

UNIVERSITY OF SOUTH FLORIDA

CURRICUMUM VITAE

—January 23, 2006—

Milton D. Johnston, Jr.
Professor
Department of Chemistry
University of South Florida
Tampa, FL 33620-5250

EQUAL EMPLOYMENT OPPORTUNITY INFORMATION:

Name: Milton D. Johnston, Jr.

Sex: Male

Race: White

Date of Birth: Nov. 4, 1943

MISCELLANEOUS INFORMATION:

Prof. Milton D. Johnston, Jr.

xxx-xx-xxxx

Home Address: 12204 N. 53rd Street, Tampa, FL 33617-1448

Campus Address: Dept. of Chemistry (CHE 205)
University of South Florida
Tampa, FL 33620-5250

Office Location/Phone: SCA 408 (974-2535)

I. GENERAL INFORMATION

Personal Data:

Milton Dwynell Johnston, Jr.

SSN: xxx-xx-xxxx

Present Rank: Professor (1994)

Tenured (1978)

Department of Chemistry/College of Arts & Sciences

Born: Nov. 4, 1943—Hillsboro, Oregon

Office Telephone Number: 813-974-2535

Home Telephone Number: 813-985-xxxx

Cell Phone Number: 813-784-xxxx

Education:

Portland State University: BA, Chemistry, 1965.

Princeton University: AM, Chemistry, 1968

Princeton University: Ph. D., Chemistry, 1969

Other Education:

JEOLCO NMR Institute (1981)

Active Learning Workshops 1991, 1995, 1996

ACS Teaching Consortium 1999

Areas of Specialization:

Physical chemist. Molecular spectroscopy. Nuclear magnetic resonance studies of NMR fast-exchange reactions. Statistical analysis of experimental data. Chemometrics. Computer programming applications and algorithm design. Two-dimensional NMR. Zero- and Multiple-Quantum NMR. Computer applications to teaching.

Honors, Awards, etc.:

Baush & Lomb Science Medal, 1961.
American Chemical Society (1965--)
Sigma Xi (1973--)
Outstanding instructor: University Experience Program (1995)
Computing award (presentation of lap top computer (2001)
Web Course Design Award (Hon. Mention) (2003)

Employment & Fellowships:

University of South Florida Faculty (1973--); Professor (1994--)
University of Houston—Sabbatical Leave Appointment (1988)
Texas A & M University (R. A. Welch Fellow, 1971-73)
University of Arizona, Research Fellow (1970-71)
Princeton University, PRF Fellow 1969
Princeton University, Monsanto Fellow 1968
Princeton University, Eastman-Kodak Fellow (1967)
Princeton University, T. A. (1966)

Other Professional or Related Activities:

Editorial Board, Preston Publications, 1975-85
Book reviewer for McGraw-Hill, 1980—
Book reviewer for Prentice-Hall, 1981—
Consulting work for Immunomed Labs, 1982-85
Consulting for Florida Progress, 1986-88
Paper reviewer for several chemical journals.
Editorial Board, Houghton-Mifflin 2005—

II. Teaching

TEACHING AND OTHER INSTRUCTIONAL ACTIVITIES:

My primary teaching duties are in Physical Chemistry and in General Chemistry. Also, I have been quite active in course development and design. The most recent work has involved extensive web teaching. At present, my major efforts are centered on teaching and teaching has been a major part of my efforts since the start of my career here at USF.

My main efforts in undergraduate and graduate teaching have been to introduce the most modern techniques in used by the chemical community while, at the same time, giving considerable time to older methods. It is my philosophy—at least a regards teaching—that we must always seek the best methods whether they are new or hoary with age! In all my courses, I attempt an eclectic approach which tries to see the “big picture” of how things are organized an interrelated rather than indulging in over specialization. This coupled with mathematical rigor has produced a large number of excellent courses.

Currently, my major work is with the second semester of General Chemistry; I am the coordinator there and supervise exams and new materials.

