Index

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1. Education

- B. Sc. Queen's University, Kingston 1965
- Ph. D. Queen's University, Kingston 1968
- Research Associate in Chemistry, Princeton 1968
- Visiting Fellow, Princeton 1970
- Sabbatical Leave, King's College, London, 1976 - 7.
- Sabbatical Leave, Research School of Chemistry, Australian National University, Canberra, 1984 - 4.
- Visiting Fellow, Research School of Chemistry, Australian National University, Canberra, 1988.
- Sabbatical Leave (6 mo), University of Calgary, 1991.
- Sabbatical Leave (6 mo), University of New England, Australian National University, Universite Louis Pasteur, 1995.

(return to Index)

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2. Employment

University of Calgary 1970-present

- Assistant Professor 1970
- Associate Professor 1975
- Professor 1980
- Professor Emeritus and Faculty Professor 2000

(return to Index)

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3. Teaching

- Undergraduate courses
  - Fall 1996,7 - Chemistry 354 (Organic Chemistry for Chemists)
  - Winter 1997,8,9 - Chemistry 357 (Organic Chemistry for Engineers)
- Graduate courses
  - Winter 1998 - Chemistry 657 (Theoretical Organic Chemistry)

Fall 2003 - Chemistry 657 (Theoretical Organic Chemistry)

- Graduate student supervision (recent)
    - Remo Dutler 1984-1989 (PhD)
    - Danya Yang 1989-1994 (PhD)
    - David A. Block 1997-2000 (MSc)
    - M. Jake Pushie 2001-Dec. 2002(MSc)
    - Patrick Brunelle 2001-2005 (PhD)
    - Duilio F. Raffa - from May 2003 - 2007 (PhD)
    - Samir Roy - from Jan. 2004 - Jan. 2010 (PhD)
    - Anahit Petoyan - from Jan. 2011 - present (MSc)
    - Stanley Opare - from Sept. 2011 - present (MSc)
- Summer student supervision (recent)
    - Jeffrey Waller 1996
    - Jerry Taylor 1997
    - Bonnie Leung 2002
    - Stephen Barry 2005
    - Nadine Hewitt 2008

(return to Index)

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4. Research Projects

- Theoretical studies of oxidative damage to peptides and proteins.
- The chemistry of Alzheimer's and other neurological diseases
- Theoretical studies of electron deficient molecules and free radicals
- Theoretical study of natural optical activity - CD and VCD

(return to Index)

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5. Research Publications

P**ublications since 1983** - A. RAUK (approximate lifetime numbering)

226. Badran, Ismail ; Rauk, Arvi ; Shi, Yujun, New Orbital Symmetry-Allowed Route for Cycloreversion of Silacyclobutane and Its Methyl Derivatives, JOURNAL OF PHYSICAL CHEMISTRY A, 2019, 123(9), 1749-1757.

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224. Banafsheh Mehrazma and Arvi Rauk, Exploring amyloid-beta dimer structure using molecular dynamics simulations, J. Phys. Chem. A, 2019, 123, 4658-4670. http://dx.doi.org/10.1021/acs.jpca.8b11251.

223. Badran, Ismail; Rauk, Arvi; Shi, Yujun, New Orbital Symmetry Allowed Route for Cycloreversion of Silacyclobutane and Its Methyl Derivatives, J. Phys. Chem. A, Manuscript ID: jp-2018-08071z.R3

222. Banafsheh Mehrazma, Stanley Opare, Anahit Petoyan and Arvi Rauk, D-Amino Acid Pseudopeptides as Potential Amyloid-Beta Aggregation Inhibitors, Molecules, 2018, 23, 2387; doi:10.3390/molecules23092387

221. Arvi Rauk, ß-N-Methylamino-L-alanine (BMAA) and Alzheimer's, J. Phys. Chem. B, 2018, 122(16):4472-4480. DOI 10.1021/acs.jpcb.8b01641

220. Stanley K. A. Opare and Arvi Rauk, Copper(I) chelators for Alzheimer's disease, J. Phys. Chem. B 2017, 121 (50), 11304-11310: DOI: 10.1021/acs.jpcb.7b10480

219. Alexander Tennant, Arvi Rauk, and Michael Wieser, Computational Modelling of the Redistribution of Copper Isotopes by Proteins in the Liver, Metallomics, 2017, 9, 1809-1819, DOI:10.1039/C7MT00248C

218. Banafsheh Mehrazma; Morgan Robinson; Stanley Opare; Anahit Petoyan; Jennifer Lou; Francis T Hane; Arvi Rauk; Zoya Leonenko, Pseudopeptide amyloid-<beta> blocking inhibitors: Molecular Dynamics and Single Molecule Force Spectroscopy study. BBA - Proteins and Proteomics. SI: Biophysics in Canada. 2017, 1865, 1707-1718. https://doi.org/10.1016/j.bbapap.2017.07.022

217. Zohreh Amini, Mohammad Hossein Fatemi and Arvi Rauk, Molecular Dynamics studies of a b-sheet blocking peptide with the Amyloid Beta Peptide of Alzheimer's Disease, Can. J. Chem. 2016, 94(10): 833-841; DOI: 10.1139/cjc-2016-0267

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215. S. K. A. Opare, A. Petoyan, B. Mehrazma, and A. Rauk, Molecular Dynamics Study of the Monomers and Dimers of N-Ac-Ab(13-23)NH2: On the Effect of pH on the Aggregation of the Amyloid Beta Peptide of Alzheimer.s Disease, Canadian Journal of Chemistry, 2016, 94(4): 273-281, 10.1139/cjc-2015-0036

214. Francis Hane, Brenda Yasie Lee, Anahit Petoyan, Arvi Rauk, and Zoya Leonenko, Testing Synthetic Amyloid-? Aggregation Inhibitor Using Single Molecule Atomic Force Spectroscopy, Journal of Biosensors and Bioelectronics, 2014, 54: 492-498: https://doi.org/10.1016/j.bios.2013.10.060

213. Samira Azimi and Arvi Rauk, Fe(III)-Heme Complexes with the Amyloid Beta Peptide of Alzheimer's Disease: QM/MM Investigations of Binding and Redox Properties, Journal of Chemical Theory and Computation, 2013, 9 (9), pp 4233-4242: DOI: 10.1021/ct400364b.

