WILLIAM B. COLLIER

Professor of Chemistry, Oral Roberts University

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TECHNICAL AREAS

Molecular spectroscopy
Infrared and Raman spectroscopy and methods
Spectral prediction and analysis
Matrix-isolation spectroscopy
Instrumentation and software development
Calculation of thermodynamic properties

Philosophy of science and origin/intelligent design studies

EDUCATION

Ph.D. in Physical Chemistry, 1983, M.S. in Physical Chemistry, 1981, Oklahoma State University; B.S. in Chemistry, Physics minor, 1977, Oral Roberts University, Tulsa, Oklahoma.

EXPERIENCE

Professor of Chemistry Oral Roberts University Department of Chemistry, Associate Professor of Chemistry, Oral Roberts University Department of Chemistry fall 1994 to summer 2000, Assistant Professor of Chemistry, Oral Roberts University Department of Chemistry, fall 1988-1994. Responsible for teaching Physical Chemistry, Chemical Instrumentation, Structure and Bonding, Quantitative Analysis, General Chemistry, lectures and labs. Manage and direct the Chemical Instrumentation and Physical Chemistry laboratories and undergraduate research. Helped create and team teach an honors level Philosophy of Science seminar class. Responsibilities include teaching various other upper division courses as needs dictate.

Chair of Oral Roberts University Tenured Faculty 2011-2012

Consultant to Road Science, Division of Amartz, Inc., 6502 S. Yale Ave, Tulsa, OK 74136, 2015

Consultant to SemMaterials, L.P., Research Center, 6502 South Yale Avenue, Tulsa, OK 74136-8368, Fourier Transform infrared spectroscopy specialist and technical services, Summer 2008.

Consulting work for Rentech Services Corporation, Denver, CO, Summer 2007

Consultant to Syntroleum Corporation, Technical Research Center, Tulsa, OK, Summer 2000 to 2005.

NSF-Research Opportunity Award to work with Dr. Stefan Franzen, North Carolina State University, Summer of 2001.

EPSCOR Grant Participant. Worked with Dr. Dale Teeters, Chairman, Dept. of Chemistry, Tulsa

University, on joint Raman Spectroscopy Research for Summers of 1999 and 2002.

Consultant to BDM-Oklahoma Petroleum Technologies, fall 1997 to fall 1998.

AWU-DOE Faculty fellowship award for summer work at NIPER during summers of 1993, 1994, 1995, 1996, 1997. Worked on predicting and assigning vibrational spectra of bicyclic heterocyclic compounds using classical and newly developed computer techniques.

Illinois Institute of Technology Research Institute, NIPER Division, National Institute for Petroleum and Energy Research, Bartlesville, Okla., 1983-1988. Fourier transform infrared and laser Raman spectroscopy. Calculation of thermodynamic functions at high temperatures. Development of high temperature vapor phase spectral collection techniques. Prediction and assignment of vibrational spectra using classical and computer aided techniques.

Oklahoma State University, graduate research assistant, 1978-1983. Research activities included developing FTIR methods of examining matrix-isolation spectra, developing computer programs to analyze complex reversible kinetic systems, performing normal mode analyses of molecular systems, and using CARS laser spectroscopy to study organic dyes.

PROFESSIONAL AFFILIATION

American Chemical Society
Fulbright Association
American Scientific Association

AWARDS

Awarded a Fellowship Appointment from the Turkish Science Agency, TÜBİTAK for Summer 2014. Working with Dr. Kubilay Balci at the Atomic and Molecular Physics Division at Istanbul University, Istanbul, Turkey on *Development of Experimental and Theoretical Techniques for Spectroscopic Study of Important Pharmaceutical Compounds using the SQM Method of Theoretical Scaling*.
Awarded a Fulbright Scholar Award for the Spring Semester of 1997. Working with Professor Geza Fogarasi of Eotvos Lorand University, Budapest, Hungary on *Research in Development of Ab Initio and Semi-empirical Scale Factors for Prediction of Vibrational Spectra for Biologically Important Heteroaromatics.*
Associated Western Universities, Inc. (AWU), AWU-DOE Faculty Fellowship at the National Institute for Petroleum and Energy Research (NIPER) for the Summers 1993, 1994, 1995, 1996, 1997,1998.
NSF-Research Opportunity Award, to work with Dr. Stefan Franzen, North Carolina State University, for the Summer of 2001 on spectroscopic predication of vibrational spectra.
International Institute of Cooperative Studies Fellow 2005 – 2006 to Eotvos Lorand University, Budapest, Hungary.
Outstanding Honors Program Faculty Award, Oral Roberts University 2011-2012.
Oral Roberts University Chemistry Department Outstanding Alumnus of the Year, awarded for the year 2000-2001.
Oral Roberts University Seed Grant 2013-14. *Computational and Matrix Isolation Techniques for Spectroscopic Study of Important Pharmaceutical Compounds using the SQM Method of Theoretical Scaling.*
EPSCOR Grant Participant. Worked with Dr. Dale Teeters, Chairman, Dept. of Chemistry, Tulsa University, on joint Raman Spectroscopy Research for Summer of 1999.

