

NIEHS CV

CURRICULUM VITAE (7-15-2017)

Name: Lee G. Pedersen

Work Address: Chemistry, CB#3290 University of North Carolina-CH, NC 27599

Date & Place of Birth: June 15, 1938; Oklahoma City, OK.

Citizenship: USA

Education:

Benedictine Heights College, Tulsa, OK.

B.S. (Chemistry) U. Tulsa, Tulsa, OK.

Ph.D. (Chemistry) U. Arkansas, Fayetteville, AK.

PROFESSIONAL EXPERIENCE and Activities:

Undergraduate Teaching Assistant, University of Tulsa, 1960-61.

Graduate Research Assistant, University of Arkansas, 1961-65.

Postgraduate Research Fellow, Columbia University, 1965-66.

Postgraduate Research Fellow, Harvard University, 1966-67.

Assistant Associate, Full Professor, University of North Carolina-CH 1967-1999

M. A. Smith Prof. Chemistry 1999-2005

Adjunct Prof. Chem. (retired from teaching, full time research) 2006-2016

Prof. Emeritus 2016-

Visiting Scientist, NIEHS, RTP, 1984-85, 1989-90, Research Chemist, NIEHS 1986-2010, visitor NIEHS 2010-present

AWARDS:

Full Four Year Scholarship, Benedictine Heights College, Tulsa, OK 1956

Full Academic Scholarship, University of Tulsa, 1958-59

NASA Predoctoral Fellowship, University of Arkansas, 1962-65

NSF Postdoctoral Fellowship, Columbia University, 1965-66

NIH Postdoctoral Fellowship, Harvard University, 1966-67

Tanner Award for Excellence in Undergraduate Teaching, University of North Carolina at Chapel Hill, 1970

Lee G. Pedersen Chair created by the University (currently held by the Dean of AS)

RECENT ACTIVITIES (Presentations)

March 2003 American Physical Soc. Invited Symposium. Issues in Modeling Blood Coagulation Complexes.

December 2003 Laboratory of Structural Biology NIEHS Issues in modeling Blood Coagulation Complexes

Jan 2004 UNC-W Symposium Speaker Modeling Blood Coagulation Proteins

Nov 4 Biophysical Symposium RTP Session Chair

Apr 2005 NIEHS Deuterium in Biology

Apr 2005 Session Chair Symposium for MKarplus NIH Washington DC

March 2006 Santa Fe Thom Dunning Appreciation Conference Speaker DNA beta polymerase

March 2006 ACS National Atlanta DNA beta Polymerase

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March 2006 ACS National Atlanta Vitamin K Mechanism Q. Mech.
May 2006 FVIIa/TF symp Chapel Hill: Comparison of FVIIa/TF and FVIIa(free).
Sept 2006 NIEHS Energy analysis for correct insertion by DNA Polymerase Beta
Dec 2006 UNC-G Chemistry Energy analysis for correct insertion by DNA Pol

Beta

Jan 2007 UNC-CH Chem Energy analysis for correct insertion by DNA Pol Beta
Sept 2007 NIEHS LSB Theoretical Study of the Vitamin K cycle
Nov 2008 NIEHS LSB Making Thrombin: Computational Issues
Apr 2010 5th FVIIa/TF Symposium NC The Ternary complex of TF/FVIIa/FXa
Aug 2010 Speaker at Whitten Symposium, Albuquerque NM (UMN) Prothrombin
Dec 2011 NIEHS LSB Prothrombin
Sept 2013 Indianapolis National Meeting. Symposium honoring Darden, York and Pedersen. Talk on Molecular Dynamics in Bioinformatics. ACS

Reviewer For Professional Journals and Granting agencies

Austrian Research Foundation
J. Computational Chemistry
J. Physical Chemistry
J. Chem. Phys.
Biochemistry
Proceedings National Acad. of Sciences (USA)
Proteins
J. Chemical Physics
J. of the Am. Soc. For Mass Spectrometry
J. Am. Chemical Soc.
J. Inorganic Biochemistry
International J. Quantum Chemistry
International Revs. Phys. Chemistry
J. Mol. Modeling
J. Mol. Graphics and Model.
J. Throm. Haem.
Throm. Haem.
BioPhysChem
PRF Grant Reviews (Theoretical Chemistry)
NSF Grant Reviews (Theoretical/Biophysical Chemistry)
NIH Program Project Reviewer

