of a novel method *per se*. Instead, his work was motivated by his wide-ranged interest in and keen insight into quantum biology, immunology and molecular modeling. His influence in this field was wide, as evidenced by an invitation from a governmental Industrial

Research Institute in Osaka, Japan, asking him to stay for a year as a visiting scientist in 1991.

Fraga had a life-long obsession. (Or, should I say, a life-long hobby?) It is the Quantum Mechanics in its intriguing form of the Schrödinger Equation. Discovery of the Quantum Mechanics could arguably be the most fantastic event in the entire history of physics. The numerical accuracy, whenever it has been tested, is truly astounding. It has now been elevated to the order of 1 part in 10^{19} ! Fraga wanted to dig into the Schrödinger Equation in his idiosyncratic way. I am gratified to learn that, toward the end of his scientific career, he published a substantial number of papers on the subject with his close collaborators, J. M. Garcia de la Vega and E. S. Fraga. The last three papers were published as recently as in 2005.

About a little more than a decade ago, one day I stumbled across a lithograph showing an old man walking with a pair of canes. Goya made the lithograph when he reached his eighty and it is entitled 'Aún aprendo,' meaning 'I still learn.' I liked the dictum of Goya and reported my finding to Fraga. Naturally he knew the dictum as a Spaniard. 'Aún aprendo.' He lived the dictum of Goya to the letter as an indomitable great mind himself.

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