A. Courses Taught

Undergraduate Courses Taught:

- CHM 2041, 2045, 2046: General Chemistry (1973-75, 1979, 1981, 1986, 1990-92, 1994--)
- CHM 3420: Elementary Phys. Chem. Lab., Coordinator (1994-2000)
- CHM4410: Physical Chem. I (Chemical Thermodynamics, 1994-2000)
- CHM 4411: Physical Chem. II (Quantum Chemistry, 1974-77, 1980-93, 1995-2003)
- CHM4412: Physical Chem. III (Kinetics) (1977, 1981, 1985-86, 1990, 1998-2002)
- CHM 4932: Math for Chemists (1976-79, 1981)
- CHM4130-31: Methods of Chemical Investigation (1976-89)

CHM 4932: Computers & Chemistry (2001)

Graduate Courses Taught:

CHM 5425: Physical Chemistry (5000 level) (1975, 1981, 1995-1999)

CHM 6038: NMR Spectroscopy (1974, 1981, 1988-90)

CHM 6411: Advanced Quantum Mechanics (1974, 1977, 1981, 1985, 1987, 1990).

CHM 6412: Statistical Mechanics (1983, 1989)

CHM 6938: Computational Chemistry (aka Computers & Chemistry) (1992, 1995-96, 2001)

B. Teaching Awards, Distinctions:

1. Selected to participate in Active Learning Workshops, 1991, 1993, 1996, 1997

2. Textbooks Published:

Computational Chemistry, An Emphasis on Practical Calculations, Milton D. Johnston, Jr., Elsevier Publication Co., Amsterdam, 1988.

3. New Courses Developed

Math for Chemists
NMR Spectroscopy
Computers & Chemistry

4. Other efforts:

Working out ways of using active learning in chemistry classes.
Extensive web development (CHM 2045, 2046, 4410, 4411, 4412, 6938)

C. Doctoral Dissertation Committees:

I have served on at least 3 committees every year since starting at USF. Below, I list only those students where I can be on the committee

chair (*i.e.*, thesis adviser).

G. Herbert Caines (1977-84)

Andrew Zektzer (1983-87)

James R. Brangan (1986-91)

Lyle Castle (1989-93)

Joanne Castle (1989-93)

D. Masters Theses

Michael Fasano (1998)

III. RESEARCH & CREATIVE ACTIVITY

A. Publications

1. Scholarly Books and Book Chapters:

“Some Aspects of the Use of Lanthanide-Induced Shifts in Organic Chemistry,” B. L. Shapiro, M. D. Johnston, Jr., R. L. R. Towns, A. D. Godwin, H. L. Pearce, T. W. Proulx, and M. J. Shapiro; *Nuclear Magnetic Resonance Shift Reagents*, R. E. Sievers, ed., Academic Press, New York (1973), pp. 227-245.

Computational Chemistry—An Emphasis on Practical Calculations, M. D. Johnston, Jr., Elsevier (1988). 680 pages.

2. Articles in Refereed Journals:

“Nuclear Magnetic Resonance Solvent Effects and Molecular Interactions,” I. D. Kuntz, Jr. and M. D. Johnston, Jr., *J. Amer. Chem. Soc.*, **89**, 6008 (1967).

“Molecular Interactions and the Benesi-Hildebrand Equation,” I. D. Kuntz, Jr., F. P. Gasparro, M. D. Johnston, Jr., and R. P. Taylor, *J. Amer. Chem. Soc.*, **90**, 4778 d(1968)

“Nuclear Magnetic Resonance Solvent Effects and Molecular Interactions. II. A Comparison of Dipolar, Hydrogen-Bonding, and Charge-Transfer Effects,” M. D. Johnston, Jr., F. P. Gasparro, and I. D. Kuntz, Jr., *J. Amer. Chem. Soc.*, **91**, 5715 (1969).

“Theoretical Studies of Solvent Effects on Nuclear Spin-Spin Coupling Constants. I. The Reaction Field Model,” M. D. Johnston, Jr. and M. Barfield, *J. Chem. Physics*, **54**, 3083 (1971).

“Theoretical Studies of Solvent Effects on Nuclear Spin-Spin Coupling Constants. II. A Cubic Closest Packed Cluster Model,” M. D. Johnston, Jr. and M. Barfield, *J. Chem. Physics*, **55**, 3483 (1971).

“Theoretical Studies of Solvent Effects on Nuclear Spin-Spin Coupling Constants. III. The Effects of Solvent Molecular Motion,” M. D. Johnston, Jr. and Michael Barfield, *Molecular Physics*, **22**, 831 (1971).

