Cynthia J. Jameson

Professor Emerita of Chemistry and Chemical Engineering, University of Illinois- Chicago
Research area: Physical Chemistry. Gas phase NMR Spectroscopy. Applications of NMR to Fundamental Studies of Adsorption and Diffusion, Xe NMR chemical shift tensors in cages, channels and other nanopores.
Ph.D., University of Illinois (Urbana), 1963.
B.S., University of the Philippines, 1958.

PROFESSIONAL EXPERIENCE
National Science and Engineering Research Council Canada Banting Postdoctoral Awards Panel 2011-2013
Visiting Scientist, Department of Material Sciences, University of Milan Bicocca, Italy 2007.
Miller Visiting Professor, University of California, Berkeley, 2002
Grant Selection Committee for Physical and Analytical Chemistry, National Science and Engineering Research Council, Canada 1995-1998
Visiting Scientist, Physical Chemistry Laboratory, Oxford University, England, 1992, 1993.
Program Officer, Experimental Physical Chemistry, National Science Foundation 1990-91
Scholar-in-Residence, Queens University, Ontario, Canada October, 1990.
Exchange Scientist, Academy of Sciences of GDR, Berlin, 1985 (National Academy of Sciences USA Inter-Academy Exchange Program).
Visiting Scientist, University of Cambridge, England, 1985, 1978.
Professor, University of Illinois at Chicago 1976-2006.
Associate Professor 1972-1976, Assistant Professor 1968-1972, UIC.
Assistant Professor, University of the Philippines, January 1966 - May 1967
Post-doctoral research, Columbia University, 1963-1965,
Post-doctoral research, University of Illinois-Urbana, 1967-1968

FELLOWSHIPS, HONORS AND AWARDS:
Camille and Henry Dreyfus Senior Scientist Mentor 2010-12
2008 Woman of the Year, University of Illinois Chicago
Miller Visiting Professor, University of California, Berkeley, 2002
2000 Vaughan Award, NMR section Rocky Mountain Conference on Analytical Chemistry
Fellow, American Association for the Advancement of Science, since 1988.
Senior University Scholar, University of Illinois 1995-1998
First Prizes, Outstanding Curriculum Development Project UIC, 1974 and 1973.
Fellowship, Winter Institute Quantum Chemistry, U of Florida & Sanibel Island, Dec. 1962
Eastman Award for The Outstanding Graduate Student in Chemistry, University of Illinois, Urbana 1962 ($1000 prize).
Pre-doctoral Fellowship, University of Illinois, Urbana, 1961-1963.
Fulbright-Hays Award, 1959 (from Philippines to U.S.A.)
Graduated “cum laude”, University of the Philippines, 1958.

NAMED LECTURESHIPS:
2016 Jean Dreyfus Boissevain Lectureship at Washington & Jefferson College
2009 Intensive Faculty Training Workshop in Quantum Chemistry at University of the Philippines

2002 Henry Emmett Gunning Lectures, University of Alberta
2000 McElvain Lecture, University of Wisconsin, Madison
2000 Vaughan Lecture, Rocky Mountain Conference NMR Symposium
1996 Dow Lecture, University of Minnesota

Ph. D. Adviser: Herbert S. Gutowsky Post-doc Adviser: Martin Karplus

LIST OF PUBLICATIONS

222. "Molecular dynamics simulations reveal how characteristics of surface and permeant affect permeation events at the surface of soft matter," P. A. Oroskar, C. J. Jameson, and S. Murad, ***Molec. Simul*.** 43(5-6), 439-466 (2017). DOI: 10.1080/08927022.2016.1268259 http://dx.doi.org/10.1080/08927022.2016.1268259
221. "Rotational behavior of PEGylated gold nanorods in a lipid bilayer system," P. A. Oroskar, C. J. Jameson, and S. Murad, ***Mol. Phys.***, 115(9-12), 1122-1143 (2017). DOI: 10.1080/00268976.2016.1248515 http://dx.doi.org/10.1080/00268976.2016.1248515
220. "Simulated permeation and characterization of PEGylated gold nanoparticles in a lipid bilayer system," P. A. Oroskar, C. J. Jameson, and S. Murad, ***Langmuir***, 32, 7541−7555 (2016). DOI: 10.1021/acs.langmuir.6b01740 http://pubs.acs.org/doi/pdf/10.1021/acs.langmuir.6b01740
219. "Using molecular simulations to develop reliable design tools and correlations for engineering applications of aqueous electrolyte solutions" K. R. Hinkle, C. J. Jameson, S. Murad, ***J. Chem. Eng. Data***, 61(4) 1578–1584 (2016). DOI: 10.1021/acs.jced.5b00945 http://pubs.acs.org/doi/pdf/10.1021/acs.jced.5b00945
218. "Fundamental intramolecular and intermolecular information from NMR in the gas phase," C. J. Jameson, a chapter in '***Gas Phase Nuclear Magnetic Resonance***', ed. M. Jaszunski and K. Jackowski, eds., Royal Society of Chemistry, London, 2016, Chap. 1, pp. 1-51. DOI: 10.1039/9781782623816-00001 ISBN-13: 978-1-78262-161-4 DOI: 10.1039/9781782623816.
217. "Recent advances in theoretical and physical aspects of NMR chemical shifts," A. C. de Dios and C. J. Jameson, ***Kimika***, 26(2), 2-31 (2015). ISSN 0115-2130 http://kimika.philippinechem.org/index.php/kimika/issue/view/30
216. "Theoretical and physical aspects of nuclear shielding," C. J. Jameson and A. C. de Dios, a chapter in ***Nuclear Magnetic Resonance***, K. Kamienska-Trela, ed., Royal Society of Chemistry, London, 2015, Vol. 44, Chap. 2, pp. 46-75. Print ISBN: 978-1-78262-052-5 pdf eISBN: 978-1-78262-275-8. DOI: 10.1039/9781782622758-00046
215. "The Xe chemical shift and chemical shift anisotropy ", C. J. Jameson, a chapter in '***Hyperpolarized Xenon-129 Magnetic Resonance: Concepts, Production, Techniques and Applications***', T. Meersman and E. Brunner, eds., Royal Society of Chemistry, London, 2015, Chap. 2, pp. 16-48. DOI:10.1039/9781782628378-00016 ISBN-13: 978-1-84973-889-7 DOI: 10.1039/9781782628378 http://pubs.rsc.org/en/Content/eBook/978-1-84973-889-7#!divbookcontent
214. "Surface-functionalized nanoparticle permeation triggers lipid displacement and water and ion leakage", P. A. Oroskar, C. J. Jameson, and S. Murad, ***Langmuir***, 31, 1074-1085 (2015). DOI: 10.1021/la503934c http://pubs.acs.org/doi/pdf/10.1021/la503934c PMID: 25549137

213. "Transport of vanadium and oxovanadium ions across zeolite membranes: A molecular dynamics study", K. R. Hinkle, C. J. Jameson, S. Murad, ***J. Phys. Chem. C*** 118, 23803-23810 (2014). http://pubs.acs.org/doi/abs/10.1021/jp507155s DOI: 10.1021/jp507155s
212. "Theoretical and physical aspects of nuclear shielding," C. J. Jameson and A. C. de Dios, a chapter in ***Nuclear Magnetic Resonance***, K. Kamienska-Trela and J. Wojcik, eds., Royal Society of Chemistry, London, 2014, Vol. 43, pp. 49-80. ISBN: 978-1-84973-955-9. DOI:10.1039/9781849738125-00049
211. "Calculation of nuclear magnetic resonance parameters", C. J. Jameson, in ***Encyclopedia of Analytical Chemistry, Instrumentation and Applications***, R. A. Meyers, ed. John Wiley: Chichester. DOI: 10.1002/9780470027318.a6109.pub2. Published online 9 January, 2014. 38 pp. http://onlinelibrary.wiley.com/doi/10.1002/9780470027318.a6109.pub2/abstract
210. "Theoretical and physical aspects of nuclear shielding," C. J. Jameson and A. C. de Dios, a chapter in ***Nuclear Magnetic Resonance***, K. Kamienska-Trela and J. Wojcik, eds., Royal Society of Chemistry, London, 2013, Vol. 42, Chap. 2, pp. 45-77. ISBN: 978-1-84973-577-3. DOI: 10.1039/9781849737678-00045
209. "Nanoparticle permeation induces water penetration, ion transport and lipid flip-flop", B. Song, H.-J. Yuan, S. V. Pham, C. J. Jameson, and S. Murad, ***Langmuir***, 28, 16989-17000 (2012). DOI 10.1021/la302879r http://pubs.acs.org/doi/abs/10.1021/la302879r PMID: 23171434
208. "Recent advances in nuclear shielding calculations," A. C. de Dios and C. J. Jameson, a chapter in ***Annual Reports on NMR Spectroscopy***, G. A. Webb, ed., Elsevier Ltd, London, 2012, Vol. 77, Chap.1, pp. 1-80. DOI:10.1016/B978-0-12-397020-6.00001-5 http://www.sciencedirect.com/science/article/pii/B9780123970206000015 (this series included in ISI for the first time).
207. "Role of surface ligands in nanoparticle permeation through a model membrane: a coarse-grained molecular dynamics simulations study," B. Song, H.-J. Yuan, C. J. Jameson and S. Murad, ***Mol. Phys***. 110, 2181-2195 (2012). http://www.tandfonline.com/doi/abs/10.1080/00268976.2012.668964#.VTfN5ORX3CI DOI:10.1080/00268976.2012.668964
206. "Theoretical and physical aspects of nuclear shielding," C. J. Jameson and A. C. de Dios, a chapter in ***Nuclear Magnetic Resonance***, K. Kamienska-Trela and J. Wojcik eds., Royal Society of Chemistry, London, 2012, Vol. 41, Chap. 2, pp. 38-55. ISBN: 978-1-84973-373-1 DOI:10.1039/9781849734851-00038
205. "Permeation of nanocrystals across lipid membranes," B. Song, H.-J. Yuan, C. J. Jameson and S. Murad, ***Mol. Phys***. 109, 1511-1526 (2011). http://www.tandfonline.com/doi/abs/10.1080/00268976.2011.569511#.VTfOUORX3CI DOI:10.1080/00268976.2011.569511
204. "Chemical shift scales on an absolute basis," C. J. Jameson, in ***Encyclopedia of Magnetic Resonance***, eds-in-chief R. K. Harris and R. E. Wasylishen, John Wiley: Chichester. DOI: 10.1002/9780470034590.emrstm0072.pub2. http://onlinelibrary.wiley.com/doi/10.1002/9780470034590.emrstm0072.pub2/abstract Published online 15 March 2011.
203. "Theoretical and physical aspects of nuclear shielding," C. J. Jameson and A. C. de Dios, a chapter in ***Nuclear Magnetic Resonance***, K. Kamienska-Trela, ed., Royal Society of Chemistry, London, 2011, Vol. 40, Chap. 2, pp. 37-54. ISBN: 978-1-84973-147-8. DOI:10.1039/9781849732796-00037

202. "Diffusion of gases across lipid membranes with OmpA channel: A molecular dynamics study," H.-J. Yuan, C. J. Jameson and S. Murad, ***Mol. Phys***. 108, 1569-1581 (2010). http://www.tandfonline.com/doi/abs/10.1080/00268976.2010.484396#.VTfZG-RX3CI DOI: 10.1080/00268976.2010.484396
201. "Theoretical and physical aspects of nuclear shielding," C. J. Jameson and A. C. de Dios, a chapter in ***Nuclear Magnetic Resonance***, G. A. Webb and K. Kamienska-Trela, eds., Royal Society of Chemistry, London, 2010, Vol. 39, Chap. 2, pp. 42-69. ISBN 978-1-847550606. DOI:10.1039/9781849730846-00042
200. "Xe NMR", C. J. Jameson, ***Encyclopedia of Magnetic Resonance***, eds R. K. Harris and R. E. Wasylishen, John Wiley: Chichester. http://onlinelibrary.wiley.com/doi/10.1002/9780470034590.emrstm1076/abstract DOI:10.1002/9780470034590.emrstm1076 Published online 15 September 2009.
199. "Exploring gas permeability of lipid membranes using coarse-grained molecular dynamics," H.-J. Yuan, C. J. Jameson and S. Murad, ***Mol. Simul***. 35, 953-961 (2009). http://www.tandfonline.com/doi/abs/10.1080/08927020902763839#.VTfZ4ORX3CI DOI: 10.1080/08927020902763839
198. "Theoretical and physical aspects of nuclear shielding," C. J. Jameson and A. C. de Dios, a chapter in ***Nuclear Magnetic Resonance***, G. A. Webb, ed., Royal Society of Chemistry, London, 2009, Vol. 38, Chap. 2, pp. 68-93. ISBN: 978-1-84755-922-7. DOI: 10.1039/b704412g
197. "Prediction of Henry's constants of xenon in cyclo-alkanes from molecular dynamics simulations," H.-J. Yuan, C. J. Jameson, S. K. Gupta, J. D. Olson and S. Murad, ***Fluid Phase Equil***. 269, 73-79 (2008). DOI:10.1016/j.fluid.2008.05.003 http://www.sciencedirect.com/science/article/pii/S0378381208001702
196. "Theoretical and physical aspects of nuclear shielding," C. J. Jameson and A. C. de Dios, a chapter in ***Nuclear Magnetic Resonance***, G. A. Webb, ed., Royal Society of Chemistry, London, 2008, Vol. 37, Chap. 2, pp. 51-67. ISBN: 978-0-85404-115-2. DOI:10.1039/B617218K
195. "Molecular dynamics simulation of ion selectivity process in nanopores," H. Liu, C. J. Jameson and S. Murad, ***Mol. Simul***. 34, 169-175 (2008). http://www.tandfonline.com/doi/abs/10.1080/08927020801966087#.VTfhk-RX3CI DOI:10.1080/08927020801966087
194. "Measuring chirality in NMR in the presence of a static electric field," J. D. Walls, R. A. Harris, and C. J. Jameson, ***J. Chem. Phys***. 128, 154502 (2008) 6 pages. DOI:10.1063/1.2888555 http://scitation.aip.org/content/aip/journal/jcp/128/15/10.1063/1.2888555 PMID: 18433230 http://www.ncbi.nlm.nih.gov/pubmed/18433230
193. "Molecular dynamics simulation of Xe chemical shifts and solubility in *n*-alkanes," H. Yuan, S. Murad, C. J. Jameson, and J. D. Olson, ***J. Phys. Chem. C***, 111, 15771-15783 (2007). DOI: 10.1021/jp0735233 http://pubs.acs.org/doi/abs/10.1021/jp0735233
192. "Theoretical and physical aspects of nuclear shielding," C. J. Jameson and A. C. de Dios, a chapter in ***Nuclear Magnetic Resonance***, G. A. Webb, ed., Royal Society of Chemistry, London, 2007, Vol. 36, Chap. 2, 50-71. ISBN: 978-0-85404-362-0. DOI:10.1039/B618338G
191. "Diastereomeric Xe chemical shifts in tethered cryptophane cages," E. J. Ruiz, D. N. Sears, A. Pines, and C. J. Jameson, ***J. Am. Chem. Soc***. 128, 16980-16988 (2006). DOI: 10.1021/ja066661z http://pubs.acs.org/doi/abs/10.1021/ja066661z PMID: 17177449