Invited Speaker to American Chemical Society Tulsa Section Meeting, University of Tulsa, Tulsa, March 16, 1999. 60 minute presentation on *Predicting Infrared and Raman Spectra*.
Invited speaker to 14th International Conference on Raman Spectroscopy, Hong Kong, August 22, 1994.
Made short list for 1995 Sir Harold Thompson Award
Publication: Heteroatom derivatives of Indene. Part 1. Vibration frequencies and a refined scaled overlay of the AM1 force field of indole, benzofuran, benzothiophene, benzoxazole and benzothiazole, by W. B. Collier and T. D. Klots, Spectrochimica Acta A, volume 51, pages 1255-1272 and Part 2. Vibrational spectra of benzothiophene and benzothiazole, pages 1273-1290, was one of seven papers on the short list for the 1995 Sir Harold Thompson Award which recognizes the best paper of the year for the journal *Spectrochimica Acta*. The journal publishes some 300 papers per year.
Honorable Mention, Innovation in Teaching, Oral Roberts University Alumni Foundation, Fall 2002.

REFEREED PUBLICATIONS

1. C. R. Legler, N. R. Brown, R. A. Dunbar, M. D. Harness, K. Nguyen, O. Oyewole, and W. B. Collier*, *Scaled Quantum Mechanical Scale Factors for Vibrational Calculations using Alternate Polarized and Augmented Basis Sets with the B3LYP Density Functional Calculation Model,* Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy 145 (2015) 15–24.
2. Lappi, S. E., Collier, W. B., and S. Franzen, *Density Functional Analysis of Anharmonic Contributions to Adenine Matrix Isolation Spectra*, J. Phys. Chem. A, 106, 2002, pp. 11446-11455.
3. Collier, W. B., I. Magdo, and T. D. Klots, *Infrared and Raman Spectra of Bicylic Molecules Using Scaled Noncorrelated and Correlated Ab Initio Force Fields*, J. Chem. Phys., 110(12) 1999, pp. 5710-5720.
4. Klots, T. D., P. Devlin, and W. B. Collier, *Heteroatom Derivatives of Indene V. Vibrational Spectra of Benzimidazole*, Spectrochimica Acta, v. 53A, 1997, pp. 2445-2456.
5. Klots, T. D., and W. B. Collier, *Vibrational Spectra, Structure, Assignment, and Ideal-Gas Thermodynamics of a Three-Ring Molecule: Dibenzofuran*, J. Mol. Struct., 380 (1996) pp. 1-14.
6. Klots, T. D., and W. B. Collier, *Heteroatom Derivatives of Indene III. Vibrational Spectra of Benzoxazole, Benzofuran and Indole*, Spectrochimica Acta, v. 51A, 1995, pp. 1291-1316.
7. Klots, T. D., and W. B. Collier, *Heteroatom Derivatives of Indene II. Vibrational Spectra of Benzothiophene and Benzothiazole, Spectrochimica Acta, v. 51A, 1995, pp. 1273-1290.*
8. Collier, W. B., and T. D. Klots, *Heteroatom Derivatives of Indene. I. Vibrational Frequencies for Indole, Benzofuran, Benzoxazole, Benzothiophene and Benzothiazole with a Refined Scaled Overlay Am1 Hamiltonian Generated Force Field*, Spectrochimica Acta, v. 51A, 1995, pp. 1255-1272.
9. Klots, T. D., and W. B. Collier, *Vibrational Assignment and Analysis for 2,3-dihydrofuran and 2,5-dihydrofuran*, Spectrochimica Acta, v. 50A, No. 10, 1994, pp.1725-1748.
10. Collier, W. B., *Vibrational Frequencies of Polyatomic Molecules. I. Indole and 2,3-Benzofuran Spectra and Analysis*, J. Chem. Physics, v. 88, No. 12, 1988, pp. 7295-7306.
11. Steele, W. V., D. G. Archer, R. D. Chirico, W. B. Collier, I. A. Hossenlopp, A. Nguyen, N. K. Smith, and B. E. Gammon, *The Thermodynamic Properties of Quinoline and Isoquinoline*, J. Chem. Thermodynamics, 20, 1233, 1988.
12. Collier, W. B., Gary Ritzhaupt, and J. P. Devlin, *Spectroscopically Evaluated Rates and Energies for Proton Transfer and Bjerrum Defect Migration in Cubic Ice*, J. Phys. Chem., v. 88, 1984, pp. 363-368.
13. Moore, J., C. Thornton, W. B. Collier, and J. P. Devlin, *Vibrational Spectra, John-Teller Distortion and the Structure of the Benzene Radical Anion*, J. Phys. Chem., v. 85, No. 4, 1981,