212. Ismail Badran, Arvi Rauk, and Yujun Shi, A theoretical study on the ring-opening of 1,3-disalacyclobutane and H2 elimination, J. Phy. Chem. A, 2012, 116, 11806-11816: DOI: 10.1021/jp3087122

211.Press, David J.; McNeil, Nicole M. R.; Rauk, A.; Back, T. G., NMR and Computational Studies of the Configurational Properties of Spirodioxyselenuranes that Act as GPx Mimetics. Are Dynamic Exchange Processes or Temperature-Dependent Chemical Shifts Involved? - J. Org. Chem., 2012, 77, 9268-9276: DOI: 10.1021/jo301846a

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209 . T. Wondimagegn and A. Rauk, The Structures and Stabilities of the complexes of biologically available ligands with Fe(II)-Porphine: an ab initio study, J. Phys. Chem. B, 2012, 116, 10301-10310: DOI: 10.1021/jp305864y

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207. Michael H. Benn, Arvi Rauk, and Thomas W. Swaddle, Measurement of the interaction of aqueous copper(II) with a model amyloid-â protein fragment — Interference from buffers. Can. J. Chem. 89: 1429–1444 (2011): DOI: 10.1139/V11-101

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204 . T. Wondimagegn and A. Rauk, The Structures and Stabilities of the complexes of biologically available ligands with Fe(III)-Porphine: an ab initio study, J. Phys. Chem. B, 115 (2011), 569-579.DOI: 10.1021/jp1090747

203. M. H. Benn, M. Parve,N. B. Perry, A. Rauk, and J. W. van Klink, H09289. Correction of a Reported Xanthone Synthesis: the Preparation of a Benzo[c]coumarin, Helv. Chim. Acta , 93 (2010) 389-394.

202. Michael Benn, Yan Yan Huang, Frank Johannsen, Michael O'Reilly, Masood Parvez, Arvi Rauk , and Ted Sorensen, Concerning the conformational preferences of the 2-cyano derivatives of oxane, thiane and selenane, Can. J. Chem., 88, 831-838 (2010).

201. Oya Ünsal Tan, Kevser Özden, Arvi Rauk and Ayla Balkan., Synthesis and Cyclooxygenase Inhibitory Activities of Some N-Acylhydrazone Derivatives of Isoxazolo[4,5-d]pyridazin-4(5H)-ones. European Journal of Medicinal Chemistry (2010), 45, 2345-2352.

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198. S. D. Barry, G. A. Rickard, M. J. Pushie, and A. Rauk The Affinity of HGGG, GHGG, GGHG, and GGGH Peptides for Copper(II) and the Structures of their Complexes. An Ab Initio Study, Can. J. Chem. in press (2009)

197. N. Hewitt and A. Rauk, The Mechanism of Hydrogen Peroxide Production by Copper-bound Amyloid Beta Peptide: A Theoretical Study. J. Phys. Chem. B, 113, 1202-1209 (2009).

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* 195. S. Sharma, A. Rauk, and A. H. Juffer,A DFT Study on the Formation of a Phosphohistidine Intermediate in Prostatic Acid Phosphatase, J. Am. Chem. Soc. 130, 9708-9716 (2008)

* 194. A. Rauk, Why is the amyloid beta peptide of Alzheimer's disease neurotoxic?, Dalton Trans. (invited Frontier, 2008, 1273-1282 (2008). [On most-accessed list for 2008]

* 193. G. A. Rickard, J. Bergès, C. Houée-Levin and A. Rauk An Ab Initio and QM/MM Study of Electron Addition on the Disulfide Bond in Thioredoxin, J. Phys. Chem. B, 112, 5774-5787 (2008)

* 192 J. Bergès, G. A. Rickard, A. Rauk and C. Houée-Levin, Proton Distribution in One-electron Reduced Thioredoxin modulated by Aspartate30. A QM/MM study. Chem. Phys. Lett, 454, 118-123 (2008).

* 191. D. F. Raffa and A. Rauk, Molecular Dynamics Study of the Beta Amyloid Peptide of Alzheimer's Disease and its Divalent Copper Complexes, J. Phys. Chem. B, 111, 3789-3799 (2007)

190. D. A. Armstrong, W. L. Waltz, A. Rauk Carbonate Radical Anion: Thermochemistry, Can. J. Chem. 84, 1614-1619 (2006)189 G. P. F. Wood, C. J. Easton, A. Rauk, and L. Radom,The Effect of Specific Residues on Competing Pathways for beta-Scission Reactions of Peptide-Backbone Alkoxyl Radicals, J. Phys. Chem. A, 110, 10316-10323 (2006).

189. G. P. F. Wood, C. J. Easton, A. Rauk, and L. Radom,The Effect of Side Chains on Competing Pathways for beta-Scission Reactions of Peptide-Backbone Alkoxyl Radicals, J. Phys. Chem. A, 110, 10316-10323 (2006).