190. “Ion permeation dynamics in carbon nanotubes,” H. Liu, S. Murad, and C. J. Jameson, ***J. Chem. Phys***. 125, 084713 (2006) 14 pages. DOI: 10.1063/1.2337289 http://scitation.aip.org/content/aip/journal/jcp/125/8/10.1063/1.2337289 PMID: 16965045
189. “Xe NMR lineshapes in channels decorated with paramagnetic centers,” D. N. Sears, L. Vukovic, and C. J. Jameson, ***J. Chem. Phys***. 125, 114708 (2006) 14 pages. DOI: 10.1063/1.2338809 http://scitation.aip.org/content/aip/journal/jcp/125/11/10.1063/1.2338809 PMID: 16999502
188. “A note on chirality in NMR spectroscopy,” R. A. Harris and C. J. Jameson, ***J. Chem. Phys***. 124, 096101 (2006). DOI: 10.1063/1.2177255 http://scitation.aip.org/content/aip/journal/jcp/124/9/10.1063/1.2177255 PMID: 16526874
187. “Theoretical and physical aspects of nuclear shielding,” C. J. Jameson and A. C. de Dios, a chapter in ***Nuclear Magnetic Resonance***, G. A. Webb, ed., Royal Society of Chemistry, London, 2006, Vol. 35, Chap. 2, pp. 52-81. ISBN: 978-0-85404-357-6. DOI:10.1039/9781847555236-00052
186. “Molecular reorientation of CD_4 in gas phase mixtures”, M. A. ter Horst, C. J. Jameson and A. K. Jameson, ***Magn. Reson. Chem***. 44, 241-248 (2006). DOI:10.1002/mrc.1756 http://onlinelibrary.wiley.com/doi/10.1002/mrc.1756/abstract PMID: 16477693
185. “Intermolecular hyperfine tensor for $Xe@O_2$. Density and temperature dependence of Xe chemical shifts in oxygen gas”, L. Vukovic, C. J. Jameson, and D. N. Sears, ***Mol. Phys***. 104, 1217-1225 (2006). DOI: 10.1080/00268970500525614 http://www.tandfonline.com/doi/abs/10.1080/00268970500525614#.VTf6BORX3CI
184. “Theoretical and physical aspects of nuclear shielding,” C. J. Jameson and A. C. de Dios, a chapter in ***Nuclear Magnetic Resonance***, G. A. Webb, ed., Royal Society of Chemistry, London, 2005, Vol. 34, Chap. 2, pp. 57-86. ISBN: 978-0-85404-352-1. DOI:10.1039/9781847553904-00057
183. “Xe NMR lineshapes in channels of peptide molecular crystals,” I. Moudrakovski, D. V. Soldatov, J. A. Ripmeester, D. N. Sears, and C. J. Jameson, ***Proc. Natl. Acad. Sci., U. S. A***., 101, 17924-17929 (2004). DOI 10.1073/pnas.0405348101 http://www.pnas.org/content/101/52/17924.abstract http://www.pnas.org/content/101/52/17924.full.pdf PMID: 15596727
182. “Molecular dynamics averaging of Xe chemical shifts in liquids,” C. J. Jameson, D. N. Sears, and S. Murad, ***J. Chem. Phys***. 121, 9581-9592 (2004). DOI: 10.1063/1.1807817 http://scitation.aip.org/content/aip/journal/jcp/121/19/10.1063/1.1807817 PMID: 15538880
181. “The Xe chemical shift tensor in silicalite and SSZ-24 zeolite,” C. J. Jameson, ***J. Am. Chem. Soc***. 126, 10450-10456 (2004). DOI: 10.1021/ja040012a http://pubs.acs.org/doi/abs/10.1021/ja040012a PMID: 15315461
180. “The Xe shielding surfaces for Xe interacting with linear molecules and spherical tops,” D. N. Sears and C. J. Jameson, ***J. Chem. Phys***. 121, 2151-2157 (2004). DOI: 10.1063/1.1758691 http://scitation.aip.org/content/aip/journal/jcp/121/5/10.1063/1.1758691 PMID: 15260769
179. “Is there a spatial correlation in the distribution of adsorbed atoms in the cages of a zeolite?,” C. J. Jameson, ***Mol. Phys***. 102, 723-727 (2004). DOI:10.1080/00268970410001699251 http://www.tandfonline.com/doi/abs/10.1080/00268970410001699251#.VTf6V-RX3CI

178. "The NMR lineshapes of Xe in the cages of clathrate hydrates," C. J. Jameson and D. Stueber, ***J. Chem. Phys***. 120, 10200-10214 (2004). DOI: 10.1063/1.1718349 http://scitation.aip.org/content/aip/journal/jcp/120/21/10.1063/1.1718349 PMID: 15268044
177. "Nuclear magnetic shielding and chirality IV. The odd and even character of the shielding response to a chiral potential," D. N. Sears, C. J. Jameson, R. A. Harris, ***J. Chem. Phys***. 120, 3277-3283 (2004). DOI: 10.1063/1.1641012 http://scitation.aip.org/content/aip/journal/jcp/120/7/10.1063/1.1641012 PMID: 15268482
176. "Theoretical and physical aspects of nuclear shielding," C. J. Jameson and A. C. de Dios, a chapter in ***Nuclear Magnetic Resonance***, G. A. Webb, ed., Royal Society of Chemistry, London, 2004, Vol. 33, Chap. 2, pp. 47-75. ISBN: 978-0-85404-347-7. DOI:10.1039/9781847553898-00047
175. "The chemical shifts of Xe in the cages of clathrate hydrate Structure I and II," D. Stueber and C. J. Jameson, ***J. Chem. Phys***. 120, 1560-1571 (2004). DOI: 10.1063/1.1632895 http://scitation.aip.org/content/aip/journal/jcp/120/3/10.1063/1.1632895 PMID: 15268283
174. "Theoretical calculations of Xe chemical shifts in cryptophane cages," D. N. Sears and C. J. Jameson, ***J. Chem. Phys*****.** 119, 12231-12244 (2003). DOI: 10.1063/1.1625364 http://scitation.aip.org/content/aip/journal/jcp/119/23/10.1063/1.1625364
173. "On using the NMR chemical shift to assess polar-nonpolar cross-intermolecular interactions," C. J. Jameson and S. Murad, ***Chem. Phys. Lett*****.** 380, 556-562 (2003). DOI:10.1016/j.cplett.2003.09.070 http://www.sciencedirect.com/science/article/pii/S0009261403016075
172. "Nuclear magnetic shielding and chirality III. The single electron on a helix model," D. N. Sears, C. J. Jameson, and R. A. Harris, ***J. Chem. Phys*****.** 119, 2694-2701 (2003). DOI: 10.1063/1.1586700 http://scitation.aip.org/content/aip/journal/jcp/119/5/10.1063/1.1586700
171. "Nuclear magnetic shielding and chirality II. The shielding tensor of a naked spin in Ne helices," D. N. Sears, C. J. Jameson, and R. A. Harris, ***J. Chem. Phys*****.** 119, 2691-2693 (2003). DOI: 10.1063/1.1586699 http://scitation.aip.org/content/aip/journal/jcp/119/5/10.1063/1.1586699
170. "Nuclear magnetic shielding and chirality I. The shielding tensor of Xe interacting with Ne helices," D. N. Sears, C. J. Jameson, and R. A. Harris, ***J. Chem. Phys*****.** 119, 2685-2690 (2003). DOI: 10.1063/1.1586698 http://scitation.aip.org/content/aip/journal/jcp/119/5/10.1063/1.1586698
169. "Calculation of the Xe chemical shift in $Xe@C_{60}$," D. N. Sears and C. J. Jameson, ***J. Chem. Phys*****.** 118, 9987-9989 (2003). DOI: 10.1063/1.1573190 http://scitation.aip.org/content/aip/journal/jcp/118/22/10.1063/1.1573190
168. "Theoretical and physical aspects of nuclear shielding," C. J. Jameson and A. C. de Dios, a chapter in ***Nuclear Magnetic Resonance***, G. A. Webb, ed., Royal Society of Chemistry, London, 2003, Vol. 32, Chap. 2, pp. 43-74. ISBN: 978-0-85404-342-2. DOI:10.1039/9781847553881-00043
167. "The ^{129}Xe nuclear shielding tensor surfaces for Xe interacting with rare gas atoms", C. J. Jameson, D. N. Sears and A. C. de Dios, ***J. Chem. Phys*****.** 118, 2575-2580 (2003). DOI: 10.1063/1.1534093 http://scitation.aip.org/content/aip/journal/jcp/118/6/10.1063/1.1534093
166. "Theoretical and physical aspects of nuclear shielding," C. J. Jameson and A. C. de Dios, a chapter in ***Nuclear Magnetic Resonance***, G. A. Webb, ed., Royal Society of

Chemistry, London, 2002, Vol. 31, Chap. 2, pp. 48-78. ISBN: 978-0-85404-337-8. DOI:10.1039/9781847553874-00048

165. "Calculations of Xe lineshapes in model nanochannels. Grand canonical Monte Carlo averaging of the ^{129}Xe NMR chemical shift tensor", C. J. Jameson, ***J. Chem. Phys.*** 116, 8912-8929 (2002). DOI: 10.1063/1.1468884 http://scitation.aip.org/content/aip/journal/jcp/116/20/10.1063/1.1468884
164. "Xe nuclear magnetic resonance lineshapes in nanochannels", C. J. Jameson and A. C. de Dios, ***J. Chem. Phys.*** 116, 3805-3821 (2002). DOI: 10.1063/1.1446424 http://scitation.aip.org/content/aip/journal/jcp/116/9/10.1063/1.1446424
163. "Theoretical and physical aspects of nuclear shielding," C. J. Jameson and A. C. de Dios, a chapter in ***Nuclear Magnetic Resonance***, G. A. Webb, ed., Royal Society of Chemistry, London, 2001, Vol. 30, Chap. 2, pp. 46-67. ISBN: 978-0-85404-332-3. DOI:10.1039/9781847553867-00046
162. "Adsorption of xenon and CH_4 mixtures in zeolite NaA. ^{129}Xe NMR and grand canonical Monte Carlo simulations," C. J. Jameson, A. K. Jameson, P. Kostikin, and B. I. Baello, ***J. Chem. Phys.*** 112, 323-334 (2000). DOI: 10.1063/1.480583 http://scitation.aip.org/content/aip/journal/jcp/112/1/10.1063/1.480583
161. "Calculation of Nuclear Magnetic Resonance Parameters", C. J. Jameson, ***Encyclopedia of Analytical Chemistry, Instrumentation and Applications***, R. A. Meyers, ed. John Wiley, London, 2000 Vol. 14, pp. 12157-12187. ISBN-13: 978-0471976707. (see update of this article in V211)
160. "Theoretical and physical aspects of nuclear shielding," C. J. Jameson and A. C. de Dios, a chapter in ***Nuclear Magnetic Resonance***, G. A. Webb, ed., Royal Society of Chemistry, London, 2000, Vol. 29, Chap. 2, pp. 41-84. ISBN: 978-0-85404-327-9. DOI:10.1039/9781847553850-00041
159. "Application of Nuclear Shielding Surfaces to the Fundamental Understanding of Adsorption and Diffusion in Microporous Solids," C. J. Jameson, A. K. Jameson, A. C. de Dios, R. E. Gerald II, H. M. Lim, P. Kostikin, ***Modeling NMR Chemical Shifts: Gaining Insights into Structure and Environment***, ACS Symposium Series 732, ed. J. C. Facelli and A. C. de Dios, Oxford University Press, Oxford, 1999, Chap. 23, pp. 335-348. DOI: 10.1021/bk-1999-0732.ch023 http://pubs.acs.org/doi/abs/10.1021/bk-1999-0732.ch023
158. "Recent Advances in Nuclear Magnetic Shielding Theory and Computational Methods", C. J. Jameson, ***Modeling NMR Chemical Shifts: Gaining Insights into Structure and Environment***, ACS Symposium Series 732, ed. J. C. Facelli and A. C. de Dios, Oxford University Press, Oxford, 1999, Chap. 1, pp. 1-23. DOI: 10.1021/bk-1999-0732.ch001 http://pubs.acs.org/doi/abs/10.1021/bk-1999-0732.ch001
157. "Theoretical and physical aspects of nuclear shielding," C. J. Jameson and A. C. de Dios, a chapter in ***Nuclear Magnetic Resonance***, G. A. Webb, ed., Royal Society of Chemistry, London, 1999, Vol. 28, Chap. 2, pp. 42-76. ISBN: 978-0-85404-322-4. DOI:10.1039/9781847553843-00042
156. "A classical dynamics study of the anisotropic interactions in NNO-Ar and NNO-Kr systems. Comparison with transport and relaxation data," M. A. ter Horst and C. J. Jameson, ***J. Chem. Phys.*** 109, 10238-10243 (1998). DOI:10.1063/1.477719 http://scitation.aip.org/content/aip/journal/jcp/109/23/10.1063/1.477719
155. "Quadrupolar spin relaxation of ^{14}N in NNO on collisions with various molecules," C. J. Jameson, M. A. ter Horst, and A. K. Jameson, ***J. Chem. Phys.*** 109, 10227-10237 (1998).

DOI:10.1063/1.477718
http://scitation.aip.org/content/aip/journal/jcp/109/23/10.1063/1.477718
154. "Conventions for tensor quantities used in nuclear magnetic resonance, nuclear quadrupole resonance and electron spin resonance spectroscopy," C. J. Jameson, ***Solid State Nucl. Magn. Reson.*** 11, 265-268 (1998). DOI:10.1016/S0926-2040(98)00029-0 http://www.sciencedirect.com/science/article/pii/S0926204098000290 PMID: 9694396
153. "Theoretical and physical aspects of nuclear shielding," C. J. Jameson, a chapter in ***Nuclear Magnetic Resonance***, G. A. Webb, ed., Royal Society of Chemistry, London, 1998, Vol. 27, Chap. 2, p.44-82. ISBN: 978-0-85404-317-0. DOI:10.1039/9781847553836-00044
152. "The role of polarization of Xe by di- and monovalent cations in ^{129}Xe NMR studies in zeolite *A*," C. J. Jameson, H. M. Lim, and A. K. Jameson, ***Solid State Nucl. Magn. Reson.*** 9, 277-301 (1997). DOI:10.1016/S0926-2040(97)00063-5 http://www.sciencedirect.com/science/article/pii/S0926204097000635 PMID: 9477456
151. "Anisotropic Xe chemical shifts in zeolites. The role of intra- and inter-crystallite diffusion," C. J. Jameson, A. K. Jameson, R. E. Gerald II, and H. M. Lim, ***J. Phys. Chem***. 101, 8418-8437 (1997). DOI: 10.1021/jp971013a http://pubs.acs.org/doi/abs/10.1021/jp971013a
150. "Competitive adsorption of xenon and krypton in zeolite NaA. ^{129}Xe NMR and grand canonical Monte Carlo simulations," C. J. Jameson, A. K. Jameson, and H. M. Lim, ***J. Chem. Phys.*** 107, 4364-4372 (1997). DOI:10.1063/1.474778 http://scitation.aip.org/content/aip/journal/jcp/107/11/10.1063/1.474778
149. "Distribution and ^{129}Xe chemical shifts of Xe_n clusters in the alpha cages of zeolite Ag*A*," C. J. Jameson and H. M. Lim, ***J. Chem. Phys.*** 107, 4373-4383 (1997). DOI: 10.1063/1.475128 http://scitation.aip.org/content/aip/journal/jcp/107/11/10.1063/1.475128
148. "The ^{129}Xe nuclear shielding surfaces for Xe interacting with linear molecules CO, N_2 and CO_2," A. C. de Dios and C. J. Jameson, ***J. Chem. Phys.*** 107, 4253-4270 (1997). DOI:10.1063/1.474800 http://scitation.aip.org/content/aip/journal/jcp/107/11/10.1063/1.474800
147. "NMR chemical shifts: theory and experiment," C. J. Jameson, a chapter in ***Optical, Electric and Magnetic Properties of Molecules***, D. C. Clary and B. J. Orr, eds., Elsevier, Amsterdam, 1997, Chap. 11, p.303-317. DOI:10.1016/B978-044482596-4/50039-7 http://www.sciencedirect.com/science/article/pii/B9780444825964500397
146. "Theoretical and physical aspects of nuclear shielding," C. J. Jameson, a chapter in ***Nuclear Magnetic Resonance***, G. A. Webb, ed., Royal Society of Chemistry, London, 1997, Vol. 26, Chap. 2, p.46-87. ISBN: 978-0-85404-312-5. DOI:10.1039/9781847553829-00046
145. "A comparative study of CO_2-Ar potential surfaces," M. A. ter Horst and C. J. Jameson, ***J. Chem. Phys.*** 105, 6787-6806 (1996). DOI: 10.1063/1.471854 http://scitation.aip.org/content/aip/journal/jcp/105/16/10.1063/1.471854
144. "Understanding NMR chemical shifts", C. J. Jameson, ***Annu. Rev. Phys. Chem.*** 47, 135-169 (1996). DOI: 10.1146/annurev.physchem.47.1.135 http://www.annualreviews.org/doi/abs/10.1146/annurev.physchem.47.1.135
143. "Theoretical and physical aspects of nuclear shielding," C. J. Jameson, a chapter in ***Nuclear Magnetic Resonance***, G. A. Webb, ed., Royal Society of Chemistry, London,

