

RICHARD VAUGHAN WILLIAMS PUBLICATIONS

Some uses of Silicon Compounds in Organic Synthesis, Ph.D. Thesis, Cambridge, 1978.

R. H. Mitchell, Y.-H. Lai, and R. V. Williams, "N-Bromosuccinimide Dimethylformamide: A Mild, Selective Nuclear Mono-Bromination Reagent for Reactive Aromatic Compounds." *J. Org. Chem.*, **1979**, *44*, 4733.

I. Fleming and R. V. Williams, "The Reaction between bis(trimethylsilyl)-cyclopentadiene and Dichloroketen, and the Diels-Alder Reactions between N-Phenylmaleimide and Two Silylated Methylcyclopentadienes," *J.C.S. Perkin, I* **1981**, 684.

L. A. Paquette and R. V. Williams, "Silicon in Organic Synthesis.12. *trans*-1-Benzenesulfonyl-2-(Trimethylsilyl)ethylene, A Diels-Alder Dienophile Equivalent of Acetylene and Monosubstituted Acetylenes," *Tetrahedron Letters*, **1981**, *22*, 4643.

R. H. Mitchell, R. V. Williams, and T. W. Dingle, "Toward the Understanding of Benzannelated Annulenes: Synthesis and Properties of [a,h]- and [a,i]-Ring Dibenzannelated Dihydropyrenes," *J. Am. Chem. Soc.*, **1982**, *104*, 2560.

R. H. Mitchell, R. V. Williams, R. Mahadevan, Y.-H. Lai, and T. W. Dingle, "Toward the Understanding of Benzannelated Annulenes: A Simple Correlation of the Diatropicity of Several Benzannelated Dihydropyrenes in terms of Bond Order Deviations with Predictions for Other Benzannulenes," *J. Am. Chem. Soc.*, **1982**, *104*, 2571.

L. A. Paquette, R. V. Williams, R. V. C. Carr, P. Charumilind, and J. F. Blount, "[1,5]Hydrogen Sigmatropy within Isodicyclopentadiene. Cycloadditive Capture of a Fleeting Isomer with Dienophiles of Low Reactivity," *J. Org. Chem.*, **1982**, *47*, 4566.

R. H. Mitchell, T. W. Dingle, P. R. West, R. V. Williams, and R. C. Thompson, "On the Possibility of New Families of $(4n+2)\pi$ Electron Biradicaloid Hydrocarbons," *J. Org. Chem.*, **1982**, *47*, 5210.

R. H. Mitchell, T. W. Dingle, and R. V. Williams, "2,3-Dimethylnaphthalene /TMEDA/n-Butyllithium: An Unusual Ambident Aromatic Nucleophile," *J. Org. Chem.*, **1983**, *48*, 903.

L. A. Paquette, A. R. Browne, C. W. Doecke, and R. V. Williams, "A Short Stereocontrolled Synthesis of [4]Peristylane," *J. Am. Chem. Soc.*, **1983**, *105*, 4113.

A. J. Fry, J. Simons, M. Tashior, T. Yamato, R. H. Mitchell, T. W. Dingle, R. V. Williams, and R. Mahadevan, "Electrochemical Reduction of Substituted 15,16-Dihydropyrenes in Dimethylformamide," *Acta Chem. Scand.*, **1983**, *837*, 445.

R. V. C. Carr, R. V. Williams, and L. A. Paquette, "Dienophilic Properties of Phenylvinyl Sulfone and *trans*-1-Benzenesulfonyl-2-(trimethylsilyl)-ethylene. Their Utilization as Synthons for Ethylene, 1-Alkenes, Acetylene, and Monosubstituted Alkynes in the Construction of Functionalized Six-membered Rings via $[4+2]\pi$ Cycloaddition Methodology," *J. Org. Chem.*, **1983**, *48*, 4976.

R. H. Mitchell, P. D. Slowey, T. Kamada, R. V. Williams, and P. J. Garratt, "The Mills-Nixon Effect - A resolution: Clear evidence for no significant bond localization in small ring annelated aromatics. The Synthesis and diatropicity of cyclobutane annelated dihydropyrenes," *J. Am. Chem. Soc.*, **1984**, *106*, 2431.