Membership in Professional Organizations

American Chemical Society, American Physical Society
American Association for Advancement of Science

Editorial Boards

World Journal of Biological Chemistry
Biophysical Chemistry

Publications in Reviewed Journals

[Ref. 125 and 139 are possibly the second and third most cited papers at UNC-CH Chemistry: >9838 and >7903 times, resp; WOS 1/16/2017. Both papers have about 1500 more citations each in Google Scholar. Mathematician Tom Darden was the “genius” behind them. Ulli Essemann (a phd student w. Max Berkowitz) took a lead role on the second and Darrin York (a g. student with me) contributed significantly to the first. JLT fairly points out, however, that some of the other papers are “dogs”; Ref. 261 (a book with Charles S. Johnson, Jr.) is a Dover Classic.) and therefore may not be a “dog”. Some of my publications are cited as L. Pedersen, some as LG Pedersen and others as L Pederson]

1. Amis, E.S. and L.G. Pedersen, *The equivalent conductance of electrolytes* Z. Physik. Chem. Neue. Folge, 1963. **36**: p. 205.
2. Morokuma, K., L.G. Pedersen, and M. Karplus, *Vibrational vs. translational activation in the (H₂, H₂) and (H₂, D₂) exchange reactions*. Journal of the American Chemical Society, 1967. **89**: p. 5064.
3. Pedersen, L.G. and K. Morokuma, *Ab initio calculations of the barriers to internal rotation of CH₃-CH₃ etc.* Journal of Chemical Physics, 1967. **46**: p. 3941.
4. Pedersen, L.G. and R.N. Porter, *A modified semiempirical approach to the H₃ potential energy surface*. Journal of Chemical Physics, 1967. **47**: p. 4751.
5. Morokuma, K. and L.G. Pedersen, *Molecular orbital studies of hydrogen bonds: an ab initio calculation for dimeric H₂O*. Journal of Chemical Physics, 1968. **48**: p. 3275.
6. Pedersen, L.G. and M. Karplus, *The structure of CH₃ and CF₃*. Journal of Chemical Physics, 1968. **48**: p. 4081.
7. Pedersen, L.G., *The barrier to internal rotation of O₂F₂*. Journal of Molecular Structure, 1969. **3**: p. 510.
8. Pedersen, L.G., D.G. Whitten, and T. McCall, *Excited states of N-hetero molecules*. Chemical Physics Letters, 1969. **3**: p. 569.
9. Pedersen, L.G., *Possible contributing structures in polywater*. Chemical Physics Letters, 1969. **4**: p. 280.
10. Pedersen, L.G. and R. Griffin, *On the structure of the li-naphthalenide anion*. Chemical Physics, 1970. **5**: p. 373.
11. Pedersen, L.G., *The structure of the triatomic free radicals HCO, HCN-, FCO*. Journal of Molecular Structure, 1970. **5**: p. 21.
12. Lee, Y.J., D.G. Whitten, and L.G. Pedersen, *Importance of 1n, a* states in N-heterocycles*. Journal of the American Chemical Society, 1971. **93**: p. 6330.
13. Pedersen, L.G., K. Gammon, and D. Hoskins, *Rotational relaxation in the H₂, Ar system. A Monte Carlo trajectory calculation*. Chemical Physics Letters, 1971. **11**: p. 407.
14. Pedersen, L.G., R.G. Hoskins, and H. Cable, *The preferred conformation of noradrenaline*. J. Pharm. Pharmacol., 1971. **23**: p.