1996, Vol. 25, 39-82 (1996). ISBN: 978-0-85404-307-1. DOI:10.1039/9781847553812-00039

142. "*Ab initio* study of van der Waals interaction of CO_2 with Ar," P. J. Marshall, M. M. Szczesniak, J. Sadlej, G. Chalasinski, M. A. ter Horst, and C. J. Jameson, ***J. Chem. Phys*.** 104, 6569-6576 (1996). DOI: 10.1063/1.471376 http://scitation.aip.org/content/aip/journal/jcp/104/17/10.1063/1.471376
141. "Competitive adsorption of xenon and argon in zeolite NaA. ^{129}Xe NMR and grand canonical Monte Carlo simulations," C. J. Jameson, A. K. Jameson, and H. M. Lim, ***J. Chem. Phys*.** 104, 1709-1728 (1996). DOI: 10.1063/1.470757 http://scitation.aip.org/content/aip/journal/jcp/104/4/10.1063/1.470757
140. "Gas phase studies of intermolecular interactions and relaxation," C. J. Jameson, ***Encyclopedia of Nuclear Magnetic Resonance***, Vol. 4, pp. 2179-2189 (1996) D. M. Grant and R. K. Harris, eds. John Wiley, London. Published online 15Mar 2007 DOI: 10.1002/9780470034590.emrstm0185 http://onlinelibrary.wiley.com/doi/10.1002/9780470034590.emrstm0185/abstract
139. "Isotope effects on chemical shifts and coupling constants", ***Encyclopedia of Nuclear Magnetic Resonance***, Vol. 4, pp. 2638-2655 (1996) D. M. Grant and R. K. Harris, eds., John Wiley, London. Published online 15 Mar 2007 DOI: 10.1002/9780470034590.emrstm0251 http://onlinelibrary.wiley.com/doi/10.1002/9780470034590.emrstm0251/abstract
138. "Chemical shift scales on an absolute basis," C. J. Jameson, ***Encyclopedia of Nuclear Magnetic Resonance***, Vol. 2, pp. 1273-1281 (1996), D. M. Grant and R. K. Harris, eds., John Wiley, London. ISBN-13: 978-0470847848. (see update of this article in V204)
137. "Early work on the ranges of chemical shifts and signs of coupling constants," C. J. Jameson, ***Encyclopedia of Nuclear Magnetic Resonance***, Vol. 1, pp. 401-402 (1996), D. M. Grant and R. K. Harris, eds., John Wiley, London. ISBN-13: 978-0470847848. DOI: 10.1002/9780470034590.emrhp0085 Published online 15 Mar 2007 http://onlinelibrary.wiley.com/doi/10.1002/9780470034590.emrhp0085/abstract
136. "Xe_n clusters in the alpha cages of zeolite K*A*," C. J. Jameson, A. K. Jameson, R. E. Gerald II, and H.-M. Lim, ***J. Chem. Phys*.** 103, 8811-8820 (1995). DOI:10.1063/1.470709 http://scitation.aip.org/content/aip/journal/jcp/103/20/10.1063/1.470709
135. "*Ab initio* studies of the nuclear magnetic resonance chemical shifts of a rare gas atom in a zeolite", C. J. Jameson and H. -M. Lim, ***J. Chem. Phys*.** 103, 3885-3894 (1995). DOI: 10.1063/1.469576 http://scitation.aip.org/content/aip/journal/jcp/103/10/10.1063/1.469576
134. "The N_2-Kr interaction: a multiproperty analysis," F. R. W. McCourt, M. A. ter Horst, and C. J. Jameson, ***J. Chem. Phys*.** 102, 5752-5760 (1995). DOI: 10.1063/1.469306 http://scitation.aip.org/content/aip/journal/jcp/102/14/10.1063/1.469306
133. "Classical trajectories on simple model potentials for N_2-Kr. Comparison with relaxation and other data," M. A. ter Horst and C. J. Jameson, ***J. Chem. Phys*.** 102, 4431-4446 (1995). DOI: 10.1063/1.469492 http://scitation.aip.org/content/aip/journal/jcp/102/11/10.1063/1.469492
132. "Theoretical and physical aspects of nuclear shielding," C. J. Jameson, a chapter in ***Nuclear Magnetic Resonance***, G. A. Webb, ed., Royal Society of Chemistry, London, 1995, Vol. 24, Chap. 2, pp. 44-75. ISBN: 978-0-85404-302-6. DOI:10.1039/9781847553805-00044

131 mistake in numbering

130. "Direct observation of distributions of mixed clusters of coadsorbed species in zeolite Na*A*." A. K. Jameson, C. J. Jameson, A. C. de Dios, E. Oldfield, and R. E. Gerald II, ***Stud. Surf. Sci. Catal*.** 98, 85-86 (1995). online 21 June 2007 (non-ISI journal) DOI: 10.1016/S0167-2991(06)81098-0 http://www.sciencedirect.com/science/article/pii/S0167299106810980

129. "^{129}Xe Magic-angle spinning spectra of xenon in zeolite NaA. Direct observation of mixed clusters of co-adsorbed species," A. K. Jameson, C. J. Jameson, A. C. de Dios, E. Oldfield, R. E. Gerald II, and G. L. Turner, ***Solid State Nucl. Magn. Reson*.** 4, 1-12 (1995). DOI:10.1016/0926-2040(94)00028-B http://www.sciencedirect.com/science/article/pii/092620409400028B PMID: 7894978

128. "Cage-to-cage migration rates of xenon atoms in zeolite Na*A* from magnetization transfer experiments and simulations," A. K. Jameson, C. J. Jameson, and R. E. Gerald II, ***J. Chem. Phys*.** 101, 1775-1786 (1994). DOI: 10.1063/1.467756 http://scitation.aip.org/content/aip/journal/jcp/101/3/10.1063/1.467756

127. "The NMR chemical shift: Insight into structure and environment," A. C. de Dios and C. J. Jameson, a chapter in ***Annual Reports on NMR Spectroscopy***, G. A. Webb, ed., Academic Press, London, 1994, Vol. 29, pp. 1-69. DOI: 10.1016/S0066-4103(08)60130-1 http://www.sciencedirect.com/science/article/pii/S0066410308601301

126. "Grand canonical Monte Carlo simulations of xenon in zeolite NaA, II. Structure of the adsorbed fluid," C. J. Jameson, A. K. Jameson, H. M. Lim, and B. I. Baello, ***J. Chem. Phys*.** 100, 5977-5987 (1994). DOI:10.1063/1.467109 http://scitation.aip.org/content/aip/journal/jcp/100/8/10.1063/1.467109

125. "Grand canonical Monte Carlo simulations of xenon in zeolite NaA," I. Distribution and ^{129}Xe chemical shifts," C. J. Jameson, A. K. Jameson, B. I. Baello and H. M. Lim, ***J. Chem. Phys*.** 100, 5965-5976 (1994). DOI: 10.1063/1.467108 http://scitation.aip.org/content/aip/journal/jcp/100/8/10.1063/1.467108

V112a. "Response to ''Comment on '14N spin relaxation studies of N2 in buffer gases. Cross sections for molecular reorientation and rotational energy transfer' '' [J. Chem. Phys. 100, 1775 (1994)]," C. J. Jameson, A. K. Jameson, M. A. ter Horst, ***J. Chem. Phys*.,** 100, 1777-1778 (1994). DOI: 10.1063/1.466557 http://scitation.aip.org/content/aip/journal/jcp/100/2/10.1063/1.466557 reply to comment on V112

124. "Theoretical and physical aspects of nuclear shielding," C. J. Jameson, a chapter in **Nuclear Magnetic Resonance**, G. A. Webb, ed., Royal Society of Chemistry, London, 1994, Vol. 23, Chap. 2, pp. 47-78. ISBN: 978-0-85186-462-4. DOI:10.1039/9781847553799-00047

123. "Theoretical and physical aspects of nuclear shielding," C. J. Jameson, a chapter in ***Nuclear Magnetic Resonance***, G. A. Webb, ed., Royal Society of Chemistry, London, 1993, Vol. 22, Chap 2, pp. 59-89. ISBN: 978-0-85186-452-5. DOI:10.1039/9781847553782-00059

122. "Overview and directions for the future," C. J. Jameson, in ***Nuclear Magnetic Shieldings and Molecular Structure***, J. A. Tossell, ed., Proceedings of the NATO Advanced Research Workshop on the Calculation of NMR Shielding Constants and Their Use in the Determination of the Geometric and Electronic Structures of Molecules and Solids, held

at College Park, Maryland, July 1992. originally published by Kluwer Academic Publishers, Dordrecht, 1993, pp. 557-560. ISBN-13: 978-0792321194. New copyright owner: Springer Science+Business Media Dordrecht ISBN 978-94-010-4722-7 DOI:10.1007/978-94-011-1652- 7 _29 http://link.springer.com/book/10.1007/978-94-011-1652-7/page/2#page-2

121. "The nuclear shielding surface: The shielding as a function of molecular geometry and intermolecular separation," C. J. Jameson and A. C. de Dios, in ***Nuclear Magnetic Shielding and Molecular Structure***, J. A. Tossell, ed., originally published by Kluwer Academic Publishers, Dordrecht, 1993, pp. 95-116. ISBN-13: 978-0792321194. New copyright owner: Springer Science+Business Media Dordrecht ISBN 978-94-010-4722-7 DOI:10.1007/978-94-011-1652-7_5 http://link.springer.com/chapter/10.1007%2F978-94-011-1652-7_5#page-1
120. "The nuclear magnetic shielding as a function of internuclear separation," C. J. Jameson and A. C. de Dios, ***J. Chem. Phys*.** 98, 2208-2217 (1993). DOI: 10.1063/1.464200 http://scitation.aip.org/content/aip/journal/jcp/98/3/10.1063/1.464200
119. "*Ab initio* calculations of the intermolecular chemical shift in nuclear magnetic resonance in the gas phase and for adsorbed species", C. J. Jameson and A. C. de Dios, ***J. Chem. Phys*.** 97, 417-434 (1992). DOI: 10.1063/1.463586 http://scitation.aip.org/content/aip/journal/jcp/97/1/10.1063/1.463586
118. "Theoretical and physical aspects of nuclear shielding," C. J. Jameson, a chapter in ***Nuclear Magnetic Resonance***, G. A. Webb, ed., Royal Society of Chemistry, London, 1992, Vol. 21, Chap. 2, pp. 36-69. ISBN: 978-0-85186-442-6. DOI:10.1039/9781847553775-00036
117. "^{129}Xe nuclear magnetic resonance studies of xenon in zeolite CaA," C. J. Jameson, A. K. Jameson, R. E. Gerald II, and A. C. de Dios, ***J. Chem. Phys*.** 96, 1690-1697 (1992). DOI: 10.1063/1.462123 http://scitation.aip.org/content/aip/journal/jcp/96/3/10.1063/1.462123
116. "Nuclear magnetic resonance studies of xenon clusters in zeolite NaA," C. J. Jameson, A. K. Jameson, R. E. Gerald II, and A. C. de Dios, ***J. Chem. Phys*.** 96, 1676-1689 (1992). DOI: 10.1063/1.462122 http://scitation.aip.org/content/aip/journal/jcp/96/3/10.1063/1.462122
115. "Gas phase NMR spectroscopy," C. J. Jameson, ***Chem. Rev*.** 91, 1375-1395 (1991). DOI: 10.1021/cr00007a005 http://pubs.acs.org/doi/abs/10.1021/cr00007a005
114. "The ^{31}P shielding in phosphine," C. J. Jameson, A. C. de Dios, and A. K. Jameson, ***J. Chem. Phys*.** 95, 9042-9053 (1991). DOI: 10.1063/1.461183 http://scitation.aip.org/content/aip/journal/jcp/95/12/10.1063/1.461183
113. "Theoretical and physical aspects of nuclear shielding," C. J. Jameson, a chapter in ***Nuclear Magnetic Resonance***, G. A. Webb, ed., Royal Society of Chemistry, London, 1991, Vol. 20, Chap. 2, pp. 48-80. ISBN: 978-0-85186-432-7. DOI:10.1039/9781847553768-00048
112. "^{14}N spin relaxation studies of N_2 in buffer gases. Cross sections of molecular reorientation and rotational energy transfer," C. J. Jameson, A. K. Jameson and M. A. ter Horst, ***J. Chem. Phys*.** 95, 5799-5808 (1991). DOI: 10.1063/1.461602 http://scitation.aip.org/content/aip/journal/jcp/95/8/10.1063/1.461602 (see reply to comment on this paper in V112a)

111. "Nuclear magnetic shielding of nitrogen in ammonia," C. J. Jameson, A. C. de Dios, and A. K. Jameson, ***J. Chem. Phys.*** 95, 1069-1079 (1991). DOI: 10.1063/1.461135 http://scitation.aip.org/content/aip/journal/jcp/95/2/10.1063/1.461135
110. "Molecular reorientation of nearly classical spherical tops. SeF_6 and TeF_6," C. J. Jameson, A. K. Jameson, and R. Terry, ***J. Phys. Chem.*** 95, 2982-2988 (1991). DOI:10.1021/j100161a010 http://pubs.acs.org/doi/abs/10.1021/j100161a010
109. "^{13}C and ^{1}H spin relaxation in CH_4 in the gas phase," C. J. Jameson, A. K. Jameson, N. C. Smith, J. K. Hwang, and T. Zia, ***J. Phys. Chem.*** 95, 1092-1098 (1991). DOI:10.1021/j100156a015 http://pubs.acs.org/doi/abs/10.1021/j100156a015

