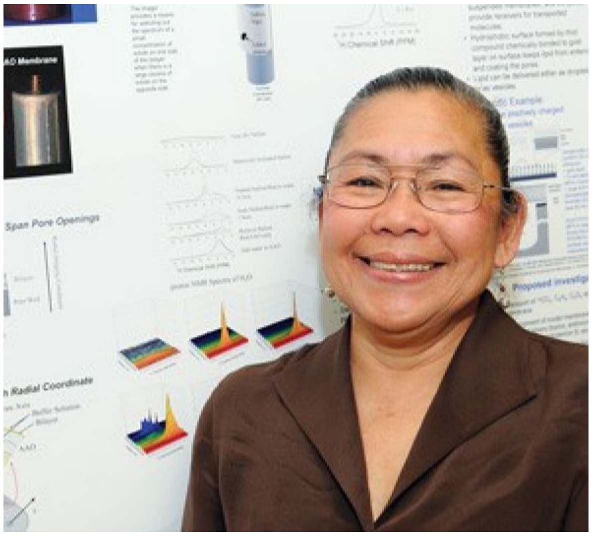


To Find CJ, Make Way for CJ

by Angel C. de Dios*

"Make Way for CJ", was a sign I remembered seeing posted on one of the faculty offices at the University of Illinois at Chicago when I was looking for Professor Cynthia Juan Jameson.

You may just find Cynthia J. Jameson or "CJ" as her students would fondly call her, working tirelessly as the prime mover of a postdoctoral institute under the Women in Science and Engineering System Transformation Program of the University of Illinois at Chicago. Or you may see her in front of a workstation writing a code that would predict spectra for ^{129}Xe in fluids, paving the way to a greater understanding of ion and molecular transport across membranes. Or you may simply find yourself admiring her garden which never fails to attract monarch butterflies every summer. Or she may just be washing dishes after serving a delicious home-cooked Filipino dish to her grandchildren. Whether you meet her in the laboratory, or at home, you will not miss the excellence, you will never overlook the fact that she always gives her very best in every effort.

CJ graduated "cum laude" at the University of the Philippines, Diliman in 1958. She loved both math and physics as an undergraduate student and her interest in math and the sciences led her to a career in science. She pursued graduate studies as a Fulbright-Hays scholar at the University of Illinois at Urbana-Champaign and received her PhD in chemistry under the direction of Herbert S. Gutowsky. She started as an assistant professor of chemistry at the University of Illinois at Chicago in 1968, at a time when female scientists were not even interviewed for faculty positions. She spent thirty eight years on the faculty and is now a professor emerita, yet still very active, of chemistry and chemical engineering.