- 216.
15. Cable, H., A. Rauch, and L.G. Pedersen, *The preferred conformation of cyclophosphamide*. J. Pharm. Pharmacol., 1973. **25**: p. 509-510.
 16. Parker, C., M.M. Bursey, and L.G. Pedersen, *Scrambling in ethane molecular ion: an indo model for hydrogen exchange before mass spectral fragmentation*. Organic Mass Spectrometry, 1973. **7**: p. 1077.
 17. Parker, C., J.R. Haas, M.M. Bursey, and L.G. Pedersen, *The ortho effect in mass spectra, insight into the tightening of activated complexes for the loss of ketene from phenyl acetates and ethylene from phenetoles from indo molecular orbital calculations*. Organic Mass Spectrometry, 1973. **7**: p. 1189.
 18. Parker, C., M.M. Bursey, and L.G. Pedersen, *Internal rotation in the molecular ions of benzoic acid and salicylic acid. An indo molecular orbital approach*. Organic Mass Spectrometry, 1974. **7**: p. 204.
 19. Bursey, M.M., R.S. Greenberg, and L.G. Pedersen, *Position of protonation of the cresols: Semi-empirical and ab initio calculations*. Chemical Physics Letters, 1975. **36**: p. 470.
 20. Carlson, G. and L.G. Pedersen, *Extension of GAUSSIAN70 to any number of atomic orbitals*. Journal of Computational Physics, 1975. **17**: p. 38.
 21. Carlson, G. and L.G. Pedersen, *An ab initio investigation of S₈*. Journal of Chemical Physics, 1975. **62**: p. 4567.
 22. Kao, J.L., M.M. Bursey, and L.G. Pedersen, *The lowest electronic states of the benzoyl ion. A molecular orbital study with configuration interaction*. Organic Mass Spectrometry, 1975. **10**: p. 38.
 23. Pedersen, L.G. and G. Carlson, *The planarity of hexachlorobenzene: an ab initio investigation*. Journal of Chemical Physics, 1975. **62**: p. 2009.
 24. Pedersen, L.G., *The correlation of partial and total scores of the SAT of the CEEB with grades in freshman chemistry*. Educational Psychological Measurement, 1975. **35**: p. 509.
 25. Putnam, J.B. and L.G. Pedersen, *Discovery of a cyclic 3'-5'guanosine monophosphate simulating factor in amoebae of dictyostelium discoideum*. Biochimica et Biophysica Acta, 1975. **411**: p. 168.
 26. Carlson, G.L., H. Cable, and L.G. Pedersen, *An ab initio investigation of ascorbic acid*. Chemical Physics Letters, 1976. **38**: p. 75.
 27. Greenberg, R.S., M.M. Bursey, and L.G. Pedersen, *Molecular orbital studies of the protonation of the methylanisoles*. Journal of the American Chemical Society, 1976. **98**: p. 4061.
 28. McLean, W., L.G. Pedersen, and R. Jarnagin, *Alkyl-metal surface complexes: methyl and lithium*. Journal of Chemical Physics, 1976. **65**: p. 2491.
 29. Pedersen, L.G. and G. Carlson, *Molecular fragment transfer in ab initio calculations*. Computers & Chemistry, 1976. **1**: p. 137.
 30. Pedersen, L.G., *Lower level freshman chemistry: how to choose the*