“Lanthanide-Induced Changes in Proton Spin-Spin Coupling Constants,” B. L. Shapiro, M. D. Johnston, Jr., and R. L. R. Towns, *J. Amer. Chem. Soc.* **94**, 4381 (1972).

“Lanthanide-induced Shifts in Proton Nuclear Magnetic Resonance Spectra. III. Lanthanide Shift Reagent-Substrate Equilibria, B. L. Shapiro and M. D. Johnston, Jr., *J. Amer. Chem. Soc.*, **94**, 8185 (1972).

“Concerning the Relative Shifting Abilities of $\text{Eu}(\text{DPM})_3$ and $\text{Eu}(\text{FOD})_3$,” B. L. Shapiro, M. D. Johnston, Jr., A. D. Godwin, T. W. Proulx, and M. J. Shapiro, *Tetrahedron Letters*, 3233 (1972).

“Lanthanide-Induced Effects in Proton NMR Spectra. VIII. ‘Scavenging’ Effects—A Problem and a Solution,” B. L. Shapiro, M. J. Shapiro, A. D. Godwin, and M. D. Johnston, Jr., *J. Magnetic Resonance*, **8**, 402 (1972).

“Solvent Dependence of Nuclear Spin-Spin Coupling Constants,” M. Barfield and M. D. Johnston, Jr., *Chemical Reviews*, **73**, 53 (1973).

“3-(α -Naphthyl)-5, 5-dimethylcyclohexanone and Derive Alcohols. Synthesis and Stereochemical Studies by Means of Lanthanide-Induced Proton Nuclear Magnetic Resonance Shifts,” B. L. Shapiro, M. D. Johnston, Jr., and T. W. Proulx, *J Amer. Chem. Soc.*, **95**, 520 (1973).

“NMR Studies and Rotational Isomerism in Fluoroacetones. I. Trifluoroacetones,” B. L. Shapiro, H.-L. Lin, and M. D. Johnston, Jr., *J. Magnetic Resonance*, **9**, 305 (1973).

“NMR Studies and Rotational Isomerism in Fluoroacetones. II. Fluoroacetone in 1,1-Difluoroacetone,” B. L. Shapiro, C. K. Tseng, and M. D. Johnston, Jr., *J. Magnetic Resonance*, **10**, 65 (1973).

“NMR Studies and Rotational Isomerism in Fluoroacetones. III. 1,3-Difluoroacetone and 1,1,3,3-Tetrafluoroacetone,” B. L. Shapiro, W. A. Thomas, J. L. McClanahan, and M. D. Johnston, Jr., *J. Magnetic Resonance*, **11**, 355 (1973).

“NMR Studies of Structure and Conformation in Some Highly Substituted Cyclohexenes. II. ^{13}C NMR Studies,” B. L. Shapiro, M. D. Johnston, Jr., and C. A. Reilly, *J. Magnetic Resonance*, **12**, 199 (1973).

“Lanthanide-Induced Shifts in Proton NMR Spectra of Cyclohexanones,” B. L. Shapiro, M. D. Johnston, Jr., and M. J. Shapiro, *Organic Magnetic Resonance*, **5**, 21 (1973).

“trans-3-(4'-Bromo-1-naphthyl)-1,1,5-trimethylcyclohexanol, $\text{C}_{19}\text{H}_{23}\text{BrO}$,” R. L. R. Towns, T. W. Proulx, B. L. Shapiro, and M. D. Johnston, Jr., *Crystal Structure Communications*, **3**, 31 (1974).

“3-Aryl-1,3,5,5-tetramethylcyclohexanols. Preparation and Stereochemical Characterizations by Proton Nuclear Magnetic Resonance,” B. L. Shapiro, M. D. Johnston, Jr., and M. J. Shapiro, *J. Organic Chemistry*, **39**, 796 (1974).

“*tert*-Butyl-7-cycloheptatrienylperacetate: The Proton NMR Spectrum and Conformational Analysis,” G. R. Jurch, Jr. and M. D. Johnston, Jr., *Organic Magnetic Resonance*, **7**, 95 (1975).

“Lanthanide-Induced Shifts in Proton Nuclear Magnetic Resonance Spectra. XI. Equilibrium Constants and Bound Shifts for Cyclohexanones and Cyclohexanols,” M. D. Johnston, Jr., B. L. Shapiro, M. J. Shapiro, T. W. Proulx, A. D. Godwin, and H. L. Pearce, *J. Amer. Chem. Soc.*, **97**, 542 (1975).