p. 350.

14. Ritzhaupt, G., W. B. Collier, C. Thornton, and J. P. Devlin, *Decoupled Vibrational Spectra for H_2O in D_2O Ice I_c*, Chem. Phys. Lett., v. 70, No. 2, 1980, p. 294.

SUBMITTED PUBLICATIONS

1. Y. Akkaya, K. Balci, Y. Goren, S. Akyuz, M. C. Stricker, D. D. Stover, G.Ritzhaupt, W. B. Collier, *A Vibrational Spectroscopy Study on Anserine and its Aqueous Solutions*, Submitted to Spectrochimica Acta A, December 2014.

OTHER PUBLICATIONS

1. Full page interview with *Magyar Nemzet*, (second largest quality daily newspaper in Hungary), on the American intelligent design movement. *Az élet kódja* (The Code of Life) by Balayány György, interviews Professor William B. Collier, *Magyar Nemzet*, June 10, 2006, p. 23, Budapest, Hungary.
2. Collier, William B., QCPE Program #631, "*FCARTP: A series of Programs used to Generate a Predicted Set of Fundamental Vibrational Frequencies (Version 1.1)*", QCPE Bulletin, 13(2), 1993.
3. Collier, William B., QCPE Program #607, "*THERPOLY: Research Grade Thermodynamic Functions for Polyatomic Molecules in the Gas Phase (Version 8.1)*", QCPE Bulletin, 11(4), 1991.
4. Steele, W. V., R. D. Chirico, W. B. Collier, R. H. Harrison, and B. E. Gammon, *Assessment of Thermodynamic Data and Needs, Including Their Economic Impact, for Development of New Fossil Fuel Refining Processes*, Topical Report NIPER-159, June 1986. Published by DOE Fossil Energy, Bartlesville Project Office. (NTIS Report No. DE-86000298.)
5. Steele, W. V., R. D. Chirico, W. B. Collier, I. A. Hossenlopp, A. Nguyen, and M. M. Strube, *Thermochemical and Thermophysical Properties of Organic Nitrogen Compounds Found in Fossil Materials*, Status Report NIPER-188, November 1986. Published by DOE Fossil Energy, Bartlesville Project Office. (NTIS Report No. DE-87001204.)
6. Steele, W. V., D. G. Archer, R. D. Chirico, W. B. Collier, I. A. Hossenlopp, A. Nguyen, and M. M. Strube, *Thermochemistry and Thermophysical Properties of Organic Nitrogen Compounds*, Status Report NIPER-281, September 1987.
7. Chirico, R. D., D. G. Archer, W. B. Collier, I. A. Hossenlopp, A. Nguyen, W. V. Steele, and M. M. Strube, *Thermochemical and Thermophysical Properties of Substances Derived from Fossil Materials*, Status Report NIPER-282, September 1987.
8. Steele, W. V., D. G. Archer, R. D. Chirico, W. B. Collier, B. E. Gammon, I. A. Hossenlopp, A. Nguyen, and N. K. Smith, *The Thermodynamic Properties of Quinoline and Isoquinoline*, Topical Report NIPER 301, November 1987. Published by DOE Fossil Energy, Bartlesville Project Office. (NTIS Report No. DE-88001218.)