V107a. "Reply to a comment on: Angular momentum relaxation in binary collisions. Comparison of cross sections," C. J. Jameson, A. K. Jameson, ***J. Chem. Phys.*** 94, 7565-7565 (1991). DOI:10.1063/1.460143 http://scitation.aip.org/content/aip/journal/jcp/94/11/10.1063/1.460143 reply to comment on V107

108. "^{19}F nuclear spin relaxation by intermolecular magnetic dipole coupling. CF_4 and SiF_4 in oxygen gas," C. J. Jameson, A. K. Jameson, and J. K. Hwang, ***J. Chem. Phys.*** 94, 172-178 (1991). DOI: 10.1063/1.460375 http://scitation.aip.org/content/aip/journal/jcp/94/1/10.1063/1.460375
107. "Angular momentum relaxation in binary collisions. Comparison of cross sections," C. J. Jameson and A. K. Jameson, ***J. Chem. Phys.*** 93, 3237-3244 (1990). DOI:10.1063/1.458856 http://scitation.aip.org/content/aip/journal/jcp/93/5/10.1063/1.458856 (See reply to comment in V107a)
106. "Absolute shielding scale for ^{31}P from gas-phase NMR studies," C. J. Jameson, A. C. de Dios and A. K. Jameson, ***Chem. Phys. Lett.*** 167, 575-582 (1990). DOI:10.1016/0009-2614(90)85472-O http://www.sciencedirect.com/science/article/pii/000926149085472O
105. "Deuterium isotope effects and bonding in carbonylvanadium complexes," D. Rehder, M. Hoch, and C. J. Jameson, ***Magn. Reson. Chem.*** 28, 138-144 (1990). DOI:10.1002/mrc.1260280209 http://onlinelibrary.wiley.com/doi/10.1002/mrc.1260280209/abstract
104. "Theoretical and physical aspects of nuclear shielding," C. J. Jameson, a chapter in ***Nuclear Magnetic Resonance***, G. A. Webb, ed., Royal Society of Chemistry, London, 1990, Vol. 19, Chap. 1, pp. 1-33. ISBN: 978-0-85186-422-8. DOI:10.1039/9781847553751-00001 http://pubs.rsc.org/en/content/chapterpdf/1990/9781847553751-00001?isbn=978-0-85186-422-8&sercode=nm
103. "The dynamic and electronic factors in isotope effects on NMR parameters," C. J. Jameson, a chapter in ***Isotopic Applications in NMR Studies***, volume 2 of the series Isotopes in the Physical and Biomedical Sciences, E. Buncel and J. R. Jones, Elsevier, Amsterdam, 1991, Chap. 1, pp. 1-54. ISBN-13: 978-0-444-89090-0.
102. "Rovibrational averaging of molecular electronic properties," a chapter in *Molecular Spectroscopy, Electronic Structure, and Intramolecular Interactions,* Part 3 of the 4-part series Theoretical Models of Chemical Bonding, Z. B. Maksic, ed., Springer-Verlag, Berlin, 1991, pp. 457-519. ISBN 3-540-52252-2. https://books.google.com/books?isbn=3540522522

101. "Theoretical and physical aspects of nuclear shielding," C. J. Jameson, a chapter in ***Nuclear Magnetic Resonance***, G. A. Webb, ed., Royal Society of Chemistry, London, 1989, Vol. 18, Chap. 1, pp. 1-33. ISBN: 978-0-85186-412-9. DOI:10.1039/9781847553744-00001 http://pubs.rsc.org/en/content/chapterpdf/1989/9781847553744-00001?isbn=978-0-85186-412-9&sercode=nm
100. "Proton relaxation in methane with oxygen gas," C. J. Jameson, A. K. Jameson, and J. K. Hwang, ***J. Phys. Chem.*** 93,. 634-638 (1989). DOI: 10.1021/j100339a028 http://pubs.acs.org/doi/abs/10.1021/j100339a028
99. "Cross-sections for the anisotropic interaction of NNO with various molecules," C. J. Jameson, A. K. Jameson, J. K. Hwang, and N. C. Smith, ***J. Chem. Phys.*** 89., 5642-5649 (1988). DOI: 10.1063/1.455570 http://scitation.aip.org/content/aip/journal/jcp/89/9/10.1063/1.455570
98. "Nuclear spin relaxation by intermolecular magnetic dipole coupling in the gas phase. ^{129}Xe in oxygen," C. J. Jameson, A. K. Jameson, and J. K. Hwang, ***J. Chem. Phys.*** 89, 4074-4081 (1988). DOI: 10.1063/1.454842 http://scitation.aip.org/content/aip/journal/jcp/89/7/10.1063/1.454842
97. "Absolute shielding scale for ^{29}Si," C. J. Jameson and A. K. Jameson, ***Chem. Phys. Lett.*** 149, 300-305 (1988). DOI:10.1016/0009-2614(88)85030-9 http://www.sciencedirect.com/science/article/pii/0009261488850309
96. "Competition of intra- and intermolecular spin relaxation mechanisms for SF_6 in oxygen gas," C. J. Jameson, A. K. Jameson, J. K. Hwang, and D. Dabkowski, ***J. Phys. Chem.*** 92, 5937-5941 (1988). DOI: 10.1021/j100332a019 http://pubs.acs.org/doi/abs/10.1021/j100332a019
95. "The effects of rovibrational averaging on the ^{93}Nb chemical shift in $[Nb(CO)_6]^-$ ion, based on NMR and vibrational spectra," C. J. Jameson, D. Rehder and M. Hoch, ***Inorg. Chem.*** 27, 3490-3495 (1988). DOI: 10.1021/ic00293a012 http://pubs.acs.org/doi/abs/10.1021/ic00293a012
94. "Relaxation cross sections for the rotational angular momentum vector in CF_4," C. J. Jameson and A. K. Jameson, ***J. Chem. Phys.*** 89, 866-870 (1988). DOI: 10.1063/1.455208 http://scitation.aip.org/content/aip/journal/jcp/89/2/10.1063/1.455208
93. "Effective collision cross-sections for SF_6 from nuclear magnetic relaxation," C. J. Jameson and A. K. Jameson, ***J. Chem. Phys.*** 88, 7448-7452 (1988). DOI: 10.1063/1.454308 http://scitation.aip.org/content/aip/journal/jcp/88/12/10.1063/1.454308
92. "Isotope effects on proton chemical shifts and coupling constants in the ammonium ions $^{15,14}NH_{4-n}D_n^+$," J. K. M. Sanders, B. K. Hunter, C. J. Jameson, G. Romeo, ***Chem. Phys. Lett.*** 143, 471-476 (1988). DOI:10.1016/0009-2614(88)87398-6 http://www.sciencedirect.com/science/article/pii/0009261488873986
91. "Theoretical and physical aspects of nuclear shielding," C. J. Jameson, a chapter in ***Nuclear Magnetic Resonance***, G. A. Webb, ed., The Royal Society of Chemistry, London, 1988, Vol. 17, Chap. 1, pp. 1-30. ISBN: 978-0-85186-402-0. DOI:10.1039/9781847553737-00001 http://pubs.rsc.org/en/content/chapterpdf/1987/9781847553737-00001?isbn=978-0-85186-402-0&sercode=nm
90. The following chapters in "***Multinuclear NMR***," J. Mason, ed. Plenum Press, 1987. ISBN: 978-1-4612-8999-9. http://link.springer.com/book/10.1007%2F978-1-4613-1783-8

Chap. 2: The Parameters of NMR Spectroscopy, C. J. Jameson and J. Mason pp. 3-50
DOI:10.1007/978-1-4613-1783-8_2
Chap. 3: The Chemical Shift, C. J. Jameson and J. Mason pp. 51-88
DOI:10.1007/978-1-4613-1783-8_3
Chap. 4: Spin-spin Coupling, C. J. Jameson pp. 89-132
DOI:10.1007/978-1-4613-1783-8_4
Chap. 16: Fluorine, C. J. Jameson pp. 437-446
DOI:10.1007/978-1-4613-1783-8_16
Chap. 18: The Noble Gases, C. J. Jameson pp. 463-478
DOI:10.1007/978-1-4613-1783-8_18

89. "^{15}N spin relaxation studies of N_2 in buffer gases. Cross sections for molecular reorientation and rotational energy transfer," C. J. Jameson, A. K. Jameson, N. C. Smith, ***J. Chem. Phys.*** 86, 6833-6838 (1987). DOI: 10.1063/1.452381 http://scitation.aip.org/content/aip/journal/jcp/86/12/10.1063/1.452381
88. "Gas phase ^{13}C chemical shifts in the zero-pressure limit. Refinements to the absolute shielding scale for ^{13}C," A. K. Jameson, C. J. Jameson, ***Chem. Phys. Lett.*** 134, 461-466 (1987). DOI:10.1016/0009-2614(87)87173-7 http://www.sciencedirect.com/science/article/pii/0009261487871737
87. "Concurrent ^{19}F and ^{77}Se or ^{19}F and ^{125}Te NMR T_1 measurements for determination of ^{77}Se and ^{125}Te absolute shielding scales," C. J. Jameson, A. K. Jameson, ***Chem. Phys. Lett.*** 135, 254-259 (1987). DOI: 10.1016/0009-2614(87)85151-5 http://www.sciencedirect.com/science/article/pii/0009261487851515
86. "Theoretical and physical aspects of nuclear shielding," C. J. Jameson, a chapter in ***Nuclear Magnetic Resonance***, G. A. Webb, ed., The Royal Society of Chemistry, London, 1987, Vol. 16, Chap. 1, pp. 1-37. ISBN: 978-0-85186-392-4. DOI:10.1039/9781847553720-00001 http://pubs.rsc.org/en/content/chapterpdf/1986/9781847553720-00001?isbn=978-0-85186-392-4&sercode=nm
85. "Isotope and temperature dependence of transition metal shielding in complexes of the type $M(XY)_6$," C. J. Jameson, D. Rehder, M. Hoch, ***J. Am. Chem. Soc.*** 109, 2589-2594 (1987). DOI: 10.1021/ja00243a008 http://pubs.acs.org/doi/abs/10.1021/ja00243a008
84. "Vibrational analysis and mean bond displacements in $M(XY)_6$ complexes," C. J. Jameson, ***J. Am. Chem. Soc.*** 109, 2586-2588 (1987). DOI: 10.1021/ja00243a007 http://pubs.acs.org/doi/abs/10.1021/ja00243a007
83. "Cross sections for transfer of rotational angular momentum in CO_2 from ^{13}C spin relaxation studies in the gas phase," C. J. Jameson, N. C. Smith, and K. Jackowski, ***J. Chem. Phys.*** 86, 2717-2722 (1987). DOI: 10.1063/1.452074 http://scitation.aip.org/content/aip/journal/jcp/86/5/10.1063/1.452074
82. "Rovibrational averaging of nuclear shielding in MX_6-type molecules," C. J. Jameson, and A. K. Jameson, ***J. Chem. Phys.*** 85, 5484-5492 (1986). DOI: 10.1063/1.451559 http://scitation.aip.org/content/aip/journal/jcp/85/10/10.1063/1.451559
81. "Temperature dependence of ^{77}Se, ^{125}Te and ^{19}F shielding and M-induced ^{19}F isotope shifts in MF_6 molecules," C. J. Jameson, A. K. Jameson, and D. Oppusunggu, ***J. Chem. Phys.*** 85, 5480-5483 (1986). DOI: 10.1063/1.451558 http://scitation.aip.org/content/aip/journal/jcp/85/10/10.1063/1.451558

80. "An *ab initio* study of the molecular electric tensor properties of N_2, HCN, acetylene and diacetylene," C. J. Jameson and P. W. Fowler, ***J. Chem. Phys.*** 85, 3432-3436 (1986). DOI: 10.1063/1.450965 http://scitation.aip.org/content/aip/journal/jcp/85/6/10.1063/1.450965
79. "Theoretical and physical aspects of nuclear shielding," C. J. Jameson, a chapter in ***Nuclear Magnetic Resonance***, G. A. Webb, ed., The Royal Society of Chemistry, London, 1986, Vol. 15, Chap. 1, pp. 1-27. ISBN: 978-0-85186-382-5. DOI:10.1039/9781847553713-00001 http://pubs.rsc.org/is/content/chapterpdf/2006/9781847553713-00001?isbn=978-0-85186-382-5&pdate=1986-11-01&sercode=nm&page=search
78. "Theoretical considerations: Spin-spin coupling," a chapter in the book ***^{31}P NMR Spectroscopy in Stereochemical Analysis*:** Organic Compounds and Metal Complexes, J. G. Verkade and L. D. Quin, Eds., VCH Publishers, Weinheim, 1987, pp. 205-230. ISBN-13: 978-0895731494 [volume 8 in the series "Methods in Stereochemical Analysis"]
77. "Nuclear spin relaxation studies of the spin-rotation interaction of ^{13}C in CO in various buffer gases," C. J. Jameson, A. K. Jameson, and K. Buchi, ***J. Chem. Phys.*** 85, 697-700 (1986). DOI: 10.1063/1.451275 http://scitation.aip.org/content/aip/journal/jcp/85/2/10.1063/1.451275
76. "Theoretical aspects of the isotope effect on nuclear shielding," C. J. Jameson and H. J. Osten, a review chapter in ***Annual Reports on NMR Spectroscopy*,** G. A. Webb, ed. Academic Press, London, 1986, Vol. 17, 1-78. DOI:10.1016/S0066-4103(08)60234-3 http://www.sciencedirect.com/science/article/pii/S0066410308602343
75. "Quadrupolar spin relaxation due to electric field gradients induced by vibrations and collisions," H. J. Osten and C. J. Jameson, ***Mol. Phys.*** 57, 553-571 (1986). DOI:10.1080/00268978600100411 http://www.tandfonline.com/doi/abs/10.1080/00268978600100411#.VTgR9-RX3CI
74. "Isotope effects on spin-spin coupling," C. J. Jameson and H. J. Osten, ***J. Am. Chem. Soc.*** 108, 2497-2503 (1986). DOI: 10.1021/ja00270a001 http://pubs.acs.org/doi/abs/10.1021/ja00270a001
73. "Rovibrational averaging of molecular magnetic properties of CH_3F, CH_2F_2, and CHF_3," C. J. Jameson and H. J. Osten, ***Mol. Phys.*** 56, 1083-1095 (1985). DOI:10.1080/00268978500102911 http://www.tandfonline.com/doi/abs/10.1080/00268978500102911#.VTgReuRX3CI
72. "Deuterium-induced ^{19}F isotope shifts in fluoroethenes," H. J. Osten, C. J. Jameson, and N. C. Craig, ***J. Chem. Phys.*** 83, 5434-5441 (1985). DOI: 10.1063/1.449713 http://scitation.aip.org/content/aip/journal/jcp/83/11/10.1063/1.449713
71. "The mean bond displacements and the derivatives of ^{19}F shielding in CF_2=CFX and CF_2=CH_2," C. J. Jameson and H. J. Osten, ***J. Chem. Phys.*** 83, 5425-5433 (1985). DOI: 10.1063/1.449712 http://scitation.aip.org/content/aip/journal/jcp/83/11/10.1063/1.449712
70. "The temperature dependence of the ^{19}F resonance in isolated F_2C=CFX molecules," C. J. Jameson, A. K. Jameson, and D. Oppusunggu, ***J. Chem. Phys.*** 83, 5420-5424 (1985). DOI: 10.1063/1.449711 http://scitation.aip.org/content/aip/journal/jcp/83/11/10.1063/1.449711
69. "Application of the reduced isotope shift to general estimation of one-bond isotope shifts in NMR," C. J. Jameson and H. J. Osten, ***J. Am. Chem. Soc.*** 107, 4158-4161 (1985). DOI: 10.1021/ja00300a012 http://pubs.acs.org/doi/abs/10.1021/ja00300a012

