

10/26/04

CURRICULUM VITAE

Bruce E. Bursten

Birthdate: March 8, 1954, Chicago

Business Address

Department of Chemistry
The Ohio State University
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Columbus, Ohio 43210
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Home Address

4067 Park Lane
Columbus, Ohio 43220
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Academic History:

Department Chair, The Ohio State University, October 1999 - September, 2003

Distinguished University Professor, The Ohio State University, October 1997 - present

Adjunct Professor of Chemistry, Kent State University, August 1996 - present Professor

of Chemistry, The Ohio State University, October, 1990 - September, 1997 Visiting

Associate, California Institute of Technology, 1988 Associated Western Universities

Sabbatical Participant, Los Alamos National

Laboratory, 1988 Associate Professor, The Ohio State University, October, 1986 -

September, 1990 Assistant Professor, The Ohio State University, September, 1980 -

September, 1986 Postdoctoral Research Associate, Texas A & M University, August,

1978 - August, 1980

Advisor: Professor F. Albert Cotton Graduate Student, University of Wisconsin -

Madison, August, 1974 - August, 1978

Advisor: Professor Richard F. Fenske Received Ph.D. in Inorganic Chemistry, August, 1978 Undergraduate Student, University of Chicago, September, 1971 - August, 1974

Received S.B. in Chemistry with Honors, August, 1974

American Chemical Society (Inorganic Division and Organometallic Subdivision)
Program Chair, 19th Central Regional Meeting, 1987
Organizer, Symposium on Density Functional Theory in Inorganic Chemistry,
American Association for the Advancement of Science
Member, User's Advisory Committee of the Environmental Molecular Sciences
Chair, Science Advisory Committee of the Environmental Molecular Sciences

Alternate Councilor, Division of Inorganic Chemistry, 1989-91

Editorial Advisory Board, *Inorganic Chemistry*, 1990-92

Secretary-Elect, Division of Inorganic Chemistry, 1992

Secretary, Division of Inorganic Chemistry, 1993-95

Executive Committee Member, Division of Inorganic Chemistry, 1997-99

Chair-Elect, Division of Inorganic Chemistry, 2000
220th National ACS Meeting, 2000

Chair, Division of Inorganic Chemistry, 2001

Executive Committee Member, Division of Inorganic Chemistry, 2002

Editorial Advisory Board, *Inorganic Chemistry*, 2002-04

Nominee for ACS Director, 2004

Guest Editor for Symposium-in-Print, *Polyhedron*, 1989

Laboratory, Pacific Northwest National Laboratory, 2000-03

Laboratory, Pacific Northwest National Laboratory, 2003-05

Awards:

University of Wisconsin Special Graduate Traineeship (9/75 - 6/76)
Procter and Gamble Fellowship (9/77 - 6/78)
McElvain Outstanding Graduate Student Award, University of
Wisconsin - Madison, 1978 NSF National Needs Postdoctoral
Fellowship (9/78 - 9/79)

Ohio State University Alumni Award for Distinguished Teaching,
1982

Finalist, Arts and Sciences Student Council Outstanding Teaching
Award, 1983

The Colleges of Arts and Sciences Student Council Outstanding
Teaching Award, 1984

Camille and Henry Dreyfus Foundation Teacher-Scholar Award,
1984-1989

Alfred P. Sloan Foundation Fellowship, 1985-1987

Selected, Outstanding Young Men of America, 1986

Associated Western Universities Sabbatical Participant, 1988

Ohio State University Distinguished Scholar Award, 1990

Finalist, Arts and Sciences Student Council Outstanding Teaching
Award, 1992

Ohio State University Academy of Teaching, 1993

Honorary Member, Chimes Junior Class Honorary Society, 1993

The Colleges of Arts and Sciences Honors Faculty Service Award,
1995

Finalist, Arts and Sciences Student Council Outstanding Teaching
Award, 1996

Ohio State University Alumni Award for Distinguished Teaching, 1996

Honorary Member, Sphinx Senior Class Honorary Society, 1996

Honorary Member, Golden Key National Honor Society, 1997

Commencement Speaker, The Ohio State University, 1998

Honorary Member, Mortar Board Senior Class Honorary Society, 1998

Honorary Member, National Society of Collegiate Scholars, 1999

Selected, Who's Who Among America's Teachers, 2000

Catalyst Award, American Chemistry Council, 2001

Ohio State University Faculty Award for Distinguished University Service, 2002

Spiers Memorial Prize and Medal, Royal Society of Chemistry, 2003

Fellow of the American Association for the Advancement of Science (AAAS), 2003

Contributed Presentations:

11th Great Lakes Regional ACS Meeting, 1977

174th National ACS Meeting, 1977; Symposium on Electronic Structure and Spectra

174th National ACS Meeting, 1977; Symposium on the Reliability of Quantum Chemical Calculations

24th Annual Conference of the National Organization for the Professional Advancement