“Structure Elucidation with Lanthanide-Induced Shifts. The Use of Bound Shifts and High-Symmetry Substrates,” M. D. Johnston, Jr., D. J. Raber, N. K. DeGennaro, A. D'Angelo, and J. W. Perry, *J. Amer. Chem. Soc.*, **98**, 6042 (1976).

“Structure Elucidation with Lanthanide-Induced Shifts. 2. Conformation Analysis of Cyclohexanecarbonitrile,”

D. J. Raber, M. D. Johnston, Jr., and M. A. Schwalke, *J. Amer. Chem. Soc.*, **99**, 7671 (1977).

“Structure Elucidation with Lanthanide-Induced Shifts. 3. Acyclic Aliphatic Nitriles,” D. J. Raber, M. D. Johnston, Jr., J. W. Perry, and G. F. Jackson, III, *J. Organic Chem.*, **43**, 229 (1978).

“Structure Elucidation with Lanthanide-Induced Shifts. 4. Bound Shifts vs. Relative Shifts,” D. J. Raber, M. D. Johnston, Jr., C. M. Campbell, C. J. Janks, and P. Sutton, *Organic Magnetic Resonance*, **11**, 323 (1978).

“Structure Elucidation with Lanthanide-Induced Shifts. 5. Evaluation of the Binding Ability of Various Functional Groups,” D. J. Raber, M. D. Johnston, Jr., C. M. Campbell, A. Guida, G. F. Jackson, III, C. M. Janks, J. W. Perry, G. J. Propeck, N. K. Raber, M. A. Schwalke, and P. M. Sutton, *Monatsh. Chem.*, **111**, 43 (1980).

“Structure Elucidation with Lanthanide-Induced Shifts. 6. Solvent Effects on Bound Shifts and Association Constants,” D. J. Raber, M. d. Johnston, Jr., G. F. Jackson, III, C. M. Janks, and J. W. Perry, *Organic Magnetic Resonance*, **14**, 32 (1980).

“Structure Elucidation with Lanthanide-Induced Shifts. 7. Development of a Reliable Method for Structure Evaluation and the Application to Organic Nitriles,” D. J. Raber, C. M. Janks, M. D. Johnston, Jr., and N. K. Raber,” *Organic Magnetic Resonance*, **15**, 57 (1981).

“Structure Elucidation with Lanthanide-Induced Shifts. 9. Bicyclo-[3,3,1]nonan-9-one,” D. J. Raber, C. M. Janks, M. D. Johnston, Jr., and N. K. Raber, *Tetrahedron Letters*, **21**, 677 (1980).

“The Synthesis and Proton NMR Spectrum of Methyl-7-cycloheptatrienyl-acetate,” G. R. Jurch, Jr., M. D. Johnston, Jr., J. W. Perry, and T. E. Detty, *J. Chemical*

Educ., **57**, 743 (1980).

“Structure Elucidation with Lanthanide-Induced Shifts. 8. Geometry of Europium-Ketone Complexes,” D. J. Raber, C. M. Janks, M. D. Johnston, Jr., and N. K. Raber, *J. Amer. Chem. Soc.*, **102**, 6591 (1980).

“Structure Elucidation with Lanthanide-Induced Shifts. 10. Generation of Atomic Coordinates: Empirical Force Field Calculations and Other Methods,” D. J. Raber, C. M. Janks, M. D. Johnston, Jr., M. A. Schwalke, B. L. Shapiro, and G. L. Behelfer, *J. Org. Chem.*, **46**, 2528 (1981).

“Structure Elucidation with Lanthanide-Induced Shifts. 11. Analysis of Alkyl-Substituted Benzonitriles,” D. J. Raber, G. H. Caines, M. D. Johnston, Jr., and N. K. Raber, *J. Magnetic Resonance*, **47**, 38 (1982).

“Structure Elucidation with Lanthanide-Induced Shifts. 12. Structural Effects on Equilibria between Ketones and $\text{Eu}(\text{fod})_3$,” D. J. Raber and M. D. Johnston, Jr., *Spectroscopy Letters*, **15**, 287 (1982).