- audience*. Journal of Chemical Education, 1976. **53**: p. 418.
31. Rehnsteiner, C., R.P. Buck, and L.G. Pedersen, *Experimental and theoretical studies on M_2X^+ ($M=Li, Na; X=F, Cl$)*. Journal of Chemical Physics, 1976. **65**: p. 1659.
 32. Peacock, W., J.B. Putnam, and L.G. Pedersen, *Massive body collisions with the solar system*. The Astronomy Quarterly, 1977. **1**: p. 201.
 33. Adamson, S.M.E. and L.G. Pedersen, *The interaction of charged disks in a dielectric medium*. Journal of Chemical Physics, 1978. **68**: p. 4333.
 34. Capitani, J.F. and L.G. Pedersen, *Rotational barriers in the guanidinium ion: an ab initio study*. Chemical Physics Letters, 1978. **54**: p. 547.
 35. Eslava, A., J.B. Putnam, and L.G. Pedersen, *An ab initio investigation of molecules with a disulfide bond: $(HS)_2$, $(CH_3S)_2$ and cystine*. International Journal of Peptide and Protein Research, 1978. **11**: p. 149.
 36. Bursey, M.M., J. Hass, D. Harvan, C. Parker, and L.G. Pedersen, *Consequences of charge reversal of gaseous formate ions. Acyloxy ion*. Journal of the American Chemical Society, 1979. **101**: p. 5489.
 37. Evans, J. and L.G. Pedersen, *A simple and inexpensive solar energy experiment*. Journal of Chemical Education, 1979. **56**: p. 339.
 38. McLean, W., J. Schultz, L.G. Pedersen, and R.C. Jarnagin, *The structure and formation of methyllithium ionic fragments*. Journal of Organometallic Chemistry, 1979. **175**: p. 1.
 39. Schultz, J., W. McLean, and L.G. Pedersen, *Surface complexes between O_2/H_2O , and lithium*. Surface Science, 1979. **83**: p. 354.
 40. Schultz, J.A., W. McLean, L.G. Pedersen, and R.C. Jarnagin, *H_2O on Li_n clusters: a theoretical study*. Chemical Physics Letters, 1979. **64**: p. 230.
 41. Sarasua, M.M., M.E. Scott, J.A. Helpert, P.B.W. Tenkortenaar, N.T. Boggs, L.G. Pedersen, K.A. Koehler, and R.G. Hiskey, *Europium Ion Coordination with Gamma-Carboxyglutamic Acid Containing Ligand Systems*. Journal of the American Chemical Society, 1980. **102**(10): p. 3404-3412.
 42. Schultz, J.A., S. Gates, L.G. Pedersen, and R.C. Jarnagin, *Methoxide Surface Complexes on Lithium*. Chemical Physics Letters, 1980. **72**(1): p. 156-161.
 43. Youngless, T.L., M.M. Bursey, and L.G. Pedersen, *Chemical-Field Ionization - Effect of Chemically Bonded Surface Groups in Field-Ionization Mass-Spectrometry*. Journal of the American Chemical Society, 1980. **102**(22): p. 6881-6882.
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45. Gottschalk, K.E., R.G. Hiskey, L.G. Pedersen, and K.A. Koehler, *A Theoretical-Study of Malonate Ion and Its Metal-Binding by Abinitio and Semi-Empirical Techniques*. *Theochem-Journal of Molecular Structure*, 1981. **1**(2): p. 197-201.
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47. Fraley, D.F., L.G. Pedersen, and M.M. Bursey, *Resistive Heating of Emitter Wires for Field Desorption and Ionization - a Theory*. *International Journal of Mass Spectrometry and Ion Processes*, 1982. **43**(2-3): p. 99-129.
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50. Madar, D.A., M.M. Sarasua, H.C. Marsh, L.G. Pedersen, K.E. Gottschalk, R.G. Hiskey, and K.A. Koehler, *The Relationship between Protein-Protein and Protein-Lipid Interactions and the Immunological Properties of Bovine Prothrombin and Several of Its Fragments*. *Journal of Biological Chemistry*, 1982. **257**(4): p. 1836-1844.
51. Schultz, J.A., S.M. Gates, L.G. Pedersen, and R.C. Jarnagin, *Surface Complexes Formed by Monohydric Alcohols on Lithium*. *Surface Science*, 1982. **118**(3): p. 634-648.
52. Bursey, M.M., R.L. Cerny, L.G. Pedersen, K.E. Gottschalk, K.B. Tomer, and T.A. Lehman, *Direct Observation of the H₂no₂-Ion*. *Journal of the Chemical Society-Chemical Communications*, 1983(9): p. 517-518.
53. Long, G.A., J.F. Capitani, and L.G. Pedersen, *A theoretical investigation of molecular NaOH*. *Journal of Molecular Structure*, 1983. **105**: p. 229.
54. McKinney, J.D., K.E. Gottschalk, and L.G. Pedersen, *A theoretical investigation of the conformation of polychlorinated biphenyls (PCB's)*. *Journal of Molecular Structure*, 1983. **104**: p. 445.
55. McKinney, J.D., K.E. Gottschalk, and L.G. Pedersen, *The polarizability of planar aromatic systems. An appli. to polychlorinated biphenyls (PCB's), dioxins and polyaromatic hydrocarbons*. *Journal of Molecular Structure*, 1983. **105**: p. 427.
56. Gates, S.M., H.M. Meyer, L.G. Pedersen, and R.C. Jarnagin, *Electronic and Geometric Structure of Acetylide Carbon on the Surface of Lithium*. *Surface Science*, 1984. **140**(2): p. 455-471.