V61a. "Erratum: The NMR isotope shift in polyatomic molecules. Estimation of the dynamic factors [J. Chem. Phys. 8, 1, 4300 (1984)]" C. J. Jameson, ***J. Chem. Phys*.** 83, 915-915 (1985). DOI:10.1063/1.449462 http://scitation.aip.org/content/aip/journal/jcp/83/2/10.1063/1.449462

68. "Rovibrational effects on nuclear shielding of apex nuclei in bent molecules," H. J. Osten and C. J. Jameson, ***J. Chem. Phys*.** 82, 4595-4606 (1985). DOI: 10.1063/1.448717 http://scitation.aip.org/content/aip/journal/jcp/82/10/10.1063/1.448717

67. "Variation of nuclear magnetic shielding of ^{19}F with intermolecular interaction and rovibrational motion in fluoroethanes," C. J. Jameson and A. K. Jameson, ***J. Magn. Reson*.** 62, 209-217 (1985). DOI:10.1016/0022-2364(85)90054-X http://www.sciencedirect.com/science/article/pii/002223648590054X

66. "Systematic trends in the variation of ^{19}F nuclear magnetic shielding with bond extension in halomethanes," C. J. Jameson and H. J. Osten, ***Mol. Phys*.** 55, 383-395 (1985). DOI: 10.1080/00268978500101411 http://www.tandfonline.com/doi/abs/10.1080/00268978500101411#.VTgQ_eRX3CI

65. "Theoretical and physical aspects of nuclear shielding," C. J. Jameson, a chapter with 116 references, in ***Nuclear Magnetic Resonance***, G. A. Webb, Ed. The Royal Society of Chemistry, London, 1985, Vol. 14, Chap. 1, pp. 1-20. ISBN: 978-0-85186-372-6. DOI:10.1039/9781847553706-00001 http://pubs.rsc.org/en/content/chapterpdf/1985/9781847553706-00001?isbn=978-0-85186-372-6&sercode=nm

64. "Correlation between the ^{19}F absolute nuclear magnetic shielding and its temperature dependence in the fluoromethanes," C. J. Jameson, ***Mol. Phys*.** 54, 73-79 (1985). DOI:10.1080/00268978500100061 http://www.tandfonline.com/doi/abs/10.1080/00268978500100061#.VTgQ0-RX3CI

63. "^{19}F nuclear magnetic shielding scale from gas phase studies II," C. J. Jameson, A. K. Jameson and J. Honarbakhsh, ***J. Chem. Phys*.** 81, 5266-5267, (1984). DOI:10.1063/1.447693 http://scitation.aip.org/content/aip/journal/jcp/81/12/10.1063/1.447693

62. "The mean bond displacements in $O{=}CF_2$ and their effect on ^{19}F nuclear magnetic shielding," C. J. Jameson and H. J. Osten, ***J. Chem. Phys*.** 81, 4915-4921, (1984). DOI:10.1063/1.447529 http://scitation.aip.org/content/aip/journal/jcp/81/11/10.1063/1.447529

61. "The NMR isotope shift in polyatomic molecules. Estimation of the dynamic factors," C. J. Jameson and H. J. Osten, ***J. Chem. Phys***. 81, 4300-4305 (1984); DOI:10.1063/1.447439 http://scitation.aip.org/content/aip/journal/jcp/81/10/10.1063/1.447439 [see also erratum JCP 83, 915 (1985), V61a]

60. "The additivity of NMR isotope shifts," C. J. Jameson and H. J. Osten, ***J. Chem. Phys*.** 81, 4293-4299 (1984). DOI: 10.1063/1.447438 http://scitation.aip.org/content/aip/journal/jcp/81/10/10.1063/1.447438

59. "The dependence of the ^{13}C and the ^{1}H nuclear magnetic shielding on bond extension in methane," H. J. Osten and C. J. Jameson, ***J. Chem. Phys*.** 81, 4288-4292 (1984). DOI: 10.1063/1.447437 http://scitation.aip.org/content/aip/journal/jcp/81/10/10.1063/1.447437

58. "^{19}F NMR chemical shifts due to intermolecular interactions in $F_2C{=}CFX$. A quantitative measure of the nuclear site effect," C. J. Jameson, A. K. Jameson and D. Oppusunggu, ***J.***

Chem. Phys. 81, 2313-2317 (1984). DOI: 10.1063/1.447921
http://scitation.aip.org/content/aip/journal/jcp/81/5/10.1063/1.447921

57. "The effect of anharmonic vibration and centrifugal distortion on nuclear shielding in linear triatomic molecules: NNO and CO_2," C. J. Jameson and H. J. Osten, ***J. Chem. Phys.*** 81, 2556-2561 (1984). DOI:10.1063/1.447988
http://scitation.aip.org/content/aip/journal/jcp/81/6/10.1063/1.447988
56. "Variation of nuclear magnetic shielding with intermolecular interactions and rovibrational motion. IX. ^{19}F in $F_2C=CH_2$ and $F_2C=CF_2$," C. J. Jameson, A. K. Jameson, and D. Oppusunggu, ***J. Chem. Phys.*** 81, 2571-2573 (1984). DOI:10.1063/1.447990
http://scitation.aip.org/content/aip/journal/jcp/81/6/10.1063/1.447990
55. "Variation of nuclear magnetic shielding with intermolecular interactions and rovibrational motion. VIII. ^{19}F in CF_3X," C. J. Jameson and A. K. Jameson, ***J. Chem. Phys.*** 81, 1198-1202 (1984). DOI: 10.1063/1.447795
http://scitation.aip.org/content/aip/journal/jcp/81/3/10.1063/1.447795
54. "Variation of nuclear magnetic shielding with intermolecular interactions and rovibrational motion. VII. ^{19}F in CF_2H_2, CF_2HCl, $CFHCl_2$, CF_2Cl_2 and $CFCl_3$," C. J. Jameson, A. K. Jameson, and D. Oppusunggu, ***J. Chem. Phys.*** 81, 85-90 (1984). DOI:10.1063/1.447356
http://scitation.aip.org/content/aip/journal/jcp/81/1/10.1063/1.447356
53. "Theoretical and physical aspects of nuclear shielding" C. J. Jameson, a chapter with 107 references, in ***Nuclear Magnetic Resonance***, G. A. Webb, Ed. The Royal Society of Chemistry, London, 1984, Vol. 13, Chap. 1, pp. 1-20. ISBN: 978-0-85186-362-7. DOI:10.1039/9781847553690-00001
http://pubs.rsc.org/en/content/chapterpdf/1984/9781847553690-00001?isbn=978-0-85186-362-7&sercode=nm
52. "Theoretical and physical aspects of nuclear shielding," C. J. Jameson, a chapter with 120 references in ***Nuclear Magnetic Resonance***, G. A. Webb, Ed. The Royal Society of Chemistry, London, 1983, Vol. 12, Chap. 1, pp. 1-19. ISBN: 978-0-85186-352-8. DOI:10.1039/9781847553683-00001
http://pubs.rsc.org/en/content/chapterpdf/1982/9781847553683-00001?isbn=978-0-85186-352-8&sercode=nm
51. "Theoretical and physical aspects of nuclear shielding", C. J. Jameson, a chapter with 132 references, in ***Nuclear Magnetic Resonance***, G. A. Webb, Ed. (Specialist Periodical Reports), The Royal Society of Chemistry, London, 1982, Vol. 11, Chap. 1, pp. 1-21. ISBN: 978-0-85186-342-9. DOI:10.1039/9781847553676-00001
http://pubs.rsc.org/en/content/chapterpdf/1982/9781847553676-00001?isbn=978-0-85186-342-9&sercode=nm
50. "Intermolecular effects of ^{1}H, ^{13}C and ^{15}N nuclear magnetic shielding in HCN", C. J. Jameson, A. K. Jameson, D. Oppusunggu, and S. Wille, ***J. Chem. Phys.*** 76, 152-162 (1982). DOI: 10.1063/1.442754
http://scitation.aip.org/content/aip/journal/jcp/76/1/10.1063/1.442754
49. "Theoretical and physical aspects of nuclear shielding", C. J. Jameson, A. chapter with 105 references in ***Nuclear Magnetic Resonance***, G. A. Webb, Ed. (Specialist Periodical Reports), The Royal Society of Chemistry, London, 1981, Vol. 10, Chap. 1, pp. 1-17. ISBN: 978-0-85186-332-0. DOI:10.1039/9781847553669-00001
http://pubs.rsc.org/en/content/chapterpdf/1981/9781847553669-00001?isbn=978-0-85186-332-0&sercode=nm

48. "Variation of chemical shielding with intermolecular interaction and rovibrational motion VI. ^{19}F in SF_4 and COF_2", C. J. Jameson, A. K. Jameson and S. Wille, ***J. Chem. Phys.*** 74, 1613-1617 (1981). DOI: 10.1063/1.441301 http://scitation.aip.org/content/aip/journal/jcp/74/3/10.1063/1.441301
47. "Temperature dependence of the ^{15}N and ^{1}H nuclear magnetic shielding of NH_3", C. J. Jameson, A. K. Jameson, S. M. Cohen, H. Parker, D. Oppusunggu, P. M. Burrell, and S. Wille, ***J. Chem. Phys.*** 74, 1608-1612 (1981). DOI: 10.1063/1.441300 http://scitation.aip.org/content/aip/journal/jcp/74/3/10.1063/1.441300
46. "Variation of chemical shielding with intermolecular interaction and rovibrational motion V. ^{15}N in N_2", C. J. Jameson, A. K. Jameson, S. Wille and P. M. Burrell, ***J. Chem. Phys.*** 74, 853-856 (1981). DOI: 10.1063/1.441135 http://scitation.aip.org/content/aip/journal/jcp/74/2/10.1063/1.441135
45. "Nitrogen nuclear magnetic shielding scale from gas phase studies", C. J. Jameson, A. K. Jameson, D. Oppusunggu, S. Wille, P. M. Burrell, and J. Mason, ***J. Chem. Phys.*** 74, 81-88 (1981). DOI: 10.1063/1.440797 http://scitation.aip.org/content/aip/journal/jcp/74/1/10.1063/1.440797
44. "^{19}F nuclear shielding scale from gas phase studies", C. J. Jameson, A. K. Jameson, and P. M. Burrell, ***J. Chem. Phys.*** 73, 6013-6020 (1980). DOI 10.1063/1.440135 http://scitation.aip.org/content/aip/journal/jcp/73/12/10.1063/1.440135
43. "Theoretical, physical and inorganic aspects of chemical shifts, C. J. Jameson and J. Mason, a chapter with 250 references, ***Nuclear Magnetic Resonance***, G. A. Webb, Ed. (Specialist Periodical Reports), The Royal Society of Chemistry, London, 1980, Vol. 9, Chap. 1, pp. 1-24. ISBN: 978-0-85186-960-5. DOI:10.1039/9781847553652-00001 http://pubs.rsc.org/en/content/chapterpdf/2006/9781847553652-00001?isbn=978-0-85186-960-5&sercode=nm
42. "Effects of intermolecular interactions and intramolecular dynamics on nuclear resonance", C. J. Jameson, ***Bull. Magn. Reson.*** 3, 3-28 (1980). https://wws.weizmann.ac.il/ISMAR/sites/ISMAR/files/bulletin/BMR_03_003-028_1981.pdf
41. "Molecular electronic property density functions: Nuclear magnetic shielding density", C. J. Jameson and A. D. Buckingham, ***J. Chem. Phys.*** 73, 5684-5692 (1980). DOI:10.1063/1.440045 http://scitation.aip.org/content/aip/journal/jcp/73/11/10.1063/1.440045
40. "Effects of vibrational anharmonicity on ^{19}F nuclear resonance in SF_6", C. J. Jameson, ***Mol. Phys.*** 40, 999-1003 (1980). DOI 10.1080/00268978000102071 http://www.tandfonline.com/doi/abs/10.1080/00268978000102071#.VTgQaeRX3CI
39. Book review of "Nitrogen-15 Nuclear Magnetic Resonance Spectroscopy," by G. C. Levy and R. L. Lichter, John Wiley and Sons, 1979, ***J. Am. Chem. Soc.*** 102, 7623 (1980).
38. "Nuclear magnetic shielding density", C. J. Jameson and A. D. Buckingham, ***J. Phys. Chem.*** 83, 3366-3371 (1979). DOI: 10.1021/j100489a011 http://pubs.acs.org/doi/abs/10.1021/j100489a011
37. "Effects of intermolecular interactions and intramolecular dynamics on nuclear resonance on NF_3, PF_3, POF_3, and PF_5", C. J. Jameson, A. K. Jameson, and S. Wille, ***J. Phys. Chem.*** 83, 3372-3378 (1979). DOI: 10.1021/j100489a012 http://pubs.acs.org/doi/abs/10.1021/j100489a012
36. "Gas to liquid shifts in NMR and the validity of the second virial coefficient of chemical shielding", C. J. Jameson, A. K. Jameson, and H. Parker, ***J. Chem. Phys.*** 70, 5916-5917