- L. A. Paquette, R. V. Williams, M. Vazeux, and A. R. Browne, "Factors Conducive to the Cascade Rearrangement of Sterically Congested and Geometrically Restricted Three-Membered Rings. Facile Synthesis of a Topologically Nonplanar Heterocycle," *J. Org. Chem.*, **1984**, *49*, 2194.
- R. H. Mitchell, M. Chaudhary, T. W. Dingle, and R. V. Williams, "Unusual macrocyclic biphenyls containing the dihydropyrene nucleus. An observation of aryl group transfer from phosphine to aryl halide using nickel complexes," *J. Am. Chem. Soc.*, **1984**, *106*, 7776.
- R. V. Lloyd, and R. V. Williams, "The bridgehead decalin radicals: Evidence for non-planarity at the radical site," *J. Phys. Chem.*, **1985**, *89*, 5379.
- R. H. Mitchell, T. K. Vinod, G. J. Bodwell, K. S. Weerawarna, W. Anker, R. V. Williams, and G. W. Bushnell, "A fusion of Metals, Cyclophanes, and Dihydropyrenes," *Pure and Applied Chemistry*, **1986**, *58*, 15.
- R. H. Mitchell, M. Chaudhary, T. Kamada, P. D. Slowey and R. V. Williams, "*cis*-Dimethyldihydropyrene synthesis: an approach utilising a Diels-Alder route to 1,2,3-trisubstituted benzenes," *Tetrahedron*, **1986**, *42*, 1741.
- H. A. Kurtz, R. V. Lloyd, and R. V. Williams, "The Bridgehead Decalin Radicals: An MM2 and MNDO Study," *J. Org. Chem.*, **1987**, *52*, 302.
- R. V. Williams, and C.-L.A. Sung, "The Unexpected Regio and Stereospecific Diels-Alder Reaction between Cyclopentadiene and 2-Benzenesulphonyl-3-trimethylsilylbicyclo[2.2.1]hepta-2,5-diene," *J. Chem. Soc., Chem. Commun.*, **1987**, 590.
- P. C. B. Page, S. Rosenthal, and R. V. Williams, "Acyl Silanes as Synthetic Intermediates: Formation of Acyl Anions and Unusual Fluoride initiated Silicon to Carbon Alkyl Group Migration," *Tetrahedron Letters*, **1987**, *28*, 4455.
- R. V. Williams, C.-L. A. Sung, H. A. Kurtz, and T. M. Harris, "Experimental evidence establishing an upper limit to the activation barrier for the butterfly bending of the double bond in *anti*-sesquinorbornene," *Tetrahedron Letters*, **1988**, *29*, 19.
- P. C. B. Page, S. Rosenthal, and R. V. Williams, "A new, one-pot synthesis of primary 2-Alkynamides" *Synthesis*, **1988**, 621.
- R. V. Williams, and H. A. Kurtz, "The quest for a neutral homoaromatic hydrocarbon. The MNDO study of Pentacyclo[7.2.1.0^{4,11}.0^{6,9}.0^{6,10}]dodeca-1,4-diene an annelated semibullvalene derivative" *J. Org. Chem.*, **1988**, *53*, 3626.
- R. V. Williams, H. A. Kurtz, and B. Farley, "The use of semiempirical energy partitioning terms in the study of through space (homoaromatic) interactions," *Tetrahedron*, **1988**, *44*, 7455.
- R. V. Williams, W. J. Ebey, X. Ji, and D. van der Helm, "The Crystal Structures of Different Diastereomers of 2-benzenesulfinylbicyclo[2.2.1]hept-5-ene. C₇H₉SOC₆H₅". *Acta Cryst.* **1989**, *B45*, 93
- R. V. Williams, and X. Lin, "New Ketene Equivalents for the Diels-Alder Reaction. Vinyl Sulphoxide Cycloadditions," *J. Chem. Soc., Chem. Commun.*, **1989**, 1872.
- R. V. Williams, G. W. Kelley, D. van der Helm, J. Loebel, and P. B. C. Page, "Experimental Evidence for the Lack of Stereoselectivity in the Electrophilic Quench of α - Sulfonyl Carbanions," *J. Org. Chem.*, **1990**, *55*, 3840.

R. V. Williams, and K. Chauhan, "New Allene Equivalents for the Diels-Alder Reaction: Vinyl Sulphoxide Cycloadditions," *J. Chem. Soc., Chem. Commun.*, **1991**, 1672.

R. H. Mitchell, M. Chaudhary, R. V. Williams, R. Fyles, J. Gibson, M. Ashwood-Smith, and A. J. Fry, "Straining Strained Molecules. III. The Spectral and Mutagenic Properties and an Alternate Synthesis of Diaceperylene and Dicyclopenta[1,2,3-cd:1',2',3'-lm]perylene," *Can. J. Chem.*, **1992**, 70, 1015.