57. Long, G.A., R.G. Hiskey, L.G. Pedersen, and K.A. Koehler, *The Role of Gamma-Carboxyglutamic Acid (Gla) in Blood-Clotting Proteins - a Theoretical-Study of Mg-Malonate Complexes*. *Theochem-Journal of Molecular Structure*, 1984. **17**(3-4): p. 173-178.
58. McKinney, J.D., G.A. Long, and L.G. Pedersen, *PCB and dioxin binding to cytosol receptors: a theoretical model based on molecular parameters*. *Journal of Quantitative Structure Activity Relationships*, 1984. **3**: p. 99.
59. Mooney, W.F., P.E. Brown, J.C. Russell, S.B. Costa, L.G. Pedersen, and D.G. Whitten, *Photochemical-Reactions in Organized Assemblies .37. Photochemistry and Photophysics of Surfactant Trans-Stilbenes in Supported Multilayers and Films at the Air Water Interface*. *Journal of the American Chemical Society*, 1984. **106**(19): p. 5659-5667.
60. Washington, K., M.M. Sarasua, L.S. Koehler, K.A. Koehler, J.A. Schultz, L.G. Pedersen, and R.G. Hiskey, *Utilization of Heavy-Atom Effect Quenching of Pyrene Fluorescence to Determine the Intramembrane Distribution of Halothane*. *Photochemistry and Photobiology*, 1984. **40**(6): p. 693-701.
61. Bursey, M.M., D.J. Harvan, L.G. Pedersen, and A.T. Maynard, *Direct Observation of the Htio3-Ion*. *Inorganic Chemistry*, 1985. **24**(26): p. 4748-4749.
62. Kabis, C.W., M.M. Sarasua, K.E. Gottschalk, C.D. Bourne, L.G. Pedersen, C.M. Jackson, R.G. Hiskey, and K.A. Koehler, *A Kinetic-Model Describing the Interaction of Bovine Prothrombin Fragment-1 with Calcium-Ions*. *Thrombosis and Haemostasis*, 1985. **53**(1): p. 19-23.
63. Maynard, A.T., R.G. Hiskey, L.G. Pedersen, and K.A. Koehler, *An Abinitio Mo Study of Calcium and Magnesium Complexes with Malonate and Formate*. *Theochem-Journal of Molecular Structure*, 1985. **25**(3-4): p. 213-221.
64. McKinney, J.D., T. A. Darden, M.A. Lyerly, and L.G. Pedersen, *Pcb and Related Compound Binding to the Ah Receptor(S) Theoretical-Model Based on Molecular-Parameters and Molecular Mechanics*. *Quantitative Structure-Activity Relationships*, 1985. **4**(4): p. 166-172.
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66. Darden, T. A., J.D. McKinney, K. Gottschalk, A.T. Maynard, and L.G. Pedersen, *A Theoretical-Study of the Minimum Energy Structures of Diethylstilbestrol and Its Analogs by Molecular Mechanics (Mm2p), Mndo, and Abinitio Calculations*. *Journal of the American Chemical Society*, 1986. **108**(2): p. 207-211.
67. Deerfield, D.W., R.A. Hoke, L.G. Pedersen, T. A. Darden, and R.G. Hiskey, *Relative Spectral Response as a Function of Sequential Ligand-Binding*. *Biochemical and Biophysical Research*

- Communications, 1986. **141**(3): p. 1207-1212.
68. Deerfield, D.W., P. Berkowitz, D.L. Olson, S. Wells, R.A. Hoke, K.A. Koehler, L.G. Pedersen, and R.G. Hiskey, *The Effect of Divalent Metal-Ions on the Electrophoretic Mobility of Bovine Prothrombin and Bovine Prothrombin Fragment-1*. *Journal of Biological Chemistry*, 1986. **261**(11): p. 4833-4839.
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70. Hoke, R.A., D.W. Deerfield, L.G. Pedersen, K.A. Koehler, and R.G. Hiskey, *Synthesis of a Gamma-Carboxyglutamic Acid Containing Heptapeptide Corresponding to Bovine Prothrombin Residues 17-23*. *International Journal of Peptide and Protein Research*, 1986. **28**(6): p. 569-578.
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- Hiskey, *Chemical Modification of Bovine Prothrombin Fragment-1 in the Presence of Tb-3+ Ions*. Journal of Biological Chemistry, 1986. **261**(23): p. 598-605.
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87. Pedersen, L.G., T.A. Darden, D.W. Deerfield, M.W. Anderson, and D.G. Hoel, *A Theoretical-Study of the Effect of Methylation or Ethylation at O-6 Guanine in the Structure and Energy of DNA Double Strands*. Carcinogenesis, 1988. **9**(9): p. 1553-1562.
88. Pollock, J.S., A.J. Shepard, D.J. Weber, D.L. Olson, D.G. Klapper, L.G. Pedersen, and R.G. Hiskey, *Phospholipid Binding-Properties of*

- Bovine Prothrombin Peptide Residues 1-45*. Journal of Biological Chemistry, 1988. **263**(28): p. 14216-14223.
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