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187. P. Brunelle, C. Schoeneich, and A. Rauk, One-Electron Oxidation of Methionine Peptides: Stability of the Three-Electron SN(Amide) Bond, Can. J. Chem. in press (accepted 2006/04/25) - CJC06076

186. Jacqueline Berges, Gail Rickards, Arvi Rauk, and Chantal Houee Levin, QM/MM study of electron addition on protein disulfide bonds, Chemical Physics Letters, 421, 63-67 (2006)

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(return to Index)

6.Papers Presented at Meetings since 1987 (approximate lifetime numbering)

103 A. Rauk, D. A. Armstrong, P. Brunelle, M. J. Pushie, D. L. Reid, C. von Sonntag, and C. J. Easton Mechanisms for Oxidative Damage to Proteins: Computational Modelling and Relevance to Alzheimer's Disease. Given at the IBOC6 Conference, Toronto, Canada, August 10th, 2002. Invited Lecture.

102. D. A. Armstrong; A. Rauk; D. L. Reid; G. V. Shustov; M. N. Schuchmann; S. Akhlaq; C. von Sonntag, H Atom transfer between Carbon-Centered and Sulfur-Centered Radicals. Given at the Institute of Nuclear Chemistry and Technology, Warsaw, Poland, August 29th, 2002. Invited Lecture.

101. D. A. Armstrong; A. Rauk; P. Brunelle, Electron Capture by Trimers: An Ab Initio Study of the Case for HCl. Given at the Ruder Boščovic Institute, Zagreb, Croatia, September 10th, 2002. Invited Lecture.

100. D. A. Armstrong; A. Rauk; P. Brunelle, Electron Capture by Trimers: An Ab Initio Study of the Case for HCl. Given at the 2nd International Symposium on Low Energy Electron-Molecule Interactions, held August 29-September 2, 2002 in Chlewiska, Poland.

99. A. Rauk, D. A. Armstrong, and M. J. Pushie, Calculating Accurate Free Energies of Solvation For Transition Metal Complexes. Methodology and Application for Determining Redox Potentials, 224th ACS National Meeting, Boston, MA, August 18-22, 2002.

98. A. Rauk, D. A. Armstrong, M. J. Pushi, P. Brunelle, and D. L. Reid, Mechanisms for Oxidative Damage to Proteins: Computational Modelling and Relevance to Alzheimer's Disease, ISBOC6, Toronto, ON, August 11-14, 2002.

97. D. L. Reid, D. A. Armstrong, A. Rauk, and C. von Sonntag, Oxidation of Peptide Backbones by Thiyl radicals. Theoretical and Experimental Studies, 20th International Symposium on the Organic Chemistry of Sulfur, Flagstaff, Arizona, July 14-19, 2002.

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94. M. J. Pushie and A. Rauk, Cu2+[Peptide] Binding Motifs - Models for Cu2+-Binding to the Prion Protein Octarepeat Domain. [Peptide] = HG, PH, and HGGG, CSC2002 (85th Canadian Society for Chemistry Conference and Exhibition), Vancouver, BC, Jun 2 - 5, 2002.

93. M. J. Pushie, A. Rauk, and D. A. Armstrong, Calculating Accurate Free Energies of Solvation For Transition Metal-Containing Complexes. Methodology and Application for Determining Redox Potentials, CSC2002 (85th Canadian Society for Chemistry Conference and Exhibition), Vancouver, BC, Jun 2 - 5, 2002.

92. D. A. Armstrong and A. Rauk, The Role of Trimers in Electron Capture by HCl: An Ab Initio Study CSC2002 (85th Canadian Society for Chemistry Conference and Exhibition), Vancouver, BC, Jun 2 - 5, 2002.

91. P. Brunelle, D. A. Armstrong, and A. Rauk, Beta-Sheet Models of Amyloid-Beta Peptide, Ernest Davidson Conference, Seattle WA, July 22-26, 2001.

90. M. J. Pushie, A. Rauk, and D. A. Armstrong, Copper(II)-Peptide Complexes Relevant to Prions and Alzheimer's Ab: A Density Functional Study, Ernest Davidson Conference, Seattle WA, July 22-26, 2001.

89. D. L. Reid, G. V. Shustov, A. Rauk, and D. A. Armstrong, Oxidative Damage to Model Peptides. A Kineti ab Initio Solution Phase Study, Ernest Davidson Conference, Seattle WA, July 22-26, 2001.

88. A. Rauk, D. P . Fairlie,and D. A. Armstrong, Computational Studies of Oxidative Damage to Proteins: Implications for Alzheimer's Disease, Ernest Davidson Conference, Seattle WA, July 22-26, 2001.

87. A. Rauk, D. P . Fairlie, D. L. Reid, and D. A. Armstrong, Mechanisms of Oxidative Damage in Ab of Alzheimer's Disease, Gordon Conference on Free Radical Reactions, Holderness, NH, July 15-20, 2001 (Invited).

86. P. Brunelle, D. A. Armstrong, and A. Rauk, Beta-Sheet Models of Amyloid-Beta Peptide, CSC2001 (84th Canadian Society for Chemistry Conference and Exhibition), Montreal, PQ, May 26 - 30, 2001.

85. M. J. Pushie, A. Rauk, and D. A. Armstrong, Copper(II)-Peptide Complexes Relevant to Prions and Alzheimer's Ab: A Density Functional Study, CSC2001 (84th Canadian Society for Chemistry Conference and Exhibition), Montreal, PQ, May 26 - 30, 2001.

84. D. L. Reid, G. V. Shustov, A. Rauk, and D. A. Armstrong, Oxidative Damage to Model Peptides. A Kineti ab Initio Solution Phase Study, CSC2001 (84th Canadian Society for Chemistry Conference and Exhibition), Montreal, PQ, May 26 - 30, 2001.

83. A. Rauk, Orbital Interaction Theory: Visually and Interactively, CSC2001 (84th Canadian Society for Chemistry Conference and Exhibition), Montreal, PQ, May 26 - 30, 2001 (Invited).