R. V. Williams, M.M.R. Todime, P. Enemark, D. van der Helm, and S.K. Rizvi, "Unusual Stereoselectivity in the Diels-Alder Addition of Cyclopentadiene with the Bicyclo[2.2.2]octene Nucleus," *J. Org. Chem.*, **1993**, 58, 6740.

R. V. Williams, and H. A. Kurtz, "Homoaromaticity," *Advances in Phys. Org. Chem*, **1994**, 29, 273.

R. V. Williams and H. A. Kurtz, "A Theoretical Investigation of Through Space Interactions. Part 3 The Semi-Empirical Study of the Cope Rearrangement in Singly Annulated Semibullvalenes," *J. Chem. Soc., Perkin Trans.*, 2, **1994**, 147.

R. V. Williams, K. Chauhan, and V. R. Gadgil, "1-Benzenesulphonyl-2-trimethylsilylacetylene: A New Acetylene Equivalent for the Diels-Alder Reaction," *J. Chem. Soc., Chem. Commun.*, **1994**, 1739.

R. V. Williams, V. R. Gadgil, K. Chauhan, D. van der Helm, M. B. Hossain, L. M. Jackman, and E. Fernandes, "1,5-Dimethyl-2,4,6,8-semibullvalenetetracarboxylic Dianhydride: A Close Approach to a Neutral Homoaromatic Semibullvalene," *J. Am. Chem. Soc.*, **1996**, 118, 4208.

J. H. Cooley and R. V. Williams, "Endo and Exo Stereochemistry in the Diels-Alder Reaction; Kinetic Versus Thermodynamic Control," *J. Chem. Educ.*, **1997**, 74, 582.

R. V. Williams, V. R. Gadgil, A. Vij, J. M. Cook, Q. Huang, and G. Kubiak, "Unexpected Stereoselectivity in the Weiss-Cook Condensation of Dimethyl 1,3-Acetonedicarboxylate with 2,3-Pentanedione," *J. Chem. Soc., Perkin Trans. 1*, **1997**, 1425.

H. Jiao, R. Nagelkerke, H. A. Kurtz, R. V. Williams, W. T. Borden, and P. von R. Schleyer, "Annulated Semibullvalenes: A Theoretical Study of How They "Cope" with Strain," *J. Am. Chem. Soc.*, **1997**, 119, 5921.

R. V. Williams, W. D. Edwards, A. Vij, R. W. Tolbert, and R. H. Mitchell, "A Theoretical Study and X-ray Structure Determination of Dimethyldihdropyrene," *J. Org. Chem.*, **1998**, 63, 3125.

R. V. Williams, V. R. Gadgil, K. Chauhan, L. M. Jackman, and E. Fernandes, "The Search for Homoaromatic Semibullvalenes. Part 5.¹ 1,5-Dimethyl-2,4,6,8-semibullvalenetetracarboxylic Dianhydride," *J. Org. Chem.*, **1998**, 63, 3302.

R. V. Williams, W. D. Edwards, V. R. Gadgil, M. E. Colvin, E. T. Seidl, D. van der Helm and M. B. Hossain "Pyramidalized Olefins : *Ab Initio* Study and X-ray Structure Determination of Bicyclo[2.2.2]octadienes," *J. Org. Chem.*, **1998**, 63, 5268.

R. V. Williams, "Semibullvalenes - Homoaromatic Bovines?" *Adv. Theor. Interesting Mol.* **1998**, 4, 157.

R. V. Williams, V. R. Gadgil, P. Luger, T. Koritsanszky, and M. Weber, "The Search for Homoaromatic Semibullvalenes. Part 6.¹ X-Ray Structure and Charge Density Studies of 1,5-Dimethyl-2,4,6,8-semibullvalenetetracarboxylic Dianhydride in the Temperature Range 123-15 K," *J. Org. Chem.* **1999**, 64, 1180.