34th Southwest Regional ACS Meeting, 1978

178th National ACS Meeting, 1979

Gordon Research Conference in Inorganic Chemistry, 1979

183rd National ACS Meeting, 1982

185th National ACS Meeting, 1983

15th Central Regional ACS Meeting, 1983

19th Great Lakes Regional ACS Meeting, 1985

191st National ACS Meeting, 1986

193rd National ACS Meeting, 1987

19th Central Regional ACS Meeting, 1987

20th Central Regional ACS Meeting, 1988

195th National ACS Meeting, 1988

196th National ACS Meeting, 1988

198th National ACS Meeting, 1989

45th Ohio State University International
Symposium on Molecular Spectroscopy, 1990

200th National ACS Meeting, 1990

201st National ACS Meeting, 1991

47th Southwest Regional ACS Meeting, 1991

203rd National ACS Meeting, 1992

47th Ohio State University International
Symposium on Molecular Spectroscopy, 1992

205th National ACS Meeting, 1993

207th National ACS Meeting, 1994

Joint 26th Central and 27th Great Lakes Regional
ACS Meeting, 1994

49th Ohio State University International
Symposium on Molecular Spectroscopy, 1994

Gordon Research Conference on Organometallic
Chemistry, 1994

208th National ACS Meeting, 1994

1994 International Conference on Raman Spectroscopy, 1994

209th National ACS Meeting, 1995

Seventh International Conference on Time-Resolved Vibrational Spectroscopy, 1995

210th National ACS Meeting, 1995

211th National ACS Meeting, 1996

29th Midwest Theoretical Conference, 1996
of Black Chemists and Chemical Engineers, 1997

213th National ACS Meeting, 1997

214th National ACS Meeting, 1997

53rd Ohio State University International Symposium on Molecular Spectroscopy, 1998

216th National ACS Meeting, 1998

217th National ACS Meeting, 1999

54th Ohio State University International Symposium on Molecular Spectroscopy, 1999

218th National ACS Meeting, 1999

55th Ohio State University International Symposium on Molecular Spectroscopy, 2000

220th National ACS Meeting, 2000

221st National ACS Meeting, 2001

222nd National ACS Meeting, 2001

223rd National ACS Meeting, 2002

225th National ACS Meeting, 2003

58th Ohio State University International Symposium on Molecular Spectroscopy, 2003

227th National ACS Meeting, 2004

Invited Presentations:

AT&T Bell Laboratories, Murray Hill,
NJ, 1979 179th National ACS Meeting,
1980; Symposium on New Quantum
Methods in Inorganic
Chemistry and Catalysis
Boston Area Organometallic Colloquium
(jointly sponsored by MIT, Harvard, and
187th National ACS Meeting, 1984;
Tutorial on Theoretical Inorganic
Chemistry -
Current State of the Art
187th National ACS Meeting, 1984;
Symposium on Theoretical Inorganic
Chemistry -
Current State of the Art

University of Texas, Austin, 1980

University of Cincinnati, 1981

University of British Columbia, 1983

University of Kentucky, 1983

Indiana University, 1983

Marietta College, 1983

University of Michigan, 1983

Ford Motor Company, 1983

University of Toronto, 1983

University of Missouri - St. Louis,
1983

Illinois State University, 1983

Monsanto Chemical Company, 1983

Kenyon College, 1983

University of Akron, 1983

Brandeis), 1984

Wright State University, 1984

University of Wisconsin - Madison,
1984

NSF Organometallic Workshop,
University of North Carolina, 1984
Procter and Gamble Company, 1984
190th National ACS Meeting, 1985; Symposium
on Organometallics of the Lanthanides,
Actinides, and Early Transition Metals
191st National ACS Meeting, 1986;
Symposium on Theory of Metal-Metal
Bonding
192nd National ACS Meeting, 1986;
Symposium on the Electronic Structure of
the
Transition State

Oxford University, 1984

University of Munich, 1984

National Research Council (C.N.R.),
Florence, Italy, 1984

NATO Advanced Study Institute on
Organo-f-element Chemistry, Maratea,
Italy, 1984

Purdue University, 1984

Columbia University, 1984

Marquette University, 1985

SUNY-Buffalo, 1985

Colorado State University, 1985

Gordon Research Conference on
Organometallic Chemistry, 1985

Northern Illinois University, 1985

University of Washington, 1985

University of Oregon, 1985

University of California, Davis, 1985

University of California, Berkeley, 1985

Stanford University, 1985

University of California, Santa Barbara,
1985

University of California, Irvine, 1985

University of California, San Diego, 1985

California Institute of Technology, 1985

University of Southern California, 1985

University of California, Los Angeles,
1985

University of Cincinnati, 1986

University of Minnesota, 1986

3M Company, 1986

17th Rare Earth Research Conference,
1986

32nd Meeting of the Research
Materials/Transplutonium Program
Committee, 1986

Kalamazoo College, 1986

DuPont Savannah River Laboratory, 1986

University of Western Ontario, 1986

University of Toledo, 1986

Himont Research and Development Center,
1987

Gordon Research Conference on Inorganic
Chemistry, 1987

33rd Meeting of the Research
Materials/Transplutonium Program
Committee, 1987

Michigan State University, 1987

DePauw University, 1987

University of Helsinki, 1987

Los Alamos National Laboratory, 1988

University of New Mexico, 1988
Utah State University, 1988

University of Utah, 1988

University of Arizona, 1988

University of Nevada - Reno, 1988

195th National ACS Meeting, 1988; ACS Nobel Laureate Signature Award Symposium
California Institute of Technology, 1988