82. A. Rauk, D. A. Armstrong, and D. P. Fairlie, Mechanisms of Oxidative Damage Related to Alzheimer's Disease, Pacifichem 2000, Waikiki, Hawaii, December 12 - 17, 2000 (Invited)

81. A. Rauk, D. A. Armstrong, and D. P. Fairlie, Mechanisms of Oxidative Damage Related to Alzheimer's Disease, CSC2000 (83rd Canadian Society for Chemistry Conference and Exhibition), Calgary, AB, May 27 - 31, 2000.

80. A. Rauk and D. A. Armstrong, The Dipole Bound Anion to Valence State Transition in HBr Dimer Anion: an Ab Initio Study, CSC2000 (83rd Canadian Society for Chemistry Conference and Exhibition), Calgary, AB, May 27 - 31, 2000.

79. D. A. Block, A. Rauk, and D. A. Armstrong, Free Energies of Solution of (alpha)-C-Radicals of Alcohols, 21 Miller Conference on Radiation Chemistry, Dooerweth, The Netherlands, April 24-29, 1999.

78. D. A. Block, A. Rauk, and D. A. Arnstrong, A Statistical Mechanical Examination of the Solvation of Acetic Acid and Glycine Zwitterion and Neutral Species, 13th Canadian Symposium on Theoretical Chemistry, Vancouver, BC, August 2 - 7, 1998.

77. D. Yu, A. Rauk, G. V. Shustov, D. A. Block, and D. A. Armstrong. Applications of MO Theory to Mechanisms of Peptide Radiolysis, presented at the 1998 Gordon Conference on Radiation Chemistry, July 6th, 1998. (Invited Paper)

76. D. A. Armstrong, D. Yu, and A. Rauk, Peptide Damage in and around Cysteine Residues: a Theoretical Study, 81st CSC Conference and Exhibition, Whistler, BC, May 31 - June 4, 1998.

75. D. A. Block, D. Yu, D. A. Armstrong, and A. Rauk, Proline alpha-C-H Bond Dissociation Energies, 12th International Symposium on High Performance Computer Systems and Applications, Ednonton, AB, May 20 - 22, 1998.

74. D. Yu, A. Rauk, and D. A. Armstrong , Products and Mechanisms of Electron Reactions with Molecule Clusters: an ab initio Approach, presented in the Department of Physics at the Technical University of Gdansk, Poland on April 20th, 1998. (Invited Paper)

73. D. Yu, A. Rauk, G. V. Shustov, D. A. Block, and D. A. Armstrong, Oxidative Damaga to the Protein Backbone: an Ab Initio Study, 11th Congress of the Polish Radiation Society, Siedlce, Poland, April 15, 1998. (Invited Paper)

72. D. Yu, A. Rauk, J. Taylor, G. V. Shustov, D. A. Block, and D. A. Armstrong, (1997) Site Specificity of Oxidative Damage in Proteins, Fifth North American Chemistry Meeting, Cancun, Mexico, 11-15, November (Invited Paper).

71. D. Yu, A. Rauk and D. A. Armstrong, (1997) Structures of Some Gas Phase Clusters and Their Roles in Electron Reactions, Lodz, Poland

70. V. Maharaj, p. Bour, A. Rauk, and H. Wieser,, (1997) Deoxyoctanucleotides and their Daunarubicin Complexes: Observed and Calculated VCD Spectra, CD '97: 6th International Conference on Circular Dichroism, Pisa, Italy, 21-24 September.

69. A. Rauk, J. L. McCann, H. Wieser, P. Bour, R. G. Kostyanovsky, I. V. Vystorop, and Y. I. Elnatanov, (1997) Skeletal Vibrational Circular Dichroism of Bicyclic Dilactones: The Fingerprint Region?, CD '97: 6th International Conference on Circular Dichroism, Pisa, Italy, 21-24 September.

68. H. Wieser, J. L. McCann, V. Maharaj, A. Rauk, and P. Bour, (1997) Vibrational Circular Dichroism - Reaching Maturity, 43rd ICASS (Invited Paper).

67. I.V.Vystorop, I.I.Chervin, A.Rauk, V.N.Voznesensky and R.G.Kostyanovsky, (1997) 13C NMR STUDY OF 2,5-DIOXABICYCLO[2.2.1]HEPTANE-3,6-DIONES, 13th International Meeting on NMR Spectroscopy University of Exeter, UK, 6-11 July,

66. J. L. McCann, A. Rauk, and H. Wieser, The infrared absorption and VCD spectra of poly(vinyl ether) containing diastereomeric menthols as pendants.

65. V. Maharaj, A. Rauk, J. H. van de Sande, and H. Wieser, Infrared absorption and VCD spectra of selected deoxyoctanucleotides complexed with daunorubicin.

64. *J. L. McCann*, A. Rauk, and H. Wieser, (1996) VCD Spectra of Optically Active Polymers, 12th European Symposium on Polymer Spectroscopy, Lyon, July 8-10. - Poster

63. *G. V. Shustov*, F. Sun, T. S. Sorensen, and A. Rauk, (1996) Optical Activity of Aldehydes, Ketenes, and Diazoalkanes: The Octant Rule Revisited. 79th CSCCE - St. John's, Newfoundland, June 23 - 26.- Oral

62. *A. Rauk*, D. Yang, J. L. McCann, H. Wieser, and G. V. Shustov, (1996) The Vibrational Optical Activity of b-Lactams. 3- and 4-Methylazetidin-2-one. 79th CSCCE - St. John's, Newfoundland, June 23 - 26.- Oral