- R. V. Williams, V. R. Gadgil, G. G. Garner, J. D. Williams, and A. Viji, "Pyramidalized Olefins: The Stereospecific Conjugate Reduction of a Bicyclo[2.2.2]octadiene," *Tetrahedron Lett.* **1999**, *40*, 2689.
- J. H. Cooley and R. V. Williams, "Qualitative Analysis in the Beginning Organic Laboratory," *J. Chem. Educ.* **1999**, *76*, 1117.
- R. V. Williams, M. E. Colvin, N. Tran, R. N. Warrenner and D. Margetic, "Exceptionally Pyramidalized Olefins: A Theoretical Study of the Cyclopropenyl Fused Tricycles - Tricyclo[3.2.1.0^{2,4}]oct-2(4)-ene, Tricyclo[3.2.1.0^{2,4}]octa-2(4),6-diene, Tricyclo[3.2.2.0^{2,4}]non-2(4)-ene and Tricyclo[3.2.2.0^{2,4}]nona-2(4),6-diene," *J. Org. Chem.* **2000**, *65*, 562.
- A. Viji, J. L. Palmer, K. Chauhan, and R. V. Williams, "The Role of Hydrogen Bonding in Pseudo-Macrocyclic Ring Formation in 2,6-dimethyl-1,3,5,7-cyclooctatetraene-1,3,5,7-tetracarboxylic Acid Monohydrate," *J. Chem. Cryst.* **2000**, *30*, 621.
- R. V. Williams, "Semibullvalenes and Related Molecules: Ever Closer Approaches to Neutral Homoaromaticity," *Eur. J. Org. Chem.* **2001**, 227.
- M. Heubes, T. Dietz, H. Quast, M. Seefelder, A. Witzel, V. R. Gadgil, and R. V. Williams, "Lifting of the Degeneracy in Semibullvalenes by Remote and Direct Substituents: A Quantitative Study Using Variable-Temperature Carbon-13 NMR Spectroscopy," *J. Org. Chem.* **2001**, *66*, 1949.
- R. V. Williams, "Homoaromaticity" *Chem. Rev.* **2001**, *101*, 1185.
- D. A. Hrovat, R. V. Williams, A. C. Goren and W. T. Borden, "B3LYP calculations on Bishomoaromaticity in Substituted Semibullvalenes," *J. Comput. Chem.* **2001**, *22*, 1565.
- R. V. Williams, J. R. Armantrout, B. Twamley, R. H. Mitchell, T. R. Ward and S. Bandyopadhyay, "A Theoretical and Experimental Scale of Aromaticity. The First Nucleus-Independent Chemical Shifts (NICS) Study of the Dimethyldihydropyrene Nucleus," *J. Am. Chem. Soc.* **2002**, *124*, 13495.
- U. Majumder, J. R. Armantrout, R. V. Williams and J. M. Shreeve "N, N-Difluorotris(*t*-butyl)silyl Amine - The First Organosilyl Difluoroamine. Synthesis and Computational Studies," *J. Org. Chem.* **2002**, *67*, 8435.
- D. B. Kimball, M. M. Haley, R. H. Mitchell, T. R. Ward, S. Bandyopadhyay R. V. Williams and J. R. Armantrout, "Dimethyldihydropyrene-Dehydrobenzoannulene Hybrids: Studies in Aromaticity and Photoisomerization," *J. Org. Chem.* **2002**, *67*, 8798.
- A. J. Boydston, M. M. Haley, R. V. Williams and J. R. Armantrout, "Diatropicity of 3,4,7,8,9,10,13,14-Octadehydro[14]annulenes: A Combined Experimental and Theoretical Investigation," *J. Org. Chem.* **2002**, *67*, 8812.
- S. Samdal, A. D. Richardson, K. Hedberg, V. R. Gadgil, M. M. Meyer and R. V. Williams, "Gas-Phase Electron-Diffraction Investigation and Quantum-Chemical Calculations of the Structure of 1,5-Dimethylsemibullvalene-2,4,6,8-tetracarboxylic Dianhydride," *Helv. Chim. Acta* **2003**, *86*, 1741.
- J. H. Cooley and R. V. Williams, "The Pyrolysis of Polystyrene," *Chem. Educator* [Online] **2003**, *8*, 1; DOI 10.1333/s00897030720a
- D. Margetic, R. V. Williams and R. N. Warrenner, "Pyramidalized Olefins: A DFT Study of the Homosquinorbornene and Sesquibicyclo[2.2.2]octane Nuclei," *J. Org. Chem.* **2003**, *68*, 9186.