Northern Illinois University, 1988

18th Rare Earth Research Conference, 1988

West Virginia University, 1988

Bowling Green State University, 1988

University of Pittsburgh, 1989

Texas A&M University Industry-University Chemistry Program, 1989

University of Maryland, 1989

Los Alamos National Laboratory, 1989

44th Northwest Regional ACS Meeting, 1989; Symposium on f-Block Organometallic
Chemistry
Calvin College, 1990

Ohio Supercomputer Center Workshop on Density Functional Theory, 1990

Great Lakes Regional ACS Meeting, 1990; Symposium on Computational Chemistry
Second World Congress of Theoretical Organic Chemists, 1990

University of Waterloo, 1990

73rd Canadian Chemical Congress, 1990; ALCAN Award Symposium
Los Alamos National Laboratory, 1990

XIVth International Conference on Organometallic Chemistry, 1990

DOE Heavy Elements Chemistry Program, 1990

Oak Ridge National Laboratory, 1990

Illinois State University, 1990

Joint Southeast/Southwest Regional ACS Meeting, 1990; Symposium on Activation of
Small Molecules by Polynuclear Metal Complexes
Los Alamos National Laboratory, 1991

201st National ACS Meeting, 1991; Symposium on High Oxidation State
Organometallics
University of Windsor, 1991

University of Delaware, 1991

United States Air Force Academy, 1991

University of Wyoming, 1991

Gordon Research Conference on Organometallic Chemistry, 1991

Xavier University, 1991

Hope College, 1991

University of Idaho, 1992

University of Nevada - Reno, 1992

Miami University, 1992

University of Wisconsin - Milwaukee, 1992

University of Wisconsin - Madison, 1992

205th National ACS Meeting, 1993;

Symposium on Fundamental Research

Problems in

Inorganic Chemistry

207th National ACS Meeting, 1994;

Symposium on Actinide, Lanthanide, and

Early

Transition Metal Chemistry

Fifth Chemical Congress of North America,

1997; Symposium on Organometallic

Chemistry of Group 3 and the f-Elements

215th National ACS Meeting, 1998;

Symposium on Metal-Metal Bonds and

Clusters, in

honor of the Priestley Medal recipient

4th Department of Energy Basic Energy

Sciences Research Conference on

Homogeneous

5th Winter Conference of the Inter-
American Photochemical Society, 1993

University of Michigan, 1993

Wayne State University, 1993

Wabash College, 1993

Ball State University, 1993

Denison University, 1994

University of Cincinnati, 1994

NSF Organometallic Workshop, 1994

Marshall University, 1994

Otterbein College, 1994

University of Illinois at
Champaign/Urbana, 1995

Gordon Research Conference on
Organometallic Chemistry, 1995

Boston College, 1995

Harvard University/MIT Joint Inorganic
Colloquium, 1995

Indiana University, 1996

University of Pennsylvania, 1996

University of North Carolina, Chapel Hill,
1996

University of Washington, 1997

University of British Columbia, 1997

Pacific Northwest National Laboratory,
1997

University of Akron, 1997

University of Arizona, 1997

Los Alamos National Laboratory, 1997

Gordon Research Conference on Inorganic
Chemistry, 1997

Michigan State University, 1997

University of Nebraska, 1997

University of Pittsburgh, 1997

University of Chicago, 1998

Catalysis and Organometallic Chemistry,
1998

Virginia Polytechnic Institute and State University, 1998

James Madison University/Bridgewater College, 1998

University of Virginia, 1998

Indiana State University, 1998

Bowling Green State University, 1998

University of Florida, 1999
9th Rocky Mountain Regional ACS Meeting, 1988; Symposium on The Interplay of Theory and Experiment in Organometallic Chemistry
217th National ACS Meeting, 1999; Symposium in honor of the recipient of the ACS Award for Distinguished Service to Inorganic Chemistry
217th National ACS Meeting, 1999; Symposium on Heavy Element Chemistry: The Convergence of the Theory & Experiment

Kent State University, 1999

Department of Energy Grand Computational Challenge Conference, 1999

Columbia University, 1999

Plenary Lecturer, Meeting of the Student Affiliate of the ACS, West Virginia University, 2000

University of Iowa, 2000

University of Illinois - Chicago, 2000

220th National ACS Meeting, 2000; Symposium on Density Functional Theory in Inorganic Chemistry
220th National ACS Meeting, 2000; Symposium in Honor of Andrew Wojcicki

Canisius College, 2000

SUNY-Buffalo, 2000

DOE Heavy Element Chemistry Contractors Meeting, 2000

Ohio University, 2001

221st National ACS Meeting, 2001; ACS Award in Organometallic Chemistry

Symposium
Gordon Research Conference on Physical Organic Chemistry, 2001

222nd National ACS Meeting, 2001; Symposium on Computational Organometallic
Chemistry
Texas A&M University, 2001

Georgia Institute of Technology, 2002