61. *A. Rauk*, D. A. Armstrong and D. Yu, (1996) Protein Modelling by Ab Initio Calculations: Susceptibility to Oxidative Damage at Gly, Ala, Ser, Thr, Cys, and Pro. 79th CSCCE - St. John's, Newfoundland, June 23 - 26.- Oral

60. D. Yu, A. Rauk, and *D. A. Armstrong*, (1996) Reactivity and Thermochemistry of Hydrazine Radical Species in Water. 79th CSCCE - St. John's, Newfoundland, June 23 - 26.- Oral

59. J. L. McCann, A. Rauk, and H. Wieser, (1996) The Vibrational Circular Dichroism Spectra of Poly(menthyl vinyl ether) and Poly(isomenthyl vinyl ether). 79th CSCCE - St. John's, Newfoundland, June 23 - 26.- Poster

58. V. Maharaj, P. Bour, A. Rauk, J. H. van de Sande, and *H. Wieser*, (1996) The Vibrational Circular Dichroism Spectra of Selected Octadeoxyribonucleotides, 79th CSCCE - St. John's, Newfoundland, June 23 - 26.- Oral

57. *V. Maharaj*, A. Rauk, J. H. van de Sande, and H. Wieser, (1996) FT-VCD Spectra of Selected Octadeoxyribonucleotides Simulated by the Coupled Oscillator Model, 16th Austin Symposium on Molecular Structure, Austin, Texas, March 4 - 6.- Poster

56. *J. L. McCann*, A. Rauk, and H. Wieser, (1996) The Vibrational Circular Dichroism Spectra of Diastereomeric Menthols, 16th Austin Symposium on Molecular Structure, Austin, Texas, March 4 - 6.- Poster

55. *V. Maharaj*, P. Bour, A. Rauk, J. H. van de Sande, and Wieser, (1996) Simulating Vibrational Circular Dichroism Spectra of Several Octadeoxyribonucleotides by Ab Initio Means, 16th Austin Symposium on Molecular Structure, Austin, Texas, March 4 - 6.- Oral

54. V. Maharaj, A. Rauk, J. H. van de Sande, and H. Wieser (1995), Computational Interpretion the FT-VCD of Selected Octadeoxynucleot ides, Pacifichem '95, Honolulu, Hawaii, December 17-22.

53. D. A. Armstrong, D. Yu, and A. Rauk, (1995) Reduction Potentials and Bond Dissociation Energies of Peptide Systems: The a-C-Centred Radical and the Peptide a-C-H Bond., 19th Miller Conference on Radiation Chemistry, Cervia/Milano, Italy, Sept. 16-21.

52. V. Maharaj, J. H. van de Sande, D. Tsankov, A. Rauk, and Wieser (1995), Toward Interpreting the FT-VCD of Selected Octadeoxynucleotides, 10th International Conference on Fourier Transform Spectroscopy, Budapest, Hungary, August 27-September 1.- Poster

51. D. Yang, A. Rauk, and H. Wieser (1995), The Absolute Stereochemistry of Cis,Cis-spiro[4.4]nonane-1,6-diol by FT-IR-VCD: Observed and Ab Initio Calculated Absorption and FT-VCD Spectra, 10th International Conference on Fourier Transform Spectroscopy, Budapest, Hungary, August 27-September 1.

50. A. Rauk, D. Yu, and D. A. Armstrong, (1995) Oxidative Damage to Peptides - Breaking the Ground , 12th Canadian Symposium on Theoretical Chemistry, Fredericton, N.B., August 5 - 11 (Invited Paper).

49. *S. A. Glover*, A. Rauk and C. A. Rowbottom, Homolytic Dissociation of Anomerically Stabilised N,N-dialkoxyamides, 1995 Gordon research Conference on Free Radical Chemistry, Plymouth, New Hampshire, July, 1995.

48. A. Rauk, I. V. Vystorop, C. Jaime, and R. G. Kostyanovsky (1995) Conformational Studies of 2,5-Dioxabycyclo[2.2.2]octane-3,6-diones. IX'th European Symposium on Organic Chemistry, Warsaw, Poland, June 18-23. Book of Abstracts, p252.

47. *D. Yu*, A. Rauk , and D. A. Armstrong (1995), T heoretical Study of Formyloxyl Radical (HCOO.) West Coast Theoretical Chemistry Conference, San Diego, March 29.

46. A. Rauk, D. Yang, and G. V. Shustov (1994) Vibrational Optical Activity of Aziridines: Electronic Factors in VCD, FACSS meeting, St. Louis, Mo., October 2-7 (Invited Paper).

45. K. F. Koehler, H. Zaddach, A. D. Kuntsevich, A. Rauk, and R. G. Kostyanovsky, Stereochemistry and the Possibility to Utilize Chemical Warfare Agents, The Second Moscow Conference on Chemical Disarmament, Demiliterization and Conversion (MOSCON94), Moscow, May 1994. - NATO

44. D. Yu, A. Rauk , and D. A. Armstrong (1994), Solution Stabilities of N-, C-, and O-Centered Radicals of Glycine 6th North American Meeting of the International Society for the Study of Xenobiotics, Raleigh, N.C., October 23-28.

43. D. Yu, A. Rauk , and D. A. Armstrong (1994), The Relative Stabilities of N-, C-, and O-Centered Radicals of Glycine Puls'94 Conference on Radiation Chemistry, Lodz, Poland, September 10-16.

42. D. Yu, A. Rauk , and D. A. Armstrong (1994), The Gas and Solution Phasec Thermochemistry of the Ions and Radicals of HCOOH and CH3COOH, Gordon Conference on Radiation Chemistry, Newport, RI July 17-22.

41. D. Yang and A. Rauk (1994) Vibrational Circular Dichroism Intensities by ab initio MP2 Vibronic Coupling Theory, 207th ACS National Meeting, San Diego, CA, March 13 - March 17.