PROFESSIONAL PRESENTATIONS

1. John A. Arriola, John P. Richards, Gary Ritzhaupt, Randy Iwanaga, William B. Collier*, *18 K Frozen Argon Matrix Isolated Spectra and Density Functional ab initio Calculation Study of the Monomer and Dimerized Spectra of Ethyl 6-methyl-2-oxo-4-phenyl-1,2,3,4-tetrahydropyrimidine-5-carboxylate.* Poster presented at the 59th Annual Pentasectional Meeting of the American Chemical Society, Oklahoma State University, Stillwater, Oklahoma, April 12, 2013.

2. John P. Richards, William B. Collier*, *Analysis of Possible Matrices for Matrix Isolation Spectroscopy at Liquid Nitrogen Temperatures*. Poster presented at the 59th Annual Pentasectional Meeting of the American Chemical Society, Oklahoma State University, Stillwater, Oklahoma, April 12, 2013.
3. Ethan A. Hacker, Gary Ritzhaupt, William B. Collier*, *97 K CO_2 matrix isolated spectra and ab inito calculation study of the monomer and dimer spectra of ethyl 6-methyl-2-oxo-4-phenyl-1,2,3,4-tetrahydropyrimidine-5-carboxylate*. Poster presented at the 58th Annual Pentasectional Meeting of the American Chemical Society, University of Tulsa, Tulsa, Oklahoma, March 9, 2013.
4. Sandra M. Clark, Lacey N. Condron, Ethan A. Hacker, Giau T. Phan, Raymee E. Sickler, Jacob A. Sweat, Celestino Velasquez, Melanie J. Wespetal, Jason L. Martin, William B. Collier*, *Accuracy of the Gill96-Perdew86 density functional with the modest, fast 3-21g(d) basis for calculating vibration frequencies with the SQM method*. Poster presented at the 58th Annual Pentasectional Meeting of the American Chemical Society, University of Tulsa, Tulsa, Oklahoma, March 9, 2013.
5. Collier, W. B., Legler, C. R., Brown, N. R., Dunbar, R. A., Harness, M. D., Nguyen, K., Oyewole, O., *Pulay SQM Scale Factors for Vibrational Frequency Prediction at the 6-311G/B3-LYP Theory Level*. Poster presented at the 57th Annual Pentasectional Meeting of the American Chemical Society, Cameron University, Lawton, OK, March 17, 2012.
6. Collier, W. B., Nguyen, K., *Solution FTIR and Ab Initio Calculation Study of the Monomer and Dimerized Spectra of Ethyl 6-methyl-2-oxo-4-phenyl-1,2,3,4-tetrahydropyrimidine-5-carboxylate and the Model Compound Dimethyl Urea.* Poster presented at the 57th Annual Pentasectional Meeting of the American Chemical Society, Cameron University, Lawton, OK, March 17, 2012.
7. Collier, W. B., C. E. Kimbrough, D. A. Bulger, M. K. Chau, J. M. Jowers, J. K. Jacobs, D. Brown, *Routine Prediction of Quality Infrared and Raman Spectra – Development of SQM Pulay Scale Factors for Model Ab Initio Chemistries, from High Theoretical Level to Low*. Poster presented at the 56th Annual Pentasectional Meeting of the American Chemical Society, ConocoPhillips Bartlesville Technology Center, Bartlesville, OK, March 12, 2011.
8. Collier, W. B., *A Visual Roadmap to the Definition of Science and its Relationship to Christianity*, Oral presentation and discussion session presented at the 63th annual meeting of the American Scientific Affiliation at George Fox University, Newberg, Oregon on August 2, 2008.
9. Collier, W. B., *Teaching the Philosophy and History of Science to Graduate Science Students in a Secular European University - Rehabilitating the Image of Christianity and Science in a Secular Environment*, Poster presentation and discussion presented at the 63th annual meeting of the American Scientific Affiliation at George Fox University, Newberg, Oregon on August 3, 2008.
10. Collier, W. B., *Teaching the Philosophy and History of Science to Graduate Science Students in a Secular European University - Rehabilitating the Image of Christianity and Science in a Secular Environment*, Oral presentation and discussion session presented at the, Scholars Coming to Faith - Vision Conference, sponsored by the International Institute for Christian Studies at Airport Hilton, Kansas City, Missouri, July 20, 2006.
11. Collier, William B., Zhang D., Liu S., Ma X., and Halsmer D. M., *Chinese Airline Pilot Trainees and Intelligent Design - Observations on Cross Cultural Evangelism using Science*, Oral presentation and discussion presented at the 60th annual Meeting of the American Scientific Affiliation at Messiah College, Grantham, Pennsylvania, August 8, 2005.
12. Collier, W. B., and R. Samuel Thorpe, *Teaching Honors Level Philosophy of Science/Origins Science in a Christian University Environment*, Oral presentation and panel discussion session presented at the 58th annual Meeting of the American Scientific Affiliation at Colorado Christian University, Lakewood, Colorado, July 27, 2003.
13. Collier, W. B., *Predicting Infrared and Raman Spectra*. Sixty minute lecture presented at the March 16, 1999, American Chemical Society Tulsa Section meeting, The University of Tulsa, Tulsa, Oklahoma.
14. Collier, W. B., T. D. Klots, and I. Magdo, *Infrared and Raman Spectra of Bicyclic Molecules using Scaled Noncorrelated and Correlated Ab Initio Force Fields*. Poster presented at the 17th Austin

