

## **James B. Foresman**

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### **Publications**

1. "Reactions of an o-Quinone Monoimide with 1,3,5-trimethoxybenzene, 2-methoxythiophene, 2-methoxyfuran, and 1-methyl-,2-methyl-, and 1-2-dimethylindoles," H.W. Heine, C. Olsson, J.D. Bergin, J.B. Foresman, E.A. Williams, J. Org. Chem. 52, 97 (1987).
2. "An Ab Initio Study of Hydrated Chloride Ion Complexes: Evidence of Polarization Effects and Nonadditivity," J.B. Foresman and C.L. Brooks, III, J. Chem. Phys. 87, 5892 (1987).
3. "Assignment of the A State in Bicyclobutadiene," V.A. Walters, C.M. Hadad, Y. Thiel, S.D. Colson, K.B. Wiberg, P.M. Johnson, J.B. Foresman, J. Am. Chem. Soc. 113, 4782 (1991).
4. "Toward a Systematic Molecular Orbital Theory for Excited States," J. B. Foresman, M. Head-Gordon, M.J. Frisch, J.A. Pople, J. Phys. Chem. 96, 135 (1992).
5. "Electronically Excited States of Ethylene," K.B. Wiberg, C.M. Hadad, J.B. Foresman, W.A. Chupka, J. Phys. Chem. 96, 10756 (1992).
6. "A Theoretical Investigation of the Rotational Barrier in Allyl and 1,1,3,3-Tetramethylallyl Ions," J.B. Foresman, M.W. Wong, K.B. Wiberg, M.J. Frisch, J. Am. Chem. Soc. 115, 2220 (1993).
7. "The Excited States of Carbonyl Compounds. I. Formaldehyde and Acetaldehyde," C.M. Hadad, J.B. Foresman, K.B. Wiberg, J. Phys. Chem., 97, 4293 (1993).
8. "Application of the CI-Singles Method in Predicting the Energy, Properties, and Reactivity of Molecules in their Excited States," J.B. Foresman and H.B. Schlegel, in *Molecular Spectroscopy: Recent Experimental and Computational Advances*, NATO-ASI Series C, 1992.
9. "Butadiene. 3. Charge Distribution in Electronically Excited States," K.B. Wiberg, C.M. Hadad, G.B. Ellison, J.B. Foresman, J. Phys. Chem. 97, 13586 (1993).
10. "Solvent Effects. 5. Influence of Cavity Shape, Truncation of Electrostatics, and Electron Correlation on Ab Initio Reaction Field Calculations," J.B. Foresman, T.A. Keith, K.B. Wiberg, J. Snoonian, M.J. Frisch, J. Phys. Chem. 100, 16098 (1996).
11. "Exploring Chemistry with Electronic Structure Methods," 2nd edition, J.B. Foresman, AE. Frisch, Gaussian, Inc., Pittsburgh, PA, 302 pages, 1993, 1996.
12. "Ab Initio Techniques in Chemistry: Interpretation and Visualization," Ch. 14 in "Using Computers in Chemistry and Chemical Education," Ed. M.L. Swift and T.J. Zielinski (ACS Books, Washington, D.C. 1997).
13. "Naphthalene and Azulene I: Semimicro Bomb Calorimetry and Quantum Mechanical Calculations," C. Salter and J.B. Foresman, J. Chem. Educ., 75, 1341 (1998).
14. "Laboratory Handbook for General Chemistry," J.E. Smith and J.B. Foresman, York College of PA, 1998, 2001.

15. "Further Solvatochromic, Thermochromic, and Theoretical Studies on Nile Red," C. M. Golini, B. W. Williams, J.B. Foresman, J. of Fluorescence, 8, 395 (1998).
16. "Computational Chemistry: A Practical Guide," by David Young; book review, J. Foresman, J. Am. Chem. Soc. 123, 10142 (2001).
17. "Assessment of TDDFT for the Calculation of Critical Features in the Absorption Spectra of a Series of Aromatic Donor-acceptor Systems," C. Jamorski, J.B. Foresman, C. Thilgen, H-P. Luthi, J. Chem. Phys., 116, 8761 (2002).
18. "Solvation of Nitrophenol Isomers: Consequences for Alkane/Water Partitioning," W.H. Steel, J.B. Foresman, D.K. Burden, Yuen Y., Lau, and R.A. Walker, J. Phys. Chem. B, 113, 759 (2009).