(1979). DOI:10.1063/1.437391
http://scitation.aip.org/content/aip/journal/jcp/70/12/10.1063/1.437391
35. "Isotope effects in ^{31}P NMR of phosphine", A. K. Jameson and C. J. Jameson, ***J. Magn. Reson.*** 32, 455-457 (1978). DOI:10.1016/0022-2364(78)90061-6
http://www.sciencedirect.com/science/article/pii/0022236478900616
34. "Effect of centrifugal distortion and anharmonic vibration on the ^{19}F chemical shielding in CH_3F", C. J. Jameson and A. K. Jameson, ***J. Chem. Phys.*** 69, 1655-1660 (1978). DOI:10.1063/1.436741
http://scitation.aip.org/content/aip/journal/jcp/69/4/10.1063/1.436741
33. "Temperature dependence of the chemical and shielding of ^{13}F nuclei in isolated CF_3H, CF_3Cl, CF_3Br and CF_3CF_3 molecules", C. J. Jameson, A. K. Jameson, and H. Parker, ***J. Chem. Phys.*** 69, 1318-1320 (1978). DOI: 10.1063/1.436675
http://scitation.aip.org/content/aip/journal/jcp/69/3/10.1063/1.436675
32. "Effect of centrifugal distortion and anharmonic vibration on the chemical shielding of ^{31}P in PH_3 and PD_3", C. J. Jameson and A. K. Jameson, ***J. Chem. Phys.*** 69, 615-621 (1978). DOI: 10.1063/1.436626
http://scitation.aip.org/content/aip/journal/jcp/69/2/10.1063/1.436626
31. "Second virial coefficient of ^{129}Xe chemical shielding in Xe interacting with CO and N_2 molecules", C. J. Jameson, A. K. Jameson, and H. Parker, ***J. Chem. Phys.*** 68, 3943-3944 (1978). DOI: 10.1063/1.436205
http://scitation.aip.org/content/aip/journal/jcp/68/8/10.1063/1.436205
30. "Variation of chemical shielding with intermolecular interactions and rovibrational motion IV. ^{11}B and ^{13}C nuclei in BF_3 and CH_4", A. K. Jameson, J. Moyer, and C. J. Jameson, ***J. Chem. Phys.*** 68, 2873-2877 (1978). DOI: 10.1063/1.436084
http://scitation.aip.org/content/aip/journal/jcp/68/6/10.1063/1.436084
29. "Variation of chemical shielding with intermolecular interactions and rovibrational motion III. ^{31}P nucleus in PH_3", C. J. Jameson, A. K. Jameson, and H. Parker, ***J. Chem. Phys.*** 68, 2868-2872 (1978). DOI: 10.1063/1.436083
http://scitation.aip.org/content/aip/journal/jcp/68/6/10.1063/1.436083
28. "Variation of chemical shielding with intermolecular interactions and rovibrational motion II. ^{15}N and ^{13}C nuclei in NNO and CO_2", C. J. Jameson, A. K. Jameson, H. Parker, S. M. Cohen, and C. L. Lee, ***J. Chem. Phys.*** 68, 2861-2867 (1978). DOI:10.1063/1.436082
http://scitation.aip.org/content/aip/journal/jcp/68/6/10.1063/1.436082
27. "The temperature dependence of chemical shielding in diatomic molecules: CO, F_2, ClF, HBr and HCl", A. K. Jameson, K. Schuett, C. J. Jameson, S. M. Cohen, and H. Parker, ***J. Chem. Phys.*** 67, 2821-2824 (1977). DOI: 10.1063/1.435147
http://scitation.aip.org/content/aip/journal/jcp/67/6/10.1063/1.435147
26. "The dependence of ^{19}F nuclear magnetic shielding on internal coordinates in CF_4, SiF_4, and BF_3", C. J. Jameson, ***J. Chem. Phys.*** 67, 2814-2820 (1977). DOI:10.1063/1.435146
http://scitation.aip.org/content/aip/journal/jcp/67/6/10.1063/1.435146
25. "Variation of chemical shielding with intermolecular interactions and rovibrational motion I. ^{19}F nuclei in BF_3, CF_4, SiF_4, and SF_6", C. J. Jameson, A. K. Jameson, and S. M. Cohen, ***J. Chem. Phys.*** 67, 2771-2774 (1977). DOI 10.1063/1.435192
http://scitation.aip.org/content/aip/journal/jcp/67/6/10.1063/1.435192

24. "Effect of interactions of non-spherical molecules on ^{129}Xe magnetic shielding", C. J. Jameson, A. K. Jameson, and S. M. Cohen, ***J. Chem. Phys*.** 66, 5226-5230 (1977). DOI:10.1063/1.433786 http://scitation.aip.org/content/aip/journal/jcp/66/11/10.1063/1.433786
23. "The isotope shift in NMR", C. J. Jameson, ***J. Chem. Phys*.** 66, 4983-4988 (1977). DOI:10.1063/1.433800 http://scitation.aip.org/content/aip/journal/jcp/66/11/10.1063/1.433800
22. "Variation of chemical shielding with internal coordinates. Applications to diatomic molecules", C. J. Jameson, ***J. Chem. Phys*.** 66, 4977-4982 (1977). DOI:10.1063/1.433799 http://scitation.aip.org/content/aip/journal/jcp/66/11/10.1063/1.433799
21. "Computer-enriched modules for introductory chemistry", C. J. Jameson, ***J. Chem. Educ*.** 54, 238-241 (1977). DOI: 10.1021/ed054p238 http://pubs.acs.org/doi/abs/10.1021/ed054p238
20. "Second virial coefficient of ^{129}Xe chemical shielding in mixture of Xe with spherical top molecules, CH_4, CF4, and SiF_4, C. J. Jameson, A. K. Jameson, and S. M. Cohen, ***J. Chem. Phys*.** 65, 3401-3406 (1976). DOI: 10.1063/1.433592 http://scitation.aip.org/content/aip/journal/jcp/65/9/10.1063/1.433592
19. "Contact interaction between ^{129}Xe and nitric oxide", C. J. Jameson, A. K. Jameson, and S. M. Cohen, ***J. Chem. Phys*.** 65, 3397-3400 (1976). DOI 10.1063/1.433591 http://scitation.aip.org/content/aip/journal/jcp/65/9/10.1063/1.433591
18. "An empirical chemical shielding function for interacting atoms from direct inversion of NMR data", C. J. Jameson, ***J. Chem. Phys*.** 63, 5296-5301 (1975). DOI:10.1063/1.431331 http://scitation.aip.org/content/aip/journal/jcp/63/12/10.1063/1.431331
17. "Absolute temperature dependence of chemical shielding of some reference nuclei", C. J. Jameson, A. K. Jameson, and S. M. Cohen, ***J. Magn. Reson*.** 19, 385-392 (1975). DOI:10.1016/0022-2364(75)90054-2 http://www.sciencedirect.com/science/article/pii/0022236475900542
16. "^{129}Xe contact shift in oxygen gas", C. J. Jameson, A. K. Jameson, and S. M. Cohen, ***Mol. Phys*.** 29, 1919-1927 (1975). DOI:10.1080/00268977500101671 http://www.tandfonline.com/doi/abs/10.1080/00268977500101671#
15. "Temperature and density dependence of ^{129}Xe chemical shift in rare gas mixtures", C. J. Jameson, A. K. Jameson, and S. M. Cohen, ***J. Chem. Phys*.** 62, 4224-4226 (1975). DOI: 10.1063/1.430304 http://scitation.aip.org/content/aip/journal/jcp/62/10/10.1063/1.430304
14. "Absolute temperature dependence of chemical shifts of lock solvents. Tetramethysilane, hexafluorobenzene and 1,4-dibromotetrafluorobenzene", A. K. Jameson and C. J. Jameson, ***J. Am. Chem. Soc*.** 95, 8559-8561 (1973). DOI: 10.1021/ja00807a010 http://pubs.acs.org/doi/abs/10.1021/ja00807a010
13. "Temperature and density dependence of ^{129}Xe chemical shift in xenon gas", C. J. Jameson, A. K. Jameson, and S. M. Cohen, ***J. Chem. Phys*.** 59, 4540-4546 (1973). DOI: 10.1063/1.1680652 http://scitation.aip.org/content/aip/journal/jcp/59/8/10.1063/1.1680652
12. "Quantum-mechanical treatment of the electronic structure and geometry of hydrogen cyanide dimer", C. J. Jameson and W. Yang, ***J. Theor. Biol*.** 35, 247-257 (1972). DOI:10.1016/ 0022-5193(72)90037-9 http://www.sciencedirect.com/science/article/pii/0022519372900379 PMID: 5039293

11. "Density dependence of ^{129}Xe NMR chemical shifts in O_2 and NO", C. J. Jameson and A. K. Jameson, ***Mol. Phys*.** 20, 957-959 (1971). DOI: 10.1080/00268977100100961 http://www.tandfonline.com/doi/abs/10.1080/00268977100100961#
10. "Density dependence of ^{129}Xe chemical shifts in mixtures of xenon and other gases", A. K. Jameson, C. J. Jameson, and H. S. Gutowsky, ***J. Chem. Phys*.** 53, 2310-2321 (1970). DOI: 10.1063/1.1674328 http://scitation.aip.org/content/aip/journal/jcp/53/6/10.1063/1.1674328
9. "On the spin-spin coupling between ^{13}C and H separated by two bonds", C. J. Jameson and M. C. Damasco, ***Mol. Phys*.** 18, 491-504 (1970). DOI:10.1080/00268977000100561 http://www.tandfonline.com/doi/abs/10.1080/00268977000100561#.VTgO4-RX3CI
8. "Signs of $^{1}K_{PC}$ and other coupling constants in phosphorus and selenium compounds", C. J. Jameson, ***J. Am. Chem. Soc*.** 91, 6232-6234 (1969). DOI:10.1021/ja01051a005 http://pubs.acs.org/doi/abs/10.1021/ja01051a005
7. "Systematic trends in the coupling constants of directly bonded nuclei", C. J. Jameson and H. S. Gutowsky, ***J. Chem. Phys*.** 51, 2790-2803 (1969). DOI: 10.1063/1.1672415 http://scitation.aip.org/content/aip/journal/jcp/51/7/10.1063/1.1672415
6. "Calculation of chemical shifts II. The xenon fluorides", C. J. Jameson and H. S. Gutowsky, ***J. Chem. Phys*.** 40, 2285-2293 (1964). DOI: 10.1063/1.1725506 http://scitation.aip.org/content/aip/journal/jcp/40/8/10.1063/1.1725506
5. "Calculation of chemical shifts I. General formulation and the Z dependence", C. J. Jameson and H. S. Gutowsky, ***J. Chem. Phys***. 40, 1714-1724 (1964). DOI:10.1063/1.1725387 http://scitation.aip.org/content/aip/journal/jcp/40/6/10.1063/1.1725387
4. "Valence bond studies of the dependence upon substituents of C^{13}-H and Si^{29}-H coupling", C. Juan and H. S. Gutowsky, ***J. Chem. Phys*.** 37, 2198-2208 (1962). DOI:10.1063/1.1732988 http://scitation.aip.org/content/aip/journal/jcp/37/10/10.1063/1.1732988
3. "Valence bond studies of internuclear coupling", H. S. Gutowsky and C. Juan, ***Disc. Faraday Soc***. 34, 52-63 (1962). DOI:10.1039/DF9623400052 http://pubs.rsc.org/EN/content/articlehtml/1962/df/df9623400052
2. "Electron coupling of nuclear spins VI. Relative signs of $J^{HH}g$, J^{HH} gem, and $J^{HH}t$ in (2.2) metacyclophane", H. S. Gutowsky and C. Juan, ***J. Chem. Phys*.** 37, 120-124 (1962). DOI:10.1063/1.1732932 http://scitation.aip.org/content/aip/journal/jcp/37/1/10.1063/1.1732932
1. "Valence bond interpretation of the additivity relations for C^{13}-proton coupling in substituted methanes", H. S. Gutowsky and C. S. Juan, ***J. Am. Chem. Soc*.** 84, 307-308 (1962). DOI: 10.1021/ja00861a037 http://pubs.acs.org/doi/abs/10.1021/ja00861a037

"Theoretical Calculations of Chemical Shifts in NMR. Application to the Xenon Fluorides." Cynthia Santos Juan 74 pp. Thesis (Ph.D.), University of Illinois at Urbana-Champaign, 1963. (Supervisor: Herbert S. Gutowsky) http://hdl.handle.net/2142/60580

PLENARY LECTURES, INVITED SYMPOSIUM LECTURES, and INVITED SEMINARS: ***(1995-present only)***

- February 1995, Argonne IL: Argonne National Labs Chemistry Division seminar, "NMR studies of rare gas clusters in zeolites. Adsorption and diffusion at the molecular level"
- March 1995, Boston MA: 36th Experimental NMR Conference, Symposium on Understanding Chemical Shifts, "Chemical shifts of rare gas clusters in zeolites"
- June 1995, La Crosse WI: ACS Great Lakes Regional Meeting Symposium on Advances and Applications of NMR, "NMR studies of rare gas clusters in zeolites. Adsorption, and diffusion at the molecular level"
- June 1995, Roskilde, Denmark: Summer School on Isotope Effects as a Tool in Basic and Environmental Science, (UNESCO), two lectures on isotope effects in NMR: "Rovibrational theory of isotope effects on molecular electronic properties" and "Isotope effects on NMR chemical shifts"
- July 1995, Denver CO: 37th Rocky Mountain Conference on Analytical Chemistry, NMR Symposium "Chemical shifts and distributions of rare gas clusters in zeolites"
- August 1995, Chicago IL: 26th Annual Meeting of the Fine Particle Society, Symposium on Multiphase Flow, Complex Media, Diffusion and Biochemical Transport, "NMR studies of rare gas clusters in zeolites. Adsorption and diffusion at the molecular level"
- September 25, 1995, Charleston, IL: Eastern Illinois University, "NMR studies of rare gas clusters in zeolites. Adsorption and diffusion at the molecular level"
- November 1995, National Research Council, Ottawa, Canada: "Understanding intermolecular NMR chemical shifts. Application to competitive adsorption in zeolites"
- December 4, 1995, Dalhousie University, Halifax, Canada: "Understanding intermolecular NMR chemical shifts. Application to competitive adsorption in zeolites"
- March 24-29, 1996, New Orleans, LA : American Chemical Society 211th National Meeting, Physical Chemistry Symposium on Adsorbed and Included Species in Zeolites, "Understanding intermolecular NMR chemical shifts. Application to competitive adsorption in zeolites"
- May 1996, Milwaukee, WI: Laboratory for Surface Studies, University of Wisconsin, "NMR studies of rare gas clusters in zeolites. Adsorption and diffusion at the molecular level"
- May 30-31, 1996, University of Minnesota Dow Lectureship in Chemistry, Minneapolis, MN: "^{129}Xe NMR Studies in Zeolites. Adsorption and Diffusion at the Molecular Level"
- Sept. 11, 1996, Chicago, IL: Illinois Institute of Technology, "^{129}Xe NMR studies in zeolites. Adsorption and diffusion at the molecular level"
- Sept. 13, 1996, Iowa City, IO: Univeristy of Iowa, "^{129}Xe NMR studies in zeolites. Adsorption and diffusion at the molecular level"
- Sept. 16, 1996, Asilomar, CA: Symposium on Understanding the Universe, R.A. Harris 60th Birthday Symposium, "Intermolecular NMR shielding surfaces and their applications"
- Oct. 24, 1996, University Park, IL: Governors State University, " ^{129}Xe NMR studies in zeolites"
- March 17, 1997, Kansas City, MO: American Physical Society National Meeting, Symposium on New Physics in Magnetic Resonance Spectroscopy, "Distribution and Dynamics of Molecules in Zeolites"
- March 27, 1997, West Lafayette, IN: Purdue University, Iota Sigma Pi Lecture, "^{129}Xe NMR studies in zeolites. Adsorption and diffusion at the molecular level"