- R. V. Williams and D. Margetić, "Pyramidalized Olefins: A DFT Study of bicyclo-[2.1.1], -[3.2.1] and -[3.2.2] Alkenes and their Fused Derivatives. Two Rare Examples of π -Facially Symmetric Pyramidal Olefins," *J. Org. Chem.* **2004**, *69*, 7134.
- R. H. Mitchell, R. Blunden, G. Hollett, S. Bandyopadhyay, R. V. Williams, B. Twamley, "13-Methyl-2,6-dithia[7]metacyclophane - A Useful Molecule to Connect VT NMR Results and Structure with Calculations," *J. Org. Chem.* **2005**, *70*, 675.
- D. A. Hrovat, E. C. Brown, R. V. Williams, H. Quast, W. T. Borden, "How Important Is Bishomoaromaticity in Determining the Relative Barrier Heights for the Degenerate Cope Rearrangements of Semibullvalene, Barbaralane, Bullvalene and Dihydrobullvalene?" *J. Org. Chem.* **2005**, *70*, 2627.
- M. Seefelder, M. Heubes, H. Quast, W. D. Edwards, J. R. Armantrout, R. V. Williams, C. J. Cramer, A. C. Goren, D. A. Hrovat and W. T. Borden "An Experimental and Theoretical Study of Stabilization of Delocalized Forms of Semibullvalenes and Barbaralanes by Dipolar and Polarizable Solvents. Observation of a Delocalized Structure that is Lower in Free Energy than the Localized Form," *J. Org. Chem.* **2005**, *70*, 3437.
- R. V. Williams, W. D. Edwards, R. H. Mitchell and S. G. Robinson "A DFT Study of the Thermal, Orbital Symmetry Forbidden, Cyclophanediene to Dihydropyrene Electrocyclic Reaction. Predictions to Improve the Dimethyldihydropyrene Photoswitches," *J. Am. Chem. Soc.* **2005**, *127*, 16207.
- T. Yoshimura, A. Inaba, M. Sonoda, K. Tahara, Y. Tobe and R. V. Williams "Synthesis and Properties of Trefoil-Shaped Tris(hexadehydrotribenzo[12]annulene) and Tris(tetradecydrotribenzo[12]annulene)," *Org. Lett.* **2006**, *8*, 2933.
- K. Tahara, T. Yoshimura, M. Sonoda, Y. Tobe and R. V. Williams "Theoretical Studies on Graphyne Substructures: Geometry, Aromaticity and Electronic Properties of the Multiply Fused Dehydrobenzo[12]annulenes," *J. Org. Chem.* **2007**, *72*, 1437.
- K. Ayub, R. Zhang, S. G. Robinson, B. Twamley, R. V. Williams and R. H. Mitchell "Suppressing the Thermal Metacyclophaneto Dihydropyrene Isomerization: Synthesis and Rearrangement of 8,16-Dicyano[2.2]metacyclophane-1,9-diene and Evidence Supporting the Proposed Biradicaloid Mechanism," *J. Org. Chem.* **2008**, *73*, 451.
- R. H. Mitchell, R. Zhang, D. J. Berg, B. Twamley and R. V. Williams "Measuring Aromaticity with the Dimethyldihydropyrene Ring Current Probe. Experimental and Computational Studies of the Fulvenes and the Strongly Antiaromatic Cyclopentadienone Reveal Large Mills-Nixon Type Bond Localization Effects. Synthesis of Fulvene Fused Dihydropyrenes," *J. Am. Chem. Soc.* **2009**, *131*, 189.
- R. V. Williams "Molecules with Labile Bonds: Selected Annulenes and Bridged Homotropilidenes," invited chapter in "Strained Hydrocarbons" ed. H. Dodziuk, Wiley-VCH, 2009.
- K. Ayub, R. Li, C. Bohne, R. V. Williams and R. H. Mitchell, "Calculation Driven Synthesis of an Excellent Dihydropyrene Negative Photochrome and its Photochemical Properties," *J. Am. Chem. Soc.* **2011**, *133*, 4040.
- P. R. Griffiths, D. E. Pivonka and R. V. Williams, "The Experimental Realization of a Neutral Homoaromatic Carbocycle," *Chem. Eur. J.* **2011**, *17*, 9193.
- R. H. Mitchell, P. Zhang, D. J. Berg and R. V. Williams, "An Experimental Estimate of the Relative Aromaticity of the Cyclooctatetraene Dianion by Fusion to Dimethyldihydropyrene," *Chem. Commun.*, **2012**, *48*, 8144.

R. V. Williams, W. D. Edwards, P. Zhang, D. J. Berg and R. H. Mitchell, "Experimental Verification of the Homoaromaticity of 1,3,5-Cycloheptatriene and the Evaluation of the Aromaticity of Tropone and the Tropylium Cation Using the Dimethyldihydropyrene Probe," *J. Am. Chem. Soc.*, **2012**, *134*, 16742.

T. C. Nugent, R. V. Williams, A. Dragan, A. V. Iosub, and A. A. Méndez, "An Investigation of the Observed, but Counter-Intuitive, Stereoselectivity Noted During Chiral Amines Synthesis via *N*-Chiral-Ketimines," *Beilstein J. Org. Chem.*, **2013**, *9*, 2103.