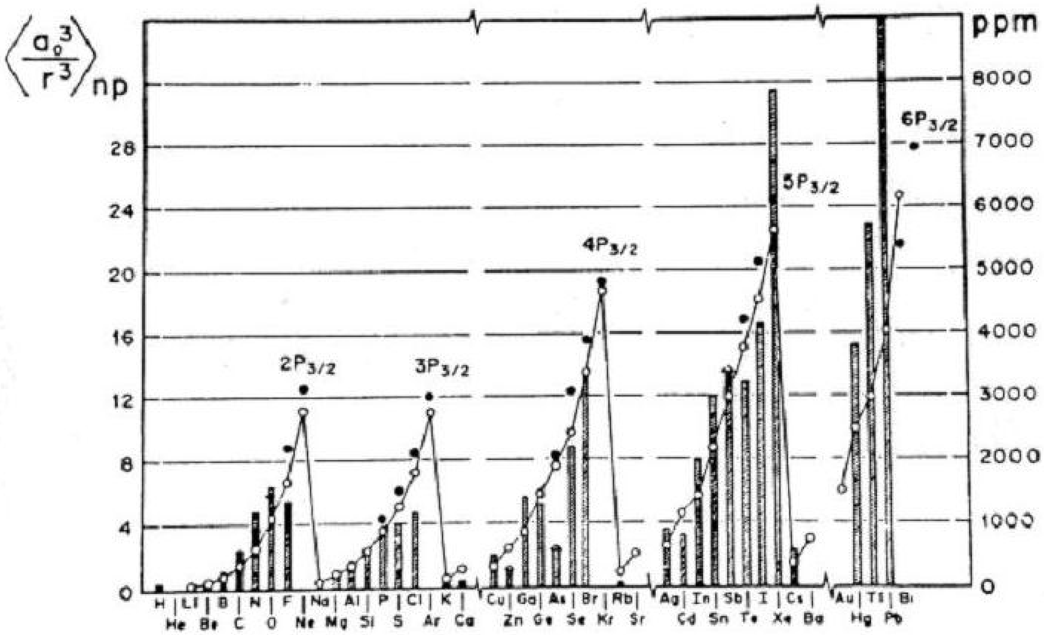
Bold Predictions

At a time when nuclear magnetic resonance (NMR) spectroscopy was still very much at its infant stage, CJ chose to predict what still remained to be seen through NMR spectroscopy. Her papers with Gutowsky; "Calculation of chemical shifts I. General formulation and the Z dependence" [1] and "Systematic trends in the coupling constants of directly bonded nuclei" [2], illustrate her visionary understanding of quantum mechanics and the emerging field of NMR spectroscopy. At a very early stage, CJ was able to map the periodic trend of NMR chemical shifts and indirect coupling constants based on first principles and the limited data that were available at that time.

Her far-seeing perspective on NMR spectroscopy continued during her tenure in Chicago. She wrote a paper on how she envisioned the NMR chemical shift to vary with internuclear separation [3]. In this general picture, she suggested that the NMR chemical shift started with the value that corresponded to the united atom, increased to a maximum at some intermediate distance, and then finally decreased to the value of the infinitely separated atoms. This prediction was later verified by *ab initio* calculations. In these seminal papers, CJ's understanding of

* Department of Chemistry, Georgetown University
Washington, DC 20057

Top figure: Cynthia J. Jameson, standing in front of her research poster on ^{129}Xe NMR and transport studies.



Periodic Table Trend of NMR Chemical Shifts. Downloaded from the web 30 May 2011. http://www.stemwomen.org/topics/PT.html

how much structural and electronic information is present in NMR parameters was very much evident. Her recent work involved the prediction of ^{129}Xe NMR line shapes of xenon gas in nanochannels [4]. In this area, she was again correct and a step ahead of the empirical observations. Her work demonstrated a significant courageous and heroic effort to bring the theoretical understanding of these parameters to a level comparable to the precision and vastness of NMR data.

Gas Phase NMR Spectroscopy

To understand the NMR parameters in great detail, CJ focused on NMR spectroscopy in the gas phase [5]. Her laboratory is one of only two research groups in the world that primarily worked on NMR in the gas phase. In the vapor phase, in partnership with her husband, A. Keith Jameson, who was a professor at nearby Loyola University, NMR data were obtained for various nuclei at varying pressures and temperatures. CJ also explored the changes in the NMR chemical shift observed upon isotopic substitution. These data enabled the extraction of both intra- and intermolecular effects on NMR parameters. The intramolecular effects originated from rovibrational averaging and were observed in the temperature dependence of the NMR spectra of the isolated molecule while the intermolecular effects manifested in the density dependence of the NMR spectra of the gas samples. Removing the intermolecular effects from the measured chemical shifts allowed for the establishment of shielding scales that corresponded to shifts of nuclei in isolated molecules. On the other hand, the temperature-dependent shifts in isolated molecules provided a glimpse on how the chemical shift was averaged over the internal motions, vibrational and rotational, of the molecules. Based on this large volume of work, several useful general trends had been discovered. It became clear, for example, how the NMR chemical shift would change with a lengthening bond distance. In addition, measurement of relaxation times in the gas phase afforded an avenue to extract effective collision cross sections, which were then utilized to gauge intermolecular potential surfaces [6]. These NMR experiments were remarkable examples of basic research that deepened our understanding of both theoretical and physical aspects of NMR and how these related to what molecules were doing.

It was in the area of small molecules in the gas phase that a strong link between the theory and experiment of NMR chemical shifts was firmly established. CJ's fundamental research in gas phase NMR spectroscopy made it feasible to apply NMR spectroscopy to more complicated systems and processes such as adsorption, diffusion, and ion and molecular transport. The gas phase NMR studies served as a strong foundation for correctly interpreting NMR chemical shifts in terms of changes in structure and environment.