### **Oral Presentations**

1. "Exploring Chemistry Using Ab Initio MO Theory," ACS National Meeting, Chicago, Aug. 1993.
2. "Molecular Visualization and Computation in Undergraduate Chemistry," ACS, Washington, Aug. 1994.
3. "Ab Initio MO Calculations Visualized on a PC," ACS National Meeting, New Orleans, March 1996.
4. "Fostering Student Understanding in Computational Chemistry," ACS, San Francisco, March 1997.
5. "Teaching Physical Chemistry," Mid-Atl Assoc of Liberal Arts Chem Teachers, Chestertown, MD, Oct. 1997.
6. "Do Undergraduates Need To Know How to Run Ab Initio MO Calculations?," ACS, Boston, Aug. 1998.
7. "The Molecular Laboratory: Student Explorations into Electronic Structure Theory," International Computational Chemistry Series, ETH Zurich, Switzerland, Oct. 1999.
8. "Exploring Organic Chemistry using Electronic Structure Theory," Dept. of Organic Chemistry, University of Geneva, Switzerland, March, 2000.
9. "Potential Energy Surfaces," lecture at the School for Computational Chemistry, Milano, Italy, July 2000.
10. "Using Computational Methods to Teach Chemistry," Gaussian Users Meeting, Honolulu, Dec. 2000.
11. "Solvent Effects in Chemistry," Chemistry Department, Moravian College, Feb. 2001.
12. "Techniques in Modern Computational Chemistry," Lebanon Valley Section of the ACS Meeting, Feb. 2001.
13. "Electronic Structure Theory in the Physical Chemistry Laboratory," American Chemical Society National Meeting, San Diego, April 2001.
14. "Theory and Experiment: Student Explorations into the Calculation and Visualization of Thermochemical and Spectroscopic Data," World Association of Theoretically Oriented Chemists, Lugano, Switzerland, Aug. 2002.
15. "Theory and Experiment: Student Exercises Designed to Increase Conceptual Understanding," American Chemical Society National Meeting, Boston, Aug. 2002.
16. "Molecular Modeling Exercises Designed to Accompany Student Lab Work," Southwest Regional ACS Meeting, Austin Texas, November 2002.
17. "Do Undergraduates Need To Be Exposed To the Cutting-Edge of Computational Chemistry?" American Chemical Society National Meeting, New Orleans, March 2003.
18. "Playing in the Sandbox: Can undergraduates learn from experimenting with molecular modeling software," co-authored with Mark Midland (U.C. Riverside), ACS national meeting, Philadelphia, 2004.

19. "Undergraduates and Gaussian: a perfect fit for developing an undergraduate research experience," Middle-Atlantic Regional Meeting, Hershey PA, 2006.
20. "Teaching Physical Chemistry the Fun and Easy Way with Density Functional Theory," American Chemical Society National Meeting, Philadelphia, August 2008.
21. "NMR measurements coupled with quantum mechanical calculations for assigning carbon-13 NMR signals in the undergraduate curriculum," American Chemical Society National Meeting, Anaheim, CA, March 2011.

### **Student Co-authored Poster Presentations**

1. "Toward more accurate computational methods to predict C-13 chemical shifts: A study of 2,2,4-trimethylpentane-1,3-diol," Pisarenko, Aleksey; Foresman, James B.; Clarke, Donald, 225th ACS National Meeting, New Orleans, LA, March 23-27, 2003.
2. "Study of N,N-(dimethylamino)benzotrile as an undergraduate physical chemistry lab: Fluorescence spectroscopy and Gaussian calculations," Beck, Jeremy M.; Foresman, James B., 229th ACS National Meeting, San Diego, CA, March 13-17, 2005.
3. "Computational analysis of zincocene, decamethylzincocene, and decamethylzincocene," Ludlow, Michelle K.; Foresman, James B., 229th ACS National Meeting, San Diego, CA, March 13-17, 2005.
4. "Comparison of rules of additivity and DFT in predicting 13C NMR shifts of anisole derivatives," Despeaux, Emily C.; Stambaugh, Amanda J.; Foresman, James B.; Halligan, Kathleen M., 237th ACS National Meeting, Salt Lake City, UT, March 22-26, 2009.
5. "Educational potential of VCD for undergraduate chemists," Stambaugh, Amanda; MacPherson, Tyler; May, Brian; Foresman, James, 239th ACS National Meeting, San Francisco, CA, March 21-25, 2010.
6. "J coupling constants of ortho substituted aromatic compounds: Comparing theory and experiment," Townsend, Julie N.; Foresman, James B., 239th ACS National Meeting, San Francisco, CA, March 21-25, 2010.
7. "Experimental and computational studies of the Mills-Nixon effect," Blaszyk, Allison N.; Foresman, James B., 239th ACS National Meeting, San Francisco, CA, March 21-25, 2010.
8. "Student explorations of the Mills-Nixon effect: kinetic measurements using FT-NMR and electronic structure calculations using Gaussian 09," Tobin, S. J.; Foresman, J.B., 241<sup>st</sup> ACS National Meeting, Anaheim, CA, March 27-31, 2011.
9. "Solvent effects in the VCD analysis of two chiral building blocks," Sapp, K.C.; Foresman, J.B., 241<sup>st</sup> ACS National Meeting, Anaheim, CA, March 27-31, 2011.