Symposium on Molecular Structure, The University of Texas at Austin, Austin, TX, March 2, 1998.

15. Collier, W. B., and T. D. Klots, *Accurate Prediction of IR and Raman Spectra of Bicyclic Molecules Using the Scaled Density Functional Calculated Ab Initio Force Field*. Presented at the 53th Southwest Regional Meeting of the American Chemical Society, Adam's Mark Hotel, Tulsa, OK, October 3, 1997.
16. Klots, T. D., and W. B. Collier, *Spectroscopy, SQM Calculations and Thermodynamics of Molecules Containing a Five-Membered-Ring at NIPER*. Presented at the 16th Austin Symposium on Molecular Structure, The University of Texas at Austin, Austin, TX, March 4, 1996.
17. Collier, W. B., and T. D. Klots, *Vibrational Frequencies for Polyatomic Molecules - Application of the Semi-empirical AM1 Hamiltonian to Mono and Bicyclo Heterocyclics and other Molecules*. Presented at the 39th Annual Pentasectional Meeting of the Oklahoma sections of the American Chemical Society, The University of Tulsa, Tulsa, OK, September 10, 1994.
18. Collier, W. B., and T. D. Klots, *Vibrational Frequencies for Polyatomic Molecules - Application of the Semi-empirical AM1 Hamiltonian to Mono and Bicyclo Heterocyclics and other Molecules*. Presented at Force Fields and Vibrational Analysis Symposium at the14th International Conference on Raman Spectroscopy, Hong Kong University of Science and Technology, Hong Kong, August 22, 1994. Invited speaker.
19. Klots, T. D., and W. B. Collier, *Vibrational Analysis of 2,5-dihydrofuran and 2.3-dihydorfuran*. Presented at the 38th Annual Pentasectional Meeting of the Oklahoma Sections of the American Chemical Society, Conoco Conference Center, Ponca City, OK, August 7, 1993.
20. Presented two, hour and a half long seminars on molecular spectroscopy at the invitation of area universities in Guiyang, Guizhou Province, People's Republic of China. The seminars were sponsored by Guizhou Institute of Technology, Guizhou University, Guizhou Normal University with faculty and graduate students from the three schools in attendance. The titles, dates, and locations of the two talks were:
    1 - Collier, W. B., *Far Infrared and Raman Vapor Phase Spectroscopy of Heterocyclic Compounds*, presented at Guizhou University on June 15, 1990.
    2 - Collier, W. B., *Determination and Calculation of Vibrational Frequencies for Polyatomic Molecules I. Indole and 2,3 Benzofuran Spectra and Analysis*, presented at Guizhou University on June 18, 1990.
21. Collier, W. B., *Vibrational Frequencies for Polyatomic Molecules*. Presented at 42nd Molecular Spectroscopy Symposium, Columbus, OH, June 1987.
22. Collier, W. B., and M. M. Strube, *Far Infrared and Raman Vapor Phase Spectroscopy of Heterocyclic Compounds*. Presented at 40th Molecular Spectroscopy Symposium at Columbus, OH, June 1985.
23. Collier, W. B., and J. P. Devlin, *Application of FT-IR Measurements to the Evaluation of Activation Energies for Proton Transfer in Protonic Solids*. Presented at 28th Annual Oklahoma Pentasectional Meeting of the American Chemical Society, Bartlesville, OK, March 20, 1982.
24. Collier, W. B., M. G. Rockley, and J. P. Devlin, *Resonant Coherent Anti-Stokes Raman Spectra of Rhodamine Dyes*. Presented at 25th Annual Oklahoma Pentasectional Meeting of the American Chemical Society, Oklahoma State University, Stillwater, OK, March 24, 1979.