True Legacy

CJ contributed significantly to the understanding of NMR parameters. Her accomplishments demonstrate a lifelong endeavor to unravel the unknown while facing life's odds and challenges. And frequently, her efforts were made in a largely uncharted territory. At one point, she established a collaboration with a scientist in East Germany with the wall still standing tall and strong. She was a visiting scientist at Oxford, Cambridge and Berkeley. In addition, CJ had served the community as a program officer at the National Science Foundation and as a member of the Grants Selection Committee of the National Science and Engineering Council of Canada. She had been a fellow of the American Association for the Advancement of Science since 1988. She was recognized as Woman of the Year in 2008 by the University of Illinois at Chicago. And most recently, she was awarded the Camille and Henry Dreyfus Senior Scientist Mentor Award. Her work has touched a vast array of areas of research in physical chemistry. She has authored and co-authored more than 200 research articles and book chapters. Indeed, the field concerning the theoretical and physical aspects of the NMR chemical shift has been transformed by her over the past forty years.

Yet, her true legacy lies in the lives of the people she has touched. CJ's own discipline and determination is a remarkable model that students could easily recognize. Her genuine interest in the material is so tangible that it effortlessly inspires students. This interest translates into a dedication that clearly sends the following very important message to the student: What the student is doing is significant. Her love for science is highly infectious. This encouragement is crucial since it is one driving force that can make students fully realize their potential as a researcher. My experience of having CJ as a mentor made me achieve things I could never have imagined to be within my reach. She worked very hard and that made me work very hard as well. She showed me how to find fulfillment in research and I learned how to treasure the endeavor as well. She expected no less than my capacity, but she provided the support that I needed.

CJ regularly meets with her students. She monitors the student's progress diligently and provides the necessary tools, background information, and guidance without spoon feeding her students. She encourages participation of everyone and never fails to acknowledge a student's contribution to the work. She promotes teamwork and cooperation as well as healthy debates and discussions. She clearly ensures that everyone understands what is going on and never compartmentalizes the research endeavors so that each member of the group knows the overall picture of the research. She brings her students to meet other scientists either in meetings, presentations or seminars. She purposely sits back and provides her students an opportunity to describe their research in these face-to-face and one-on-one meetings. Although she promptly guides a student who may need an additional push, she is very quick in praising a student when it is deserved. Co-authorship in peer-reviewed journals is a hard-earned award in her group. Co-authorship means a student has indeed provided a significant contribution to the paper, from start to finish. The fact that in spite of this stringent requirement, CJ has managed to share authorship with students is a clear demonstration of how tremendously successful she is in mentoring students.

You might find her preparing female scientists for a job search and interview. Or she might just be in the Philippines, like in 2008 when she singlehandedly prepared and delivered an intensive course in Quantum Chemistry and Molecular Spectroscopy which was urgently needed by 38 university instructors who would teach undergraduate physical chemistry courses. And her legacy will remain in the lives of the students whose hearts she has touched and inspired. In CJ's laboratory, NMR chemical shifts were first completely understood in small molecules in the gas phase. Later, NMR chemical shifts in proteins would likewise be understood [7].

[1] C. J. Jameson and H. S. Gutowsky, J. Chem. Phys. 40, 1714-1724 (1964).
[2] C. J. Jameson and H. S. Gutowsky, J. Chem. Phys. 51, 2790-2803 (1969).
[3] C. J. Jameson, J. Chem. Phys. 63, 5296-5301 (1975).
[4] C. J. Jameson, J. Chem. Phys. 116, 8912-8929 (2002).
[5] C. J. Jameson, Chem. Rev., 91, 1375-1395 (1991).
[6] C. J. Jameson, Encyclopedia of Nuclear Magnetic Resonance, Vol. 4, pp. 2179-2189 (1996) D. M. Grant and R. K. Harris, eds. John Wiley, London.
[7] A.C. de Dios, J.G. Pearson, and E. Oldfield, Science, 260, 1491-1496 (1993).