“Structure Elucidation with Lanthanide-Induced Shifts. 14. Structural Effects of Equilibria between Nitriles and $\text{Eu}(\text{fod})_3$,” D. J. Raber, W. E. Beaumont, and M. D. Johnston, Jr., *Spectroscopy Letters*, **15**, 329 (1982).

“HP-41 Jacobi Matrix Diagonalization,” M. D. Johnston, Jr., *PPC Calculator Journal*, **9:3**, 9 (1982).

“Calculation of Bond Angles, Lengths, and Dihedral Angles on a Pock Calculator,” G. H. Caines and M. D. Johnston, Jr., *Computers and Chemistry*, **7**, 99 (1983).

“The Lanthanide-Induced-Shift-Assisted Determination of Proton Spin-Lattice Relaxation Times,” M. D. Johnston, Jr., G. H. Caines, and Andrew S. Zektzer, *J. Magnetic Resonance*, **60**, 415 (1984).

“A Rigorous Statistical Analysis of Errors Incurred in the Study of Intermolecular Fast-Exchange Equilibria by NMR Spectroscopy,” M. D. Johnston, Jr., A. P. Marvhand, and A. E. Earlywine, *J. Magnetic Resonance*, **69**, 467 (1986).

“New Pulse Sequence for Long-Range Two-Dimensional Heteronuclear NMR Chemical Shift Correlation,” A. S. Zektzer, M. J. Quast, G. S. Linz, G. E. Martin, J. D. McKenney, M. D. Johnston, Jr., and R. N. Castle, *Magnetic Resonance in Chemistry*, **24**, 1083 (1986).

“Double Quantum Filtered Zero Quantum Coherence Two-Dimensional NMR with Broadband Proton Decoupling,” L. R. Saltero, M. D. Johnston, Jr., R. N. Castle, and G. E. Martin, *J. Magnetic Resonance*, **81**, 406 (1989).

“Total Assignment of the ^1H and ^{13}C NMR Spectra of Dinaphtho-[1,2-b:1',2'd]thiophene Through the Concerted Use of Two-Dimensional NMR Techniques,” M. D. Johnston, Jr., M. Salazar, D. K. Kruger, R. N. Castle, and G. E. Martin, *Magnetic Resonance in Chemistry*, **26**, 838 (1989).

“Total Assignment of the ^1H and ^{13}C NMR Spectra of Phenanthro-[9,10-b]thiophene: Concerted Use of Two-Dimensional NMR Techniques,” M. D. Johnston, Jr., M. Salazar, L. D. Sims, A. S. Zektzer, R. N. Castle, and G. E. Martin, *Magnetic Resonance in Chemistry*, **27**, 318 (1989).

“Establishing Long Range Connectivities in Polynuclear Aromatics Through the Use of Two-Dimensional MLEV-17 Based Isotropic Mixing,” M. D. Johnston, Jr. and G. E. Martin, *Magnetic Resonance in Chemistry*, **27**, 529 (1989).

“A Reassignment of the ^{13}C -NMR Spectrum of the Alkaloid Ajmaline Through the Use of Two-Dimensional NMR Techniques,” M. D. Johnston, Jr., L. R. Soltero, and G. E. Martin, *J. Heterocyclic Chem.*, **25**, 1803 (1988).

“Total Assignment of the Proton NMR Spectrum of Dinaphtho-[1,2-b:2',3'-d]thiophene,” M. D. Johnston, Jr., G. E. Martin, and R. N. Castle, *J. Heterocyclic Chem.*, **25**, 1593 (1988).

“Running 2D Homonuclear Hartmann-Hahn (HOHAHA) Experiments on NT-Series Spectrometers, M. D. Johnston, Jr., L. D. Sims, A. S. Zektzer, L. R. Soltero, and G. E. Martin, *Relaxation Times*, **5**, 3 (1988).

“Double Quantum Filtered Zero Quantum Coherence with Broadband Homonuclear F_1 Decoupling,” L. R. Soltero, G. E. Martin, M. D. Johnston, Jr., and R. N. Castle, *J. Heterocyclic Chem.*, **26**, 741 (1989).

“Assignment of the ^1H and ^{13}C NMR Spectra of Naphtho[1',2':4,5]-thieno[2,3-c]quinoline Using Two-Dimensional NMR Spectroscopy,” Lyle W. castle, Andrew S. Zektzer, and Milton D. Johnston, Jr., *Magnetic Resonance in Chemistry*, **30**, 779 (1992).