OTHER PRESENTATIONS

1. Presented a nine session one hour adult education class on Wednesday nights at Kirk of the Hill Presbyterian Church, Tulsa Oklahoma, entitled, *Science Christianity Philosophy and Modern Myths*

Class: *A quick gentle Christian worldview tour and appraisal of the western secular worldview*, at the invitation of Kirk of the Hills Associate Pastor Sean Farver Kirk started, March 10, 2010

2. Presented an hour long sermon and PowerPoint presentation at my home church, Bread of Life, Tulsa, on *Christianity and Philosophy from Athens to America*, (a scriptural exposition on Paul's Areopagus, Mars Hill sermon and its implications for confronting today's secular philosophies), June 9, 2008 at the invitation of the church elders.

3. Presented an hour long presentation and talk on, *Christian Worldview, Irreducible Complexity, and the Metaphysical Naturalist Worldview*, to Kirk of the Hills Presbyterian Church, Tulsa, on February 9, 2005 at the invitation of Pastor Dr. Tom Grey.

ARRANGING AND MANAGING SPECIAL GUEST SPEAKERS AND MINI-CONFERENCES

1. Contacted and arranged for special guest speaker, Dr. Walter L. Bradley, to speak on campus at several different university forums. Dr. Bradley is distinguished Professor of Engineering at Baylor University coming from Texas A&M University where he was director of the nationally recognized Polymer Technology Center and Department Head of Mechanical Engineering. The talks and times were: Oral Roberts University; Learning Resources/Graduate Center, Tuesday, March 31, 2009**,** 8:00 pm, *Is There Scientific Evidence for the Existence of God (Advanced Version);* 8:50 am, *Science and Engineering in Service of the Poor: How Can We Possibly Make a Difference?* 11:00 am University Chapel Speaker, Christ's Chapel, *Is There Scientific Evidence for the Existence of God;* 12:30 pm, Luncheon Meeting for Faculty and Staff, Holy Spirit Room – Christ's Chapel; *On Being a Christian Professor in the Academy.*

2. Contacted and arranged for special guest speaker, Dr. Angus Menuge, to speak in several ORU classes and the Honors brown bag luncheon for the university faculty, honor students and students. Dr. Angus Menuge is Professor of Philosophy at Concordia University Wisconsin and with Gene Edward Veith, directs the Cranach Institute. Dr. Menuge is the author of *Agents Under Fire: Materialism and the Rationality of Science*, editor of three books, including *Reading God's World: The Vocation of Scientist*. He assisted the editors William Dembski and Michael Ruse in the preparation of *Debating Design: From Darwin to DNA* (Cambridge University Press, 2004). He served as an expert witness for the Science Education Standards Hearings in Topeka, Kansas, May, 2005. The talks and times were: Oral Roberts University; Learning Resources/Graduate Center, Tuesday, April 8, 2008**,** 9:30 am, *Refuting the Case for Methodological Materialism;* 12:30 pm, *Getting to the Point in Christian Apologetics*; 2:30 pm, *ID, Darwinism and Psychological Unity;* 7:30 pm *Philosophy through Story Telling in the Works of C. S. Lewis.*

