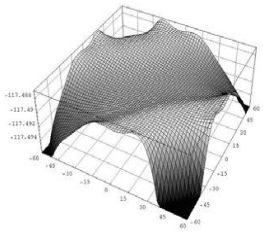
Weston Thatcher Borden
Welch Professor
Theoretical and Organic Chemistry



Dr. Borden received B.A., M.A., and Ph.D. degrees from Harvard University in 1964, 1966, and 1968, respectively. He also spent a year studying theoretical chemistry at Cambridge University in 1964-65. Dr. Borden became an Assistant Professor at Harvard in 1968. In 1973 he moved to the University of Washington, where he remained for the next 31 years, before joining the UNT faculty in 2004. Dr. Borden is Associate Editor of the Journal of the American Chemical Society. He has been the recipient of Fellowships from the Sloan and Guggenheim Foundations, from the Japanese Society for Promotion of Science, and from the University of Melbourne. He has received a Senior Scientist Award from the Alexander von Humboldt Foundation, a Cope Senior Scholar Award from the American Chemical Society, and the 2011 James Flack Norris Award in Physical-Organic Chemistry, also from the American Chemical Society. He has also been elected a Fellow of the American Association for the Advancement of Science and of the American Chemical Society.

Research

Professor Borden's group uses electronic structure calculations to interpret the results of experiments and to propose experimental tests of these interpretations. The computational research in Professor Borden's group is aimed not only at making quantitative predictions but also at developing a qualitative understanding of organic and organometallic chemistry.

The Borden group has published the results of ab initio and DFT calculations on many different types of molecules and reactive intermediates, including carbenes, nitrenes, carbocations, mono-, di-, and triradicals, radical anions and cations, silenes, silylenes, phosphenes and phosphinidenes. Potential surfaces for the rearrangements of both reactive intermediates (e.g., carbenes and nitrenes) and stable molecules (e.g. cyclopropane and derivatives of 1,5-hexadiene) have been computed and interpreted. Since moving to UNT, the Borden group has also been investigating the role that quantum mechanical tunneling, both by hydrogen and by carbon, plays in organic reactions.

The computational research in Professor Borden's group has led to extensive collaborations with many other research groups, not only in the U.S. and Canada, but also in Europe and Japan.

Selected Publications

- "Calculations of the Effects of Methyl Groups on the Energy Differences Between Cyclooctatetraene and Bicyclo[4.2.0]octa-2,4,7-triene and Between Their Iron Tricarbonyl Complexes." X. Bao, D. A. Hrovat, and W. T. Borden, J. Org. Chem. 77, 956 (2012).
- "H. C. Longuet-Higgins – The Man and His Science" in Pioneers of Quantum Chemistry, A. Wilson and T. Strom, Eds., ACS Books, in press.
- "The Molecular Orbitals of the Oxocarbons $(CO)_n$, n = 2 – 6. Why Does $(CO)_4$ Have a Triplet Ground State?" X. Bao, X. Zhou, C. F. Lovitt, A. Venkatraman, D. A. Hrovat, R. Gleiter, R. Hoffmann, and W. T. Borden, J. Am. Chem. Soc. 134, 10259 (2012).
- "Cooperative and Competitive Effects Associated with Fe(CO)3 Binding to Annelated Benzenes" X. Bao, D. A. Hrovat, and W. T. Borden, Chemical Science 4, 516 (2012).
- "Synchronized Aromaticity as an Enthalpic Driving Force for the Aromatic Cope Rearrangement." D. J. Babinski, X. Bao, M. El Arba, B. Chen, D. A. Hrovat, W. T. Borden, and D. E. Frantz, J. Am. Chem. Soc. 134, 16139 (2012).
- "Like $(CO)_4$, Do $(CS)_4$ and $(CSe)_4$ Have a Triplet Ground State?" X. Bao, D. A. Hrovat, and W. T. Borden, Chem. Eur. J. 19, 5687 (2013).
- "Negative Ion Photoelectron Spectroscopy Confirms the Prediction that $(CO)_5$ and $(CO)_6$ Each Has a Singlet Ground State." X. Bao, D. A. Hrovat, W. T. Borden, and X.-B. Wang, J. Am. Chem. Soc. 135, 4291 (2013).
- "The Ground State of $(CS)_4$ Is Different from that of $(CO)_4$: An Experimental Test of a Computational Prediction by Negative Ion Photoelectron Spectroscopy." J. Zhang, D. A. Hrovat, Z. Sun, X. Bao, W. T. Borden, and X.-B. Wang, J. Phys. Chem. A, 117, 00000 (2013)
- "How to Make the $\sigma^{\square}\pi^2$ Singlet the Ground State of Carbenes." B. Chen, A. Y. Rogachev, D. A. Hrovat, R. Hoffmann, and W. T. Borden, W. T. J. Am. Chem. Soc. 135, 00000 (2013).

For more information, contact:
E-mail: borden@unt.edu
Phone: (940) 565-3658
Website: http://chemistry.unt.edu/people/weston-t-borden