40. *A. Rauk* and T. B. Freedman (1994), Chiroptical Techniques and their Relationship to Biological Molecules, Big or Small. 1994 Sanibel Symposium, Ponte Vedra, Florida, February 11-19 (Invited Paper).

39. D. Yu, D. A. Armstrong, and A. Rauk (1994), The Structures and Thermochemical Properties of the Radicals and Ions of HCOOH and CH3COOH, 77th CSCCE, Winnipeg, May 29-June 2.

38. D. A. Armstrong, D. Yu, and A. Rauk (1994), Thermochemistry and Kinetics of Some Radical Redox Reactions, 77th CSCCE, Winnipeg, (Invited Paper), May 29-June 2.

37. G. V. Shustov and A. Rauk (1993) , Aziridinones (a-Lactams) as the Simplest Models of the Intrinsic Chiral Non-planar Amide Chromophore, 5th International Conference on Circular Dichroism, Pingree Park, Colorado, August 18 - August 22.

36. A. Rauk, F. Sun, T. S. Sorensen, and G. V. Shustov (1993) , The Role of Excited State Geometry on the Optical Activity of Ketones, Ketenes, and Diazoalkanes, 5th International Conference on Circular Dichroism, Pingree Park, Colorado, August 18 - August 22.

35. D. Yang and A. Rauk (1993) Calculations of Vibrational Circular Dichroism Spectra Using ab initio Post-SCF Vibronic Coupling Theory, 5th International Conference on Circular Dichroism, Pingree Park, Colorado, August 18 - August 22.

34. D. Yang and A. Rauk (1993) Calculations of Vibrational Circular Dichroism Spectra Using ab initio Post-SCF Vibronic Coupling Theory, 8th American Conference on Theoretical Chemistry, Rochester, New York, June 28 - July 2.

33. D. A. Armstrong D. Yu, and A. Rauk (1993) A Theoretical Study on Solvation Energies of NH4+ and NH3+, 76th Canadian Society for Chemistry Conference and Exhibition, Sherbrooke, Que. May 30 - June 3.

32. D. Yu, A. Rauk and D. A. Armstrong (1993) Redox and Thermodynamic Properties of Amino Radicals. MillerConference on Radiation Chemistry, April 3 - 8, Windermere Hydro Hotel, England.

31. A. Rauk, D. Yu and D. A. Armstrong (1992) The Mechanism of Electron Loss from Anions in the Gas Phase. 75th Canadian Chemical Conference and Exposition, May 31 - June 4, Edmonton, Alberta (Invited Paper).

30. A. Rauk and D. Yang (1992) Ab Initio Infrared and Vibrational Circular Dichroism Intensities in 3-Ring Heterocycles. Comparison with Experiment. 75th Canadian Chemical Conference and Exposition, May 31 - June 4, Edmonton, Alberta (Invited Paper).

29. D. Yang and A. Rauk (1992) Ab Initio Vibronic Coupling Theory using the Distributed Origins with Origins at Nuclei Gauge. 75th Canadian Chemical Conference and Exposition, May 31 - June 4, Edmonton, Alberta.

28. D. A. Armstrong, D. Yu, and A. Rauk (1992) The Calculation of Electron Affinities and Thermodynamic Properties of some Diatomic Species. 75th Canadian Chemical Conference and Exposition, May 31 - June 4, Edmonton, Alberta.

27. D. Yu, A. Rauk, and D. A. Armstrong (1992) The Energy Profile for Electron Transfer between H2NCH2 and CO2. 75th Canadian Chemical Conference and Exposition, May 31 - June 4, Edmonton, Alberta.

26. A. Rauk, Y. Chen and E. Tschuikow-Roux (1991) Fluorinated Ethyl Radicals:Structures, IR Spectra, and Thermodynamic Functions, 7th International Congress on Quantum Chemistry, July 2 - 5, Menton, France.

25. A. Rauk and D. Yang (1991) VCD Spectra of Oxiranes and Thiiranes - Ab Initio VCT with 6-31G*(0.3) Basis Set, First Canadian Symposium on Computational Chemistry, May 19 - 22, Orford, Quebec.

24. F. Maurer, R. A. Shaw, R. Dutler, A. Rauk, and H. Wieser (1990) Charge Flow Contributions to Infrared Absorption and Vibrational Circular Dichroism Intensities of 1-d-Ethanol 45th Ohio State University Symposium on Molecular Spectroscopy, Columbus, Ohio.

23. Y. Chen, A. Rauk, and E. Tschuikow-Roux (1990) Structures, Barriers for Internal Rotation, Vibrational Frequencies, and Thermodynamic Functions of a,b-Difluoroethyl, a,b,b-Trif luoroethyl Radical and a,b,b,b-Tetrafluoroethyl Radicals: An Ab Initio Study, 20th International Symposium on Free Radicals, September 3 - 7, Susono, Shizuoka, Japan.

22. A. Rauk and D. Yang (1990) The VCD and IR Spectra of 2-Methylaziridine: Ab Initio Vibronic Coupling Theory with the 6-31G*(0.3) Basis set., The 10th IUPAC Conference on Physical Organic Chemistry, Aug 5 - 10, Haifa, Israel.

21. Y. Chen, A. Rauk, and E. Tschuikow-Roux (1990) Structures, Barriers for Rotation, Vibrational Frequencies, and Thermodynamic Functions of CH2FCH2, CHF2CH2, and CF3CH2 Radicals: An Ab Initio Study, 23rd International Symposium on Combustion, July , Orleans, France.