3. Contacted and arranged for the special guest speaker, John Calvert, J.D., to speak in several ORU classes. John Calvert J.D. is the manager of IDNet, and co-founder of the Kansas group that changed the state of Kansas science education standards. The talks and times were: Oral Roberts University; Learning Resources/Graduate Center; Monday, April 2, 2007, 7:00 PM, Philosophy of Science and other combined classes, *Materialism: Its assault on our conscience and liberty;* Tuesday, April 3, 2007, 9:30 AM Comparative Government, Philosophy of Science, History of Theology (combined classes), *Intelligent Design and Materialism: their Impact on Government and Human Rights;* 10:50 AM Public Policy class, *Promoting Good Public Policy in a Materialistic Culture;* 12:10 PM Zios 81st and Lewis, *Faculty Lunch: Q&A*, 2:30 PM Government 101, *A Primer on Intelligent Design and Materialism: Why they are important to government;* 4:00 PM Combined Education Classes, *Two Models for Teaching Origins Science: The Kansas Experience.*

4. Presented a movie film showing and serious critique of the 1960 movie, *Inherit the Wind, to the campus community, April 12, 2008*. Dr. Paul Vickery of History and Humanities assisted me by impersonating H. L. Mencken, a famous newspaper reporter of the Scopes Trial. About 200-300 students showed up. This event was pre-publicity to generate student interest for the upcoming Phillip Johnson event.

5. *Arranged and hosted (in conjunction with the Faculty Christian Worldview Committee and others) the internationally known founder of the Intelligent Design Movement and best selling author of "Darwin on Trial"; emeritus UC Berkeley Professor of Law Phillip Johnson at three events at ORU on April 14*. The first event was a special faculty staff luncheon/talk that was attended by over 120 faculty and staff. The second event was a public lecture by Phillip Johnson in Christ's Chapel, *Design vs Naturalism: What is at Stake for our Culture?***,** that was attended by over 1000 faculty, students, and residents of Tulsa. The third event was a Worldview Supper/Consultation session attended by Phillip Johnson and select interested faculty and staff of ORU. The main second event in Christ's Chapel received a two-thirds page, front page article in the religion section of Tulsa's main newspaper, the Tulsa World.

6. *Arranged and hosted, Dr. Michael Keas,* of Oklahoma Baptist University as a special guest lecturer for the Philosophy of Science class and for a special faculty luncheon with Dr. Keas. His topic and luncheon discussion on, *The Meaning of the Cambrian Explosion*, was hosted on March 11, 2003. He is an Associate Fellow of the Discovery Institute based in Seattle, Washington.

RECENT RESEARCH AND WORK SPECIALIZATIONS

Origin Studies, Christianity and the Philosophy of Science

I am working on articles and research dedicated to understanding a post-critical Polanyian based philosophy that can reformulate modern scientific philosophy along lines less dedicated to scientism, and more open to theistic based rationality. My reading in the scientific and epistemological philosophy of Michael Polanyi and other leading scientists and philosophers of science has convinced me that our modern science textbooks are filled exclusively with simplistic Baconian induction explanations of the scientific method. Many really good scientists know; and all philosophers of science agree that these textbook explanations are at best inaccurate shells of the real thing, and quite possibly outright lies. How did we arrive at this state of affairs in scientific education, and what should be done to correct it? How does my faith interact in this process and where should science go in the future? How is our study of the origin of life impacted by our philosophical presuppositions? Where would we go if a Polanyian perspective was more widely embraced? I am currently investigating tentative answers and possibilities for these questions.

Molecular Spectroscopy - Vibrational Assignments of Molecules

Our research in this area applies vibrational analysis to problems in the pharmaceutical and energy industry. For example; ethyl 6-methyl-2-oxo-4-phenyl-1,2,3,4-tetrahydropyrimidine-5-carboxylate (**etpPC**) is a pharmaceutically interesting Biginelli condensation reaction product. The urea moiety on the dihydro-priminidinone ring is responsible for dimerization of **etpPC** in solution. We study the vibrational spectra of compounds like these matrix isolated in inert argon gas at 18 K. There it is easier to isolate the spectra of the monomers and dimers apart from the extensive hydrogen bonding that greatly complicates the liquid and solid phase spectra of compounds like this. By using SQM scaled ab initio calculated infrared and Raman spectra calculated *in silico*, with software developed in this lab, it is possible to make reasonable normal mode assignments even when several conformers are present. This vibrational analysis allows us to make predictions about the native conformal states of the molecule and how they might possibly interact under pharmaceutical conditions. The prediction of vibrational spectra for larger molecules is currently found through ab initio calculation of the vibrational frequencies and intensities, typically with density functional theory. A scaling procedure usually brings the calculated frequencies into near agreement with the experimental observed harmonic frequencies. The best scaling procedure uses the Pulay Scaled Quantum Mechanical (SQM) method of scaling the calculated force constants in internal coordinate space on specific coordinate types. This method was programmed and adapted for use on large molecules in a series of software packages named FCART01, FCART06; with the latest release being Fcart version 7.0. It is being released to the research and educational public through http://www.fcart.wbcollier.com. Future work will extend the vibrational and computational methods to additional large molecules and other molecules of chemical interest. The energy industry is interested in developing a comprehensive thermodynamic database of fossil fuel components. Using the SQM methods developed earlier we have obtained the complete fundamental vibrational assignment of bi and tricyclic heteroaromatic compounds. The traditional methods of collecting the infrared and Raman spectra are difficult for these high boiling point compounds. New cell designs and sampling techniques were constructed and used for obtaining the low-frequency vapor spectra of these compounds.