- April 17, 1997, Oxford, OH: Miami University of Ohio, "^{129}Xe NMR studies in zeolites. Adsorption and diffusion at the molecular level"
- Sep. 26, 1997, Bloomington, IL: Illinois State University, "^{129}Xe NMR studies in zeolites. Adsorption and diffusion at the molecular level"
- Oct. 24, 1997, Eau Claire, WI: University of Wisconsin at Eau Claire, "^{129}Xe NMR studies in zeolites. Adsorption and diffusion at the molecular level"
- Nov. 25, 1997, College Station, TX: Texas A and M University, "^{129}Xe NMR studies in zeolites. Adsorption and diffusion at the molecular level"
- March 31, 1998, Dallas, TX: American Chemical Society 215th National Meeting, "Recent developments in the fundamental understanding of adsorption and diffusion in microporous solids"
- July 27-30, 1998, Denver CO: 40th Rocky Mountain Conference on Analytical Chemistry, NMR Symposium, " Understanding intermolecular chemical shifts. Applications to competitive adsorption in zeolites"
- August 23-27, 1998, Boston, MA: American Chemical Society 216th National Meeting, two invited talks: "Recent advances in nuclear magnetic shielding theory and computational methods", and " Intermolecular chemical shifts as a tool for fundamental understanding of adsorption and diffusion in microporous solids," in the Symposium on Modeling Chemical Shifts of the Division of Computational Chemistry.
- September 10, 1998, Ann Arbor, MI: University of Michigan, "^{129}Xe NMR studies in zeolites. Adsorption and diffusion at the molecular level"
- September 14-18, 1998, Smolenice, Bratislava, Slovak Republic: International Conference on Quantum Chemical Calculations of NMR and EPR Parameters "Application of Nuclear Shielding Surfaces to the Fundamental Understanding of Adsorption and Diffusion in Microporous Solids"
- September 25, 1998, Stony Brook, NY: SUNY, "^{129}Xe NMR studies in zeolites. Intermolecular Shifts as a Tool for Fundamental Understanding of Adsorption and Diffusion in microporous solids,"
- April 28, 1999, Morgantown, WV: West Virginia University , "^{129}Xe NMR Studies in Zeolites. Toward a Fundamental Understanding of Adsorption and Diffusion in Microporous Solids,"
- June 2, 1999, Toronto, Canada: 82nd Canadian Society for Chemistry Conference, Symposium on Nuclear Magnetic Resonance, "Understanding Intermolecular Chemical Shifts. Applications to Competitive Adsorption in Zeolites,"
- June 4, 1999, Ottawa, Canada: National Research Council, Steacie Institute for Molecular Sciences Colloquium, "Distributions of Molecules in Confined Geometries,"
- May 4, 2000, Madison, WI: University of Wisconsin McElvain Lecture , "^{129}Xe NMR Studies in Zeolites. Toward a Fundamental Understanding of Adsorption and Diffusion in Microporous Solids,"
- June 24, 2000, Ubana, IL: Herbert Gutowsky Memorial Symposium, "Chemical Shifts and Spin Spin Couplings,"
- June 27-30, 2000, Sestri Levante, Italy: XEMAT 2000, First International Meeting on Optical Polarization and Xenon NMR of Materials, "Understanding Xe Chemical Shifts," Plenary Lecture
- July 16-19, 2000, Argonne National Laboratory, IL: SMASH 2000. Small Molecule NMR Conference, "The NMR Chemical Shift" Plenary Lecture

- July 30-Aug. 3, 2000, Denver, CO: 42nd Rocky Mountain Conference on Analytical Chemistry, NMR Symposium, The Vaughan Award Lecture: " What types of Information can Intermolecular NMR Chemical Shifts Provide?"
- Jan. 19, 2001, University of California at Berkeley, CA: Alex Pines Group Seminar: "Xe NMR lineshapes in nanochannels"
- March 11-16, 2001, Orlando, FL: 42nd Experimental NMR Conference, "Xe chemical shifts in nano-channels"
- June 17-22, 2001, Bristol RI: Gordon Research Conference on Magnetic Resonance, "Xe shielding tensor in nano-channels and cavities"
- Feb. 7, 2002, University of California at Davis, CA: "Xe NMR lineshapes in nanochannels"
- Feb. 12, 2002, University of California at Berkeley, CA: "Xe NMR lineshapes in nanochannels"
- Apr. 24, 2002, University of Akron, OH: "Xe NMR lineshapes in nanochannels and cavities"
- July 22, 2002, Sonderkolloquium anlässlich des 65. Geburtstages von Herrn Prof. Dr. Reiner Radeglia, Adlershofer Analytisches Kolloquium, Berlin: "Xe NMR lineshapes in nanochannels and cavities"
- Oct. 2-4, 2002, The Harry Emmett Gunning Lecture Series, University of Alberta, Edmonton, Canada: "The nucleus as a reporter, the NMR chemical shift", "Adsorption and diffusion in nanopores", "Probing nanochannels with xenon"
- November 9, 2002, University of Notre Dame, IN: Chicago Area NMR Discussion Group, "Xe NMR lineshapes in nanochannels"
- May 29-31, 2003, La Colle-sur-Loup (Nice) France: XEMAT 2003, Second International Symposium on Xenon NMR of Materials, "Understanding Xe Chemical Shifts," Plenary Lecture
- July 27-31, 2003, Denver, CO: 45th Rocky Mountain Conference on Analytical Chemistry, NMR Symposium, "Xe chemical shifts in channels, cages and voids"
- August 10-15, 2003, Ottawa, Canada: 39th IUPAC Congress and 86th Conference of the Canadian Society for Chemistry, "Xe Chemical Shifts in Channels, Cages and Voids"
- Oct. 23-24, 2003, Chicago: Midwest Symposium Bruker Biospin, "Xe NMR in channels, cages and other nanopores"
- Oct. 27, 2003, University of Oregon: "Xe NMR in channels, cages and other nanopores"
- Nov. 18, 2003, Ohio State University: "Xe NMR in channels, cages and other nanopores"
- Feb. 3, 2004, Michigan State University: "Xe NMR in channels, cages and other nanopores"
- Sept. 24, 2004, University of Windsor, Canada: "Xe NMR in channels, cages and other nanopores"
- November 6, 2004, Loyola University: Chicago Area NMR Discussion Group, "Xe NMR lineshapes in peptide nanochannels"
- September 11, 2005, 4th Alpine Conference on Solid State NMR, Chamonix Mont-Blanc, France: "The Xe chemical shift in channels, cages, and other nanopores"
- October 18, 2005, University of Florida: "Xe NMR lineshapes in channels, cages and other nanopores"
- December 7, 2005, University of Delaware: ""Xe NMR in channels, cages and other nanopores"
- December 15, 2005, Symposium on Applications of NMR Spectroscopy in Materials Science, Pacifichem 2005, Honolulu: "Xe NMR informs on channels and cavities in solid materials"

- June 1-3, 2006, XEMAT III 2006, Ottawa, Canada: “The average chemical shift tensor of Xe atom as a probe of materials”
- November 11, 2006, University of Wisconsin-Madison, Chicago Area NMR Discussion Group, “Diastereomeric Xe chemical shifts in tethered cryptophane cages”
- February 6, 2007, Università Degli Studi Di Milano “Bicocca” Dipartimento di Scienza dei Materiali, Milan, Italy, “Exploring channels, cages and other nanopores with small molecules“
- January 8, 2008, 10th Eurasia Conference in the Chemical Sciences Jan. 7-11, 2008, Philippine International Convention Center, Manila Philippines, keynote address in the Spectroscopy Session.
- May 22-24, 2008, Philippine American Academy of Science and Engineering meeting, Georgetown University, Washington, D. C.
- March 23 - April 4, 2009, Intensive Faculty Training Workshop in Quantum Chemistry, sponsored by Commission on Higher Education, Philippines.
- June 7-11, 2009 XEMAT IV 2009, Kuusamo, Finland, “Understanding The Xe NMR Spectra In Well-Defined Environments To Reveal Structural And Dynamic Information In More Complex Environments”
- July 19-23, 2009, 51st Rocky Mountain Conference on Analytical Chemistry, NMR Symposium, Snowmass-Aspen, Colorado, “Understanding Xe NMR Spectra in Porous Solids”
- August 10-12, 2009, 55th ICASS, Kingston, Ontario, Understanding Xe NMR Spectra In Pores And Channels
- Best Practices in Diversity Recruitment and Retention of Faculty and Staff GCHERC Conference, University of Chicago, May 21, 2010, “Two Models of Faculty Search Committee Education: University of Illinois at Chicago (UIC) and the University of Wisconsin-Madison” Eve Fine, Research and Workshop Developer, Women in Science and Engineering Leadership Institute (WISELI), University of Wisconsin-Madison Cynthia J. Jameson, Professor Emerita, Department of Chemistry and Chemical Engineering, UIC, Constantine Megaridis, Professor, Mechanical and Industrial Engineering, UIC, Jennifer Sheridan, Executive and Research Director, WISELI, University of Wisconsin-Madison
- November 12-15, 2013, Washington, DC, Gender Summit 3- North America, Supporting Academic Women in STEM: The Post-Doc Institute, Nov. 14, 2013, Session on Improving Career-Life Balance. http://gender-summit.com/gs-past-speakers4/103-speakers-to-date/gs3-north-america-speakers/463-jameson
- March 23-28, 2014 55th ENC, Boston, 50+ Years of Trying to Understand NMR Chemical Shifts and Coupling Constants, after-dinner talk March 27, 2014.
- April 7-12, 2014, University of California at Berkeley, Alexander Pines Group, Xenon Atom: The Spy Who Came In From The Cold, April 11, 2014.
- July 13-17, 2014, 56th Rocky Mountain Conference on Analytical Chemistry. NMR Symposium, Copper Mountain Colorado,
- April 9-14, 2016 Jean Dreyfus Boissevain Lectureship at Washington & Jefferson College, a private liberal arts college in Washington, Pennsylvania, a series of lectures including: ”A Shielding Tutorial. Understanding the Chemical Shift Tensor”, “Mechanisms of Spin-Spin Coupling”, “Relativistic Effects on Nuclear Shielding”, “Why So Few? Unconscious biases and how they affect the advancement of women in academia in the STEM fields”

- May 3-8, 2017 University of Delaware. Physical Chemistry Colloquium “The inside scoop on the nature (symmetry, size, shape, dynamic distortion, presence of paramagnetic entities, chirality) of nanocavities and channels in porous materials via Xe atom NMR” and talks for NMR groups “A shielding tutorial. Understanding the chemical shift tensor” and “Mechanisms of spin-spin coupling”

SUMMARY OF PROF. JAMESON’S RESEARCH

The NMR chemical shift has been a very sensitive and extremely useful tool for chemists for discriminating between electronic environments. This intrinsic sensitivity to environment at nuclear sites becomes even more obvious as ever higher magnetic fields spread out the unique environments in the frequency scale. Jameson has contributed significantly to a fundamental understanding of the NMR chemical shift as a molecular electronic property. One characteristic of Jameson’s work is her interest in general trends and over-arching relationships, not just specific systems. Her contributions have usually involved providing the basis for a fundamental understanding of a limited body of data, and on this basis, predicting a systematic global pattern which emerges much later. In her early work, while searching for an explanation for the huge ^{129}Xe chemical shifts in the xenon fluorides, at a time when NMR shifts had been measured for only a very few nuclei in a limited number of compounds, she predicted that the range of chemical shifts should vary from one nucleus to another in the Periodic Table in the same way that r^{-3} average value for the p electron (or d for transition series) in the free atom. Accumulated data on nuclei in all parts of the Periodic Table now demonstrate this periodic behavior in a dramatic way. That seminal study forms the basis for the now commonly known scaling of chemical shifts of one type of nucleus to that of another type in analogous compounds and for the comparative sensitivities of different NMR nuclei to their electronic environment.

The NMR chemical shift is a difference between two values of the nuclear magnetic shielding. Part of the motivation of Jameson’s work in NMR in the gas phase has been to understand the way in which intermolecular interactions affect the nuclear magnetic shielding, in other words, the exploration of the nuclear magnetic shielding surface, analogous to the intermolecular potential energy surface. The observed resonance signal of a ^{129}Xe nucleus in xenon gas, for example, is a weighted average over the shielding surface corresponding to various Xe-Xe distances. She predicted the general shape of the intermolecular shielding surface, based on insight gained from the temperature dependence of the density coefficients of the chemical shifts measured in gases in her laboratory. The shape is not unlike the shape of a potential energy surface, deshielding relative to the infinitely separated situation, reaching a minimum at shorter distances, then becoming more shielded as the united atom (zero separation) limit is approached. No *ab initio* calculations had provided such a picture, and the calculations that did appear in the literature showed an intermolecular shielding function that was the wrong sign in the interesting separations, and monotonically deshielding as the distance between the interacting pair decreased, going to unphysically large negative values at short distances. Only recently (1993) have Jameson’s *ab initio* calculations shown that in the rare gas pair the shape of the purely theoretical shielding surface is indeed of a shape much like that predicted by Jameson nearly twenty years earlier. Almost all the reported studies of the effects of molecular collisions on the NMR chemical shift in the gas phase have emerged from Jameson’s laboratory. Her work forms the basis for the wide application of Xe NMR shifts for probing various polycrystalline surfaces, zeolites, other porous solids, and polymers.

The other nuclear magnetic shielding surface is the intramolecular one. This concept has emerged out of two separate but related phenomena: the observed temperature dependence of the NMR chemical shift in the gas in the limit of zero density and the small but ubiquitous NMR isotope shifts. All but one of the reported experiments observing phenomena of the first type were carried out in the Jameson laboratory. A global view of the large volume of isotope shift data, expressed in the same theoretical framework as used for the temperature dependence of the chemical shift in the isolated molecule was provided by Jameson in two papers in 1977. The nuclear magnetic shielding surface is the collection of values of shielding corresponding to the various geometries of the molecule. Weighted averaging over this surface occurs as the molecule undergoes rotation and vibration, according to the probabilities of various geometries, as expressed by the anharmonic vibrational wavefunctions. This interpretation provides a connection between the very easily measured isotope shifts and the product of two factors: a dynamic factor which depends on masses and force constants and an electronic factor which is a measure of the sensitivity of the shielding at the resonant nucleus to a small perturbation at the location of the isotopic substitution. The full theory involves many such terms containing these two factors; the leading term provides an interpretation of a very large collection of isotope shift data in a simple yet global way. Moreover, it leads to the interesting idea that isotope shifts provide important electronic information that depends on the electronic pathway between the two points, in the same way as does chemical shifts arising from functional group substitution, but are so benign as to not disturb the electronic distribution in the way that chemical group substitution does. With this model, Jameson predicted a large number of trends in the derivatives of the shielding surfaces at the equilibrium geometry of the molecule, all of which have recently been verified by *ab initio* calculations of the derivatives.

Jameson has determined absolute values of nuclear shielding for ^{19}F, ^{13}C, ^{15}N, ^{29}Si, ^{31}P, ^{77}Se, and ^{125}Te in the gas in the zero-density limit (virtually in the isolated molecule) for many compounds, thereby providing quantities which are much closer to what is calculated theoretically than the usual differences (chemical shifts) measured in condensed phases. These absolute shielding scales place all measured chemical shifts on an absolute basis, providing more stringent tests of high level quantum mechanical calculations. Other areas of interest have included NMR spin-spin coupling constants. Very early on she provided a simple model which predicted absolute signs of one-bond couplings and the changes in sign for pairs of nuclei as one goes across the Periodic Table when only a handful of such signs were known. The same model provides the basis for the shapes of spin spin coupling surfaces and isotope effects on J couplings. In summary, using NMR chemical shifts and coupling constants as examples, Jameson has drawn attention to the role of two important contributions to molecular electronic properties in general: intermolecular effects and rovibrational averaging, which should be considered in any comparisons of the experimental quantities with *ab initio* calculations, and she has made the general concept of molecular electronic property surfaces an important tool in the understanding of macroscopic observables.

Her work on spin relaxation studies in the gas phase provides a measure of the rate constants associated with either the reorientation of a molecular frame or the changes in the rotational angular momentum vector of a molecule upon collision with another. Each is an independent sensitive measure of the anisotropy of the intermolecular interaction potential of the collision pair. The relation between these two rates has been predicted by many theoretical models for molecular reorientation in liquids. Jameson's gas phase experiments test these models in the gas limit where the model predictions differ substantially from each other. From her lab has emerged the largest body of data on such rate constants (or the related cross

sections) for over a hundred different collision pairs as a function of temperature; the observed molecules are linear or spherical tops such as N_2, CO, CO_2, NNO, CH_4, CF_4, SiH_4, SiF_4, SF_6, SeF_6, and TeF_6. By using two different nuclei as probes, Jameson and her group have obtained both types of cross sections for the same collision pair and with a simple model she provided explanations for the general patterns observed in both cross sections. Her classical trajectory calculations are beginning to reproduce these quantities, thereby fulfilling the original promise of spin relaxation in the gas phase as a very sensitive test of the anisotropy of the intermolecular potential.