“Spin-Spin Coupling of ^{19}F with ^{13}C Transmitted Through Nonbonded Interactions: Observation and Characterization using a Series of Fluoro-Substituted Polynuclear Aromatic Heterocycles Containing a Large Bay-Region,” Lyle W. Castle, J.-K. Luo, and M. D. Johnston, Jr., *Magnetic Resonance in Chemistry*, **30**, (1992).

“Assignments of the ^1H and ^{13}C NMR Spectra of Pseudo-Symmetric Heterocycles Using the HMQC-TOCSY Experiment to Differentiate Overlapping Spin Systems,” Lyle W. Castle, M. D. Johnston, Jr., C. L. Camoutsis, and R. N. Castle, *J. Heterocyclic Chem.*, **29**, 1805 (1992).

Refereed Computer Programs in General Circulation:

These are free programming packages and are all in more or less general use in the chemical community. All are available for use on a PC and all are interactive in nature.

MOLPIX: This is a large programming package for the producing of molecular coordinates and molecular structures starting from just bond lengths, bond angles, and dihedral angles. It has been in circulation since 1983 and has received quite favorable reviews. It allows the user to produce a structure on screen and then to translate or rotate it in any way desired. This was the first major programming package developed by me and has proved quite useful.

FFTUTOR: This is a program which allows a person to produce nearly any mathematical function desired and then produce its Fourier transform. A novel aspect of this program is that the operations of the

Cooley-Tukey algorithm are displayed as they are carried out. A major feature of this program is the extensive use of interactive graphics.

COSYSIM: This is a program to produce COSY 2D-NMR spectra on a computer screen or on to a printer. This is an extremely useful pedagogical tool in teaching the fundamentals of one of the simpler, yet most important, modern NMR experiments.

LISA: This is a program which analyzes NMR fast-exchange equilibria. As such, it affords an introduction to an area of NMR which has been exploited by just a few specialists. The handling of complex equilibria has applications to more than just NMR and this programming package allows entrance to these more advanced and interesting applications.

NMRCALC: This program provides simulations for NMR spectra for up to seven spins. Here, the student is introduced to the intricacies of matrix manipulations involving quantum mechanical spin operators. At the same time, the user can produce sample spectra for almost any conceivable set of NMR chemical shifts and coupling constants. Energy level diagrams can also be produced and the program is a practical introduction into the intricacies of handling these. Graphics are used extensively in several areas. Among these are the display of energy level diagrams, expectation level diagrams, “stick” spectra, and Lorentzian spectra.

Miscellaneous Nonrefereed Publications:

“The Purification of LSR’s,” M. D. Johnston, Jr., TAMUNMR Newsletter, No. 190, 24 (1974).

“LIS of Some Sulfur-Containing Compounds,” M. D. Johnston, Jr. and G. R. Jurch, Jr., TAMUNMR Newsletter, No. 196, 39 (1975).

“Much Ado About Nothing or A Comedy of Errors—The Temperature Dependence of LIS,” M. D. Johnston, Jr., TAMUNMR Newsletter, No. 213, 12 (1977).

“Pocket Calculator NMR Spectral Analysis (LAOCOON-1/2?),” M. D. Johnston, Jr., TAMUNMR Newsletter, No. 225, 13 (1977).

“Two-Step Equilibria the Fastest Way,” M. D. Johnston, Jr., TAMUNMR Newsletter, No. 237, 25 (1978).

“Doing Statistical Fits,” M. D. Johnston, Jr., TAMUNMR Newsletter, No. 250, 4 (1979).

“Sample Mixing mit den Walterssplasern,” J. P. Walters and M. D. Johnston, Jr., TAMUNMR Newsletter, No. 260 (1980).

“90°-pulses Easily,” M. D. Johnston, Jr., TAMUNMR Newsletter, No. 271, 18 (1981).

“A Hindered Rotation Unmasked by an LSR,” M. D. Johnston and D. J. Raber, TAMUNMR Newsletter, No. 281, 37 (1982).

“Effect of LSR’s on Coupling Constants,” D. J. Raber and M. D. Johnston, Jr., TAMUNMR Newsletter, No. 283, 34 (1982).