20. A. Rauk, R. Dutler, D. Yang (1989) IR and VCD Intensities of Model Systems CH3OH, CH3NH2, NH2NH2, NH2OH, and HOOH, The 1989 International Chemical Congress of the Pacific Basin Societies, Dec 17 - 22, Honolulu, Hawaii.

19. R. Dutler and A. Rauk, (1989) VCD and IR Intensities of Deuterated Oxiranes. An Ab Initio Study. 72nd Canadian Chemical Conference and Exposition, June 4 - 8, Victoria, B.C.

18. R. Dutler, A. Rauk, T. S. Sorensen and S. M. Whitworth, (1989) Unsymme trical Tertiary Carbocations. 72nd Canadian Chemical Conference and Exposition, June 4 - 8, Victoria, B.C.

17. A. Rauk, R. Dutler, S. M. Whitworth, and T. S. Sorensen, (1989) Ab Ibitio Search for the Structure of the 4-Protoadamantyl Cation. 10th Canadian Symposium on Theoretical Chemistry, August 24 - 30, Banff, Alberta.

16. R. Dutler, R. A. Shaw, H. Wieser, and A. Rauk, (1989) IR and VCD of a-d-Ethanol, 10th Canadian Symposium on Theoretical Chemistry, August 24 - 30, Banff, Alberta.

15. A. Rauk, R. Dutler, D. Yang (1988) IR and VCD Intensities of Model Systems CH3OH, CH3NH2, NH2NH2, NH2OH, and HOOH and the Deuterated Species, ND2ND2, DOOH, and DOOD: A Theoretical Study using the Vibronic Coupling Formalism, 10th Canadian Symposium on Theoretical Chemistry, August 24 - 30, Banff, Alberta.

14. R. Dutler and A. Rauk (1988) How to Pass Through a Looking Glass: On the Feasibility of Asymmetric Synthesis Using Circularly Polarized Light, SuperComputer Symposium '88, Edmonton, June 19-21, 1988.

13. R. A. Shaw, C. Castro, R. Dutler, A. Rauk, and H. Wieser (1987) The Vibrational Spectra and Ab Initio STO-3G and 3-21G Harmonic Force Fields of Norbornane, Norbornene, Norbornadiene, 7-Oxanorbornane, and 7-Thianorbornane, EUCMOS XVIII, XVIIIth European Conference on Molecular Spectroscopy, August 30 - September 4, Amsterdam.

12. R. Dutler and A. Rauk (1987) Ab Initio Computation of Infrared and Vibrational Circular Dichroism Absorption Intensities American Conference on Theoretical Chemistry, July 17-24, Gull Lake, Minnesota.

11. R. Dutler and A. Rauk (1987) Quantum Chemistry at the University of Calgary, Supercomputer Symposium '87, June 15-16, Calgary.

10. R. Dutler and A. Rauk (1987) A Theoretical Exploration into the Efficacy of Circularly Polarized IR Light in Inducing Conrotatory Electrocyclic Reactions of Some Asymmetrically Substituted Cyclobutenes 70'th Canadian Chemical Conference, June 6-11, Quebec City.

9. A. Rauk (1987) Optical Activity of N-Halooxaziridines:Vibronic Effects, 70'th Canadian Chemical Conference, June 6-11, Quebec City. Books A. Rauk (1994) Orbital Interaction Theory of Organic Chemistry: Wiley-Interscience, New York, NY, 1994.

(return to Index)

7. Monographs, etc

137A. A. Rauk (1998) VCD (Vibrational Circular Dichroism), entry in Encyclopedia of Computational Chemistry, Schleyer, P. v. R.; Allinger, N. L.; Clark, T.; Gasteiger, J.; Kollmann, P.; Schaefer III, H. F.; Schreiner, P. R., Eds. J. Wiley, New York, NY, 1998.

137B. A. Rauk (1998) ECD (Electronic Circular Dichroism), entry in Encyclopedia of Computational Chemistry, Schleyer, P. v. R.; Allinger, N. L.; Clark, T.; Gasteiger, J.; Kollmann, P.; Schaefer III, H. F.; Schreiner, P. R., Eds. J. Wiley, New York, NY, 1998.

(return to Index)

8. Electronic Conference Presentations

James M. Coxon*, Robert G.A.R. Maclagan, Arvi Rauk, Aaron J. Thorpe and Dale Whalen (1996), Molecular gymnastics of oxiranes in acid,Electronic Conference on Heterocyclic Chemistry, 24 June - 22 July 1996.(http://www.ch.ic.ac.uk/ectoc/echet96/papers/023/index.htm)

(return to Index)

9. Books

A. Rauk (2000) Orbital Interaction Theory of Organic Chemistry, 2nd Edition: Wiley-Interscience, New York, NY, 2000.

A. Rauk (1994) Orbital Interaction Theory of Organic Chemistry: Wiley-Interscience, New York, NY, 1994.

(return to Index)

10. Other Scholarly Activity

Editorships and Advisory Boards

Associate Editor - Journal of Alzheimer's Disease 2002 - 2003
Editor (Theoretical) - Canadian Journal of Chemistry 1999-present
Advisory Board - Canadian Journal of Chemistry 1996-1999
Advisory Board -Estonian Academy of Sciences 1996-present

Conferences Organized

Scientific Program Chair - 66'th Canadian Chemical Conference, Calgary, 1983
Chairman (with B. Clark) - 10th Canadian Symposium on Theoretical Chemistry, Banff, 1989.
Scientific Program Chair - 83'rd Canadian Chemical Conference, Calgary, 2000
Symposium Organizer - Pacifichem2005, Hawaii, 2005

Seminars

1988 -Seminar:

Vibrational Optical Activity: Theory with a Little Practise presented at:

- University of New England, Armidale, Australia
- University of Aukland, Aukland, New Zealand
- Whiteshell Nuclear Research Establishment, Pinawa, Manitoba
- University of Manitoba, Winnipeg, Manitoba
- University of Regina, Regina Saskatchewan
- University of Saskatchewan, Saskatoon, Saskatchewan

1989 - Seminar:

Vibrational Optical Activity: Theory with a Little Practise presented at:

- University of Alberta, Edmonton, Alberta

1990 - Seminar:

The Structures of Organic Molecules from a Theoretical Interpretation of Vibrational Circular Dichroism Spectroscopy presented at:

- University of Erlangen-Nurnburg, West Germany

1991 - Seminar:

The Structures of Organic Molecules from a Theoretical Interpretation of Vibrational Circular Dichroism Spectroscopy presented at:

- Simon Fraser University - April 4.
- Estonian Academy of Sciences, Tallinn - June 17
- Tartu University, Tartu - June 20
- Academy of Sciences of the USSR, Moscow - June 27

Seminar:

Orbital Interaction Theory: Organic Chemistry the Easy Way presented at:

- Estonian Academy of Sciences, Tallinn - June 18
- Tartu University, Tartu - June 21
- University of Moscow, Moscow - June 28

1992 - Seminar:

Finally, a spectroscopic method for the determination of absolute configurations! Vibrational Circular Dichroism. presented at:

- University of Saskatchewan, Saskatoon, Saskatchewan - July 7.

1994 - Seminar:

Chiroptical Techniques and their Relationship to Biological Molecules, Big or Small.

- University of Calgary: Chem 603 seminar - February 4
- Moscow State University, Moscow - May 31

Seminar:

Orbital Interaction Theory of Organic Chemistry presented at:

- Estonian Academy of Sciences, Tallinn - May 23

1995 - Seminar:

Orbital Interaction Theory of Organic Chemistry presented at:

- University of New England, Armidale, Australia - Feb 26
- University of Queenslqnd, Brisbane, Australia - March 3
- University of Tasmania, Hobart, Australia - April 6

Seminar:

Chiroptical Techniques and their Relationship to Biological Molecules, Big or Small.

- University of New England, Armidale, Australia - March 26
- Research School of Chemistry, ANU, Canberra, Australia - May 4
- Universite Louis Pasteur, Strasbourg, France - May 31

Seminar:

Quantum Chemical Research of the Rauk Group presented at:

- Research School of Chemistry, ANU, Canberra, Australia - April 27

Seminar:

Oxidative Damage to Peptides - Breaking the Ground coauthors - Dake Yu and David A. Armstrong - presented at:

- Universite de Nice, Nice, France - June 6
- Universite Louis Pasteur, Strasbourg, France - June 15

- **1996** - Seminar:

- Physical Chemistry Today, Chem 601 seminar, Uof C, Nov 1.
- **1997** - Seminar: A Chemist's Adventures with Mathematics, Department of Mathematics, Uof C, March 13

- **1999** - Seminar:

Integrating Monte Carlo Solvation Studies with Quantum Mechanical Thermochemistry: Carbon Free Radicals - coauthors - David A. Block, and D. A. Armstrong - presented at:
University of Canterbury, Christchurch, NZ - January 25.
Research School of Chemistry, ANU, Canberra, Australia - February 24
University of Queensland, Brisbane, Australia - March 18.
University of New England, Armidale, Australia - April 1.

Seminar:
Research into Oxidative Damage to Proteins at the University of Calgary - coauthors - David A. Block, and D. A. Armstrong - presented at:
Research School of Chemistry, ANU, Canberra, Australia - February 3

Seminar:
Modelling Oxidative Damage to Beta Sheet Structure - coauthors - J. Berges and D. A. Armstrong - presented at:
Heart Research Institute, Sydney, Australia - February 26
3D Centre, Brisbane, Australia - April 22

- **2000** - Seminar:

Mechanisms of Oxidative Damage Related to Alzheimer's Disease - coauthors - D. A. Armstrong and D. P. Fairlie - presented at:
Universite Rene Descartes Paris V, Laboratoire de Chimie et Biologie - June 16

Seminar:
Glutathione, 4-Hydroxynonenal, and the Beta Amyloid Peptide: A Progress Report on the Theoretical Investigation of Their Interrelationship in Mediating Cytotoxicity
coauthors - D. A. Armstrong and J. Berges - presented at:
Universite Pierre et Marie Curie Paris VI, Laboratoire de Chimie Theorique - June 20

- **2001** - Seminar:

Computational Studies of Oxidative Damage to Proteins: Implications for Alzheimer's Disease - coauthors - D. A. Armstrong and D. P. Fairlie - presented at:
University of Regina, Sask., March 30.
University of Toronto, Ont, April 9.
Queen's University, Kingston, Ont, April 10.
Cornell University, Ithaca, NY, April 12. (Invited)

Seminar:
From Free Radical Chemistry of Proteins to a Model of Alzheimer's Disease - coauthors - P. Brunelle, D. P. Fairlie, and D. A. Armstrong - presented at:
Dalhousie University, NS, Aug. 24. (Invited)
University of Calgary, AB, Sept. 21.
University of Saskatchewan, Sask., Oct. 9. (Invited)

- **2002** - Seminar:

Mechanisms for Oxidative Damage to Proteins: Computational Modelling and Relevance to Alzheimer's Disease
coauthors - David A. Armstrong, Patrick, Brunelle, M. Jake Pushie, Darren L. Reid, Clemens von Sonntag, Christopher J. Easton
presented at:
Concordia University, Montreal, PQ, Oct 25, 2002 (Invited)

(return to Index)

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11. Hobbies and Interests

- Hiking in the mountains
- Tennis
- Growing indoor plants (especially Orchids)

(return to Index)