Her recent work in zeolites, the crystalline materials widely used for separations, oil recovery, and catalysis, capitalizes on Jameson's acknowledged leadership in the field of interpretation of gas phase NMR chemical shifts and is something sorely needed for advancing the understanding of how xenon interacts with the zeolite past the empirical state it had been in. Her studies of distribution and dynamic behavior of adsorbed species in what had been traditionally called "microporous" solids addresses a topical problem of both basic and technological importance. Actually the pores are in the nano-scale. What makes this research unusual is the combination of a detailed molecular level understanding of the fundamental processes with an awareness of the relevance of the results to potential technological applications. The PI has established an international reputation in the fields of ^{129}Xe NMR and zeolites and the PI is the leading expert in theoretical understanding of chemical shifts. The unique and powerful aspect of this research program is the combination of NMR experiments with theoretical calculations and simulations. Jameson's group at the University of Illinois at Chicago integrates Monte Carlo simulations (GCMC), ab initio quantum calculations and NMR experiments. Such a combination is essential if any fundamental advances in the understanding of distributions and dynamics in microporous solids are to occur. The prior work focused on zeolite NaA, a well-characterized crystalline system Jameson's lab has determined directly the distribution of Xe atoms in the cavities of a microporous solid by observing individually the trapped clusters Xe, Xe_2, Xe_3, ..., Xe_8 in NMR. The chemical shifts of the clusters vary with temperature as they undergo changes in configurations within the cavities. For the first time Jameson has reproduced the observed distributions, the cluster chemical shifts, and the temperature dependence by a computer simulation using only potential energy and shielding surfaces, with no adjustable parameters. These are the most detailed tests yet of any computer simulation, the observed quantities depend on the equilibrium distribution of the xenon between the bulk gas and inside the zeolite (the adsorption isotherm), the distribution of the adsorbed xenon among the cages (the cluster sizes and their fractions) and the distribution of the atoms of a given cluster within a cage (the chemical shift of the cluster depends on this). Her simulations provide these quantities and are tested by the detailed experiments in the same lab. This judicious choice of system where individual clusters Xe_n are observable in the ^{129}Xe NMR spectrum avoids having to interpret exchange-averaged spectra, where all the contributions are convoluted into a single chemical shift value. Thus, these investigations provide a basic understanding and the results highlights the subtleties and intricacies of the contributions of various intermolecular interactions to the Xe shielding function. The investigation of pore sizes, cation substitutions and distributions, alumina-silica ratio are all important issues relevant to applications in catalysis and separation science. The systematic approach used in this laboratory is the most sensible way to develop a quantitative understanding of the behavior of Xe in microporous solids in general. For example, the complete substitution of K^+ for Na^+ ion in the zeolite, while leaving the zeolite framework unchanged, verified the magnitude of the alkali ion contributions to the ^{129}Xe chemical shift in experimental and theoretical studies as detailed

as that in NaA. In another experimental breakthrough, the divalent cation contributions were determined by magic angle spinning NMR experiments in the same A zeolite framework where the Na+ ions were incrementally substituted by Ca^{2+} ions. In the same spectrum the individual progressions of Xe_n peaks were observed for cages containing no Ca^{2+} ion, one, two, or three Ca^{2+} ions, thereby observing directly the distributions of Xe atoms among cages of one type, as well as the competition between cages of different types for the sorbate atoms. Simulations successfully reproduced all observed trends and verified the importance of the role of electric polarization of the Xe atom by cations in any zeolite.

In another set of experiments and simulations, Jameson's lab has determined the rate of cage-to-cage migration of xenon atoms in a zeolite. By attaching a magnetic label to the Xe atoms in Xe_6 for example, it is possible to follow in time the appearance and disappearance of this label in all the other clusters, as the Xe atom leaves cavities of Xe_6 and go elsewhere. The time evolution of all peaks following a perturbation of one peak is simulated successfully when the rate constants are correctly chosen, One of the most exciting and significant results of this work is that the microscopic cage-to-cage migration rates k_{mn} vary with cluster sizes, m and n. Simulations using these rate constants also lead to the correct equilibrium distribution of xenon atoms among the cavities, as they should, verifying the consistency of the detailed dynamic information with the detailed equilibrium information. This work provides the most detailed picture yet of the process of diffusion within a microporous solid. These studies demonstrate that simulations can provide strict constraints on the quantitative interpretation of the experimental results. This represents an important contribution because Xe NMR is used empirically to characterize solids and polymers (usually in the fast exchange limit).

Competitive adsorption is a very important issue in the technological applications of zeolites. Jameson's experiments and simulations of binary mixtures in zeolites has provided a very detailed picture of competitive adsorption and diffusion as never before possible, right down to directly observing for the first time mixed clusters such as XeKr, Xe_2Kr, ... Xe_6Kr. In other cases where the co-adsorbed molecules (such as Ar, CO, CH_4, CO_2) are in fast exchange, she has directly determined the average number of co-adsorbed molecules in the same cage as exactly n Xe atoms for a given loading of the two sorbates. This level of detail is unprecedented in the entire history of adsorption studies. Although a large amount of ^{129}Xe NMR data in zeolites and other porous media have been reported over the past dozen years, Jameson's studies are the first to provide a quantitative theoretical understanding by reproducing detailed experimental results entirely from first principles.

A fundamental understanding of the processes of adsorption and diffusion within microporous solids is very important to their technological applications. Although a large number of scientists and engineers all over the world have been involved in such studies, only now with Jameson's recent papers have the most detailed experiments and quantitative interpretation of adsorption and diffusion processes been put forth. Given her style of doing science, it comes as no surprise that the concept of the intermolecular shielding surfaces developed by her from *ab initio* and gas phase studies make such detailed interpretations possible in heterogeneous systems which are completely consistent with her body of previous work in NMR of gas phase binary mixtures.

Jameson has developed a well-conceived systematic program to address fundamental aspects of adsorption at the molecular level in porous media. The broad scale of the attack on a well-defined problem in a well-characterized system has been particularly fruitful, combining as it does theoretical chemical shift calculations as a function of interatomic distances with GCMC calculations and comparing both with detailed experimental results under a variety of conditions.

Her work on kinetics and on Monte Carlo analysis of population distributions are completely original. The research has already led to significant new knowledge. The kind and variety of information obtained are unique. Jameson's work has convincingly demonstrated that information, unprecedented in its detail and fundamental significance can be extracted from such NMR experiments. This is the first major entree into the structure and dynamics of inclusion compounds in general, which are obviously relevant to the understanding and development of catalytic systems for industry. Jameson's thoughtful approach to the fundamental problems addressed will continue to have substantial impact upon progress in the field.

Jameson has established that the NMR lineshape of a confined molecule reflects the average NMR tensor properties which in turn reflect the geometry and the internal structure of the confining pore or channel and the intermolecular interaction of the molecule with the wall atoms of the confining structure. This was accomplished by making theoretical predictions of line shapes as a function of shape and size of the cage or channel, electronic nature of the wall atoms, the extent of hydrogen bonding of cage atoms, the point group symmetry of the cage, as a function of temperature and of occupancy. In a series of papers, she and her group have used a combination of quantum mechanical shielding surfaces and grand canonical Monte Carlo simulations to predict the line shapes and the systematic changes which are observed with temperature, with occupancy, in a wide range of zeolitic materials (Linde type A zeolites, silicalite, SSZ-24, ALPO4-11, etc.), a large number of clathrate hydrate cages of four different ice structures, organic cages of four types of cryptophanes and C_{60}, self-assembled nanochanneled molecular crystals such as TPP and dipeptides (prior to observations in this case), and also in channels decorated with paramagnetic centers.

A series of fundamental studies on model systems (carried out in collaboration with R. A. Harris at Berkeley) elucidates the relation between the nuclear magnetic shielding (which gives rise to the NMR chemical shift) and the intrinsic chirality of a molecule or environment, establishes the relation between odd and even parts of the potential and the various symmetric and antisymmetric components of the shielding tensor, and proves that a chiral potential alone is sufficient to provide discrimination of various diastereomers via their chemical shifts. These fundamental studies in simple model systems leads to reliable assignments of diastereomeric chemical shifts observed for Xe atom in derivatized cryptophane cages, including the Xe biosensor diastereomers.

Predictions of the chemical shifts of Xe in liquid solutions including water, alkanes, perfluoroalkanes and perfluorooctylbromide using molecular dynamics provide the first ever calculations of such shifts which for decades had been interpreted entirely in terms of the refractive index of the solvent. The ability to reproduce the chemical shift of Xe in aqueous solution by molecular dynamics simultations is particularly gratifying, since the shielding surfaces have been obtained from ab initio calculations for the Xe shielding in various ice cages in the clathrate hydrates, taking into account not only the cage water molecules, but the complete set of waters in the next shell of hydrogen bonding partners, as well as the electrostatic contributions from the remaining water molecules in the entire crystal. Not only solubilities and other average properties such as NMR chemical shifts of Xe in solutions can be obtained, but also rates of dynamic processes such as exchange, reorientation, and hydrated ion permeation of channels, including competitive transport studies of hydrated ions in carbon nanotube models for nanochannels.

Coarse-grained molecular dynamics simulations of model lipid-bilayer membranes which are self-assembled from an isotropic mixture permit the studies of permeation processes across

these membranes, providing important insight into mechanisms of transport of Xe and other small molecules such as O_2 and CO_2 across these membranes, with or without a transmembrane protein channel such as OmpA; penetration of gold nanocrystals and ligand-coated gold nanoparticles cause changes in the membrane physical and structural properties, and cause molecular-level events such as creation of pores (water columns), ion transport along the water-filled pores, lipid flip-flops, and lipid displacement from the membrane, revealing the molecular-level mechanisms for these events under various conditions.

SUMMARY OF PROF. JAMESON'S WORK IN ADVANCING WOMEN IN SCIENCE & ENGINEERING

In the late sixties, Professor Jameson was one of a handful of tenure-track women faculty in Chemistry departments in Ph. D. granting institutions, starting as an Assistant Professor in the Department of Chemistry at the University of Illinois at Chicago (then known as U of I Chicago Circle) in 1968, she was a tenured Associate Professor in 1972 and full professor in 1976, Professor Emeritus January 2006. Mentoring of students, undergraduate and graduate was a natural part of her academic activities. Her pre-and post-retirement activities towards advancing women in science and engineering careers, particularly in academic careers, became a significant part of the UIC ADVANCE program. Among these activities were the following.

(a) She developed of a series of workshops for science and engineering post-doctoral fellows, designing and planning the series which ran roughly once a month for two years, inviting and preparing the speakers, panelists, reviewers, mock search committees, etc., preparing the materials (presentations, hand-outs, checklists), moderating each one, and in many instances doing the presentations as well. A summary of the post-doc workshops, known as '*The Post-Doc Institute*' may be found at http://stemwomen.org/pdi.html and a copy of the original plan may be found at http://stemwomen.org/career/c14.pdf . Materials developed by Prof. Jameson for women preparing for an academic career may be found at http://www.stemwomen.org/career.html. These include the job search, a bibliography of gender issues in academe, key news articles on gender gap studies, and preparing for an academic career.

(b) She carried out training workshops for individual departmental Faculty Search Committees (customized with sub-field dis-aggregated data for each of 11 science and engineering departments, plus additional other departments who requested them) and also hiring workshops for college executives (heads and directors) of Liberal Arts and Sciences and the general faculty of College of Engineering). The workshops are on awareness and mitigation of the possible effects of unconscious bias in evaluation and decision-making in the hiring and promotion of faculty. The training workshop for faculty search committees initially developed for UIC by the founder of Women in Science and Engineering System Transformation (WISEST), Dr. Claudia Morrissey, was further developed by Prof. Jameson and other WISEST Facilitators who were members of *SUCCEED* (Supporting UIC's Commitment to a Community of Excellence, Equity & Diversity).
Some examples of these materials may be found at: http://www.stemwomen.org/search.html
A comparison of the SUCCEED approach with the WISELI approach for faculty search workshops, "Two Models of Faculty Search Committee Education: UI-Chicago and UW-Madison", can be found at: http://wiseli.engr.wisc.edu/docs/Present_HERC_2010.pdf.

(c) She co-developed with Claudia Morrissey the 32-page '*Faculty Search Toolkit*', a comprehensive set of strategies and examples for an evidence-based and inclusive faculty

search/hire. Copies of this Toolkit are used in other universities, e.g., 6 institutions in LA: http://www.institute.loni.org/lasigma/mentoring/WISESTSearchCommitteeToolkit.pdf. Case studies illustrating the successful application of these strategies were documented and presented as exemplars in SUCCEED workshops.

(d) Prof. Jameson developed the workshops for promotion/tenure committees of the College of Liberal Arts and Sciences, the College of Engineering, and the campus-wide Faculty Promotion/Tenure Committees, examples of which may be found at: http://www.stemwomen.org/PandT.html

(e) She developed the website plan and provided the content of the Facilitators' version of the WISEST website.

(f) She developed materials for STEM faculty development, examples of which may be found at: http://stemwomen.org/acad.html and materials for post-docs and prospective faculty which may be found at: http://www.stemwomen.org/job.html and http://www.stemwomen.org/pdi.html

Selected On-line pages:

- Retired(?) professor wins grant for student mentoring UIC News 4/14/10 http://www.uic.edu/depts/cemsl/Retired()%20professor%20wins%20grant%20for%20student%20mentoring.htm
- Celebrating Woman of the year UIC News 11/19/08 http://www.uic.edu/htbin/cgiwrap/bin/uicnews/articledetail.cgi?id=12573
- Woman of the Year: Cynthia Jameson. Forging a path in science UIC News 11/05/08 http://www.uic.edu/htbin/cgiwrap/bin/uicnews/articledetail.cgi?id=12529
- Chemists take closer look at useful xenon gas UIC News 03/02/05 http://www.uic.edu/htbin/cgiwrap/bin/uicnews/articledetail.cgi?id=9369
- Cynthia Jameson wouldn't take no for an answer UIC News 11/20/96 http://www.uic.edu/htbin/cgiwrap/bin/uicnews/articledetail.cgi?id=3870
- 1995 University Scholars: Cynthia Jameson UIC News 11/15/95 http://www.uic.edu/htbin/cgiwrap/bin/uicnews/articledetail.cgi?id=3308
- 'To Find CJ Make Way for CJ', by Angel C. de Dios, Philippine Science Letter, vol. 4, no. 2, pp 88-90, 2011. http://www.philsciletters.org/pdf/2011n2.14.pdf
- Gender Summit 3- North America, Supporting Academic Women in STEM: The Post-Doc Institute, Nov. 14, 2013, Session on Improving Career-Life Balance. http://gender-summit.com/gs-past-speakers4/103-speakers-to-date/gs3-north-america-speakers/463-jameson

- CJJ Home page http://www.stemwomen.org/
- CJJ's research http://www.stemwomen.org/cjj.html
- Preparing for an academic career http://www.stemwomen.org/career.html and linked pages.
- UIC faculty page for CJJ https://chem.uic.edu/chemistry/people/emeritus-faculty/cynthia-j-jameson
- Web of Science Researcher ID: http://www.researcherid.com/rid/G-4097-2012
- LinkedIn profile: https://www.linkedin.com/in/cynthia-j-jameson-78ba7763/
- Google Scholar Citations: https://scholar.google.com/citations?hl=en&user=BY5TvD0AAAAJ