“LSR Impurities—Na NMR Monitoring,” M. D. Johnston, Jr. and G. H. Caines, TAMUNMR Newsletter, No. 292, 24 (1983).

GRANTS & CONTRACTS:

Faculty Release-Time Award, 1974 (USF).

Research Corporation Grant (1977-81).

Summer Faculty Research Grant (USF) (1980).

Sabbatical Award (USF/Univ. of Houston) (1988).

PRESENTATIONS OF PAPERS/MAJOR SPEECHES:

“Solvent Effects on Nuclear Spin-Spin Coupling Constants,” Los Angeles ACS National Meeting, 1971. (With M. Barfield)

“Aspects of Lanthanide-Shift Reagents,” 13th Experimental NMR Conference, Asilomar, California (Invited talk), 1972. (With B. L. Shapiro)

“Applications of LIS to Molecular Structure Determination,” Dallas ACS National Meeting, 1973. (With B. L. Shapiro)

“Applications of LSR’s to Structure Determination,” New Orleans ACS National Meeting, 1977.

“Applications of Bound Shifts to NMR Spectroscopy and the Liquid State,” SERACS, Tampa, 1978.

“NMR Spectroscopy,” Sigma Xi presentation (invited), Tampa, 1977.

“‘Q-Sort,’ An Algorithm for Handling Statistical Analyses of Complex Equilibria,” Seattle ACS National Meeting, 1983. (With J. P. Walters).

“Statistical Analysis and Anisotropy Effects of LIS,” Seattle ACS National Meeting, 1983 (with G. H. Caines).

“Determination of Spin-Lattice Relaxation Times for the Solution Species, S, LS and LS₂ Using the LSR, Eu(fod)₃,” Washington, DC ACS National Meeting, 1983 (with G. H. Caines).

“Rigorous Statistical Analysis of the Errors Incurred in Studying Fast-Exchange Equilibria by NMR Spectroscopy,” SERACS Meeting, Charlotte, NC, 1983.

“Nonlinear Regression and Multi-Step Chemical Equilibria,” Miami Beach, FL National ACS Meeting, 1985.

“Application of Binuclear (Ln-Ag) Shift Reagents to Sulfur Heterocycles,” Miami Beach, FL, ACS National Meeting, 1985 (with A. Zektzer).

“FFTUTOR—An Interactive Computing Package for Studying Fourier Transforms,” Anaheim, CA, ACS National Meeting, 1986.

“PHITTER—A Computer Package for Studying pH Equilibria,”
SERACS Regional ACS Meeting, Orlando, FL, 1987.

“Stimulating Simulations—Applications of Microcomputers to the
Study of Dynamics Processes,” M. D. Johnston, Jr., North Texas State
University Departmental Seminar (invited), Denton, TX, 1988.

“Total Assignment of the Proton and Carbon NMR Spectra of a
Potential Mutagen Through the Use of Two-Dimensional NMR
Techniques,” M. D. Johnston, Jr. and Gary E. Martin, MALTO
(Medicinal Chemistry & Pharmacognosy Meeting, Auburn, AL, 1988.

“Establishing Long Range Connectivities in Polynuclear Aromatics
Through the Use of Two-Dimensional MLEV-17 Based Isotropic
Mixing,” M. D. Johnston, Jr. and Gary E. Martin, ACS National
Meeting, Los Angeles, CA, 1988.

“A Reassignment of the ^{13}C NMR Spectrum of the Alkaloid
Ajmaline Through the Use of Two-Dimensional NMR Techniques,”
M. D. Johnston, Jr., G. E. Martin, and L. R. Soltero, SERACS
Regional ACS Meeting, Atlanta, GA, 1988.

“The Simulation of Two-Dimensional NMR Spectra,” M. D.
Johnston, Jr., SERMACS Regional ACS Meeting, Winston-Salem,
NC 1989.

“Applications of Concerted 2D-NMR Methods to Organic Structural
Elucidation,” M. D. Johnston, Jr., USF Chem. Dept. seminar, 1989.

“Spin-Spin Coupling of ^{19}F with ^{13}C Transmitted Through Nonbonded
Interactions: Observation and Characterizations using a Series of
Fluoro-Substituted Polynuclear Aromatic Heterocycles Containing a
Large Bay Region,” with Lyle Castle. This talk was given at the
University of Oregon in August, 1990, and at the Experimental NMR
Conference (Asilomar, CA) in April, 1992.