Matrix - Isolation Spectroscopy

Recent work with matrix isolation has focused on the energetics of heteroaromatic ring systems and the vibrational analysis of large pharmaceutically interesting molecules as described previously. We have found that vacuum deposited amorphous or crystalline adenine mixed with D_2O at 100 K does not exchange its

labile protons and deuterons upon annealing at 185 K; but H_2O and D_2O within the mix do. This is very suggestive of a long range proton conduction mechanism in the crystalline D_2O that is not disrupted by the extensive inclusion of adenine. The research goals are to develop new structure prediction tools using quantum mechanical calculation of vibrational properties, to understand proton conduction in biologically important molecules, and provide experimental models for checking computational chemistry calculations.

Programming and Instrumentation Development

Our lab is working on extending the range and scope of the Pulay SQM method of scaling calculated force constants. This includes finding new SQM scale factors for the newer more extensive basis sets and functionals that have become feasible for current spectroscopic calculation of spectra. We recently have extended the SQM method to 13 new polarized and augmented basis sets based on the 6-31G and 6-311G double and triple split valence basis sets using a B3LYP density functional. We have modestly improved the overall accuracy of the method while providing 13 new basis sets with polarizations and augmentation schemes that can greatly improve the modelling of complex hydrogen bonded dimer, trimers and n-mers of molecules, and improve the structural and spectral accuracy in predicting the properties of larger molecules with difficult functional groups. These results were released in a comprehensive software package named Fcart version 7.0; that is available to the research public.

Recent work has focused on integrating previously written Fortran programs packages with Visual Basic GUI front ends that graphically display the molecule with mouse selected rotational orientations and sizes, and controls the overall data manipulation and output and extending the computational features. Two extensive Fortran packages were written to aid the molecular spectroscopist in calculating accurate thermodynamic functions and to assist the spectroscopist in obtaining accurate zero-order predictions of vibrations for large molecules using ab-initio molecular orbital force field calculations. These two program packages were submitted to the Quantum Chemistry Program Exchange at the University of Indiana for general distribution to interested parties. Since the demise of the QCPE software exchange, I have written and extended the originally submitted Pulay SQM scaling package FCARTP, to FCART01, FCART06, and lately Fcart version 7.0, adding new features so that it accepts input from various public domain and commercial ab-initio molecular orbital structure programs, and displays the results in ways that professional spectroscopists can use to advance their research. It is being distributed via my own webpage.

A Visual Basic instrument control program was written to drive the digital control and digital data acquisition from a Fast Fourier Transform Infrared Spectrometer. The FFT of the data, display, manipulation and printing of the spectrum was user controlled and implemented from within the control program. Many similar instrument control programs have been written and implemented to control HPLC gradients elution, NMR data collection and control, and Raman Spectrometer control, data collection and manipulation.

Commercial Consulting

I have consulted with various companies, SemMaterials, L.P. of the SemGroup corporation, Tulsa, OK, RenTech Corporation, Denver, CO; Syntroleum Corporation, Tulsa; OK; BDM-Oklahoma Petroleum Technologies, Bartlesville, OK; on method development for analytical services, GC, FTIR, IR, HPLC, UV-Vis, and other methods, data analysis and experimental design, and the development of novel spectroscopic methods for thermodynamic analysis and database development.