“Parabolic Orbitals of Hydrogen, the ‘Other’ Solution to the
Schrödinger Equation,” M. D. Johnston, Jr., ACS National Meeting,
San Diego, CA, 1994.

“Conductimetric Titrations: A New Look at an Old Technique,” M. D. Johnston, Jr., ACS National Meeting, Orlando, FL, 1995.

“Nonconventional Exact Solutions to the Schrödinger Equation: Particles in a box in an Electric Field,” M. D. Johnston, Jr., ACS National Meeting, Anaheim, CA 1999.

“The Schrödinger Equation and Some Unique Two-Dimensional Systems,” M. D. Johnston, Jr., San Francisco, CA, National ACS Meeting, 2000.

“A Comparison of WebCT and BlackBoard in Teaching Chemistry,” San Diego National ACS Meeting, San Diego, CA 2001.

“Foolproof Algorithms for pH Calculations,” Orlando, 2002, National ACS Meeting.

IV. Service

Major Civic & Public Service Activities

Asolo Angels (Sarasota)
Symphony Guild (Tampa)
Taoist Tai Chi Association of North America

University, College, Departmental Committees:

Chemistry Department (* Denotes Chair)

Curriculum Committee (*) (1974-75)
Safety committee (*) (1978-86)
Advisory Committee (*) (1979-85; 1989-1992)
(Chaired 1981-83)
Graduate Council (1979-84)
Computer Committee (*) (1983--)
Library Committee (1988-2002)
Undergraduate Council (*) (2003-2005)
Coordinator, General Chemistry (2003--)

College of Natural Sciences/College of Arts & Sciences:

Tenure Committee (1981)
Academic Computing Committee (1994--) (Vice Chair in 1999)

University of South Florida:

Community College Committee (1980-83)
Faculty Senate (1980)
USF Faculty/Staff Club Committee (1993-1998) President, 1995-96

Other Relevant Activities:

Coordinator for Chemistry Dept. "Methods of Chemical Investigation" (1979-1989)

NMR Lab Coordinator (1973-1990)

Instructor in University Experience courses at USF (1990-95)

Founding member of USF Faculty/Staff Club

Mentor in the new program involving African-American Students (1992)

University Food Service Committee (1994-95)

MISCELLANEOUS GOALS AND ACHIEVEMENTS:

Since 1966, I have been actively pursuing research problems in one form or another which involve applications of NMR to problems of chemical interest. The work has ranged from experimental to theoretical. My main efforts have been centered toward the development of new techniques and the gaining of new insights into various chemical problems. It should be noted that what I have been doing is to develop my own techniques and methods rather than, for instance, using other people's canned programs and then pass myself off as a theoretician. Rather, I have tried (I feel successfully) to keep my work original, interesting, and of high quality. This cuts down the number of possible publications but, given the limitations inherent over the years in working at USF, I have still managed to turn out a great deal of original, useful, and stimulating work.

My main field of interest is NMR spectroscopy. In this area, my primary interests involve the study of fast-exchange equilibria, the study of applications of LSR's, and the application of 2D NMR techniques to the solutions of significant problems of chemical interest. In this work, I have produced much original work of good quality regarding molecular structure, equilibrium dynamics, kinetics and theoretical problems; I now list some of main achievements along these lines.

- 1) Development of a generalized collision complex model for dipole-dipole, hydrogen-bonding, and charge-transfer interactions as observed by NMR.
- 2) A theoretical description of medium effects upon NMR spin-spin coupling constants.
- 3) Delineation of the interaction mechanism between lanthanide shift

reagents (LSR's) and organic substrates. Both experimental and statistical methods for the analysis of these interactions were developed.

- 4) The analysis of relaxation pathways in NMR spectroscopy. Developed methods for separating strongly coupled reactions from weakly coupled ones.
- 5) Made some inroads in the concerted use of 2D NMR methods.

Currently, my work is getting more mathematical and I am working extensively on computer simulations of strongly coupled spin systems.

Along different lines, I have been quite active in writing and producing web pages for courses ranging from Gen. Chem. to P. Chem. to advanced computer applications. This work has gained a great deal of respect from people outside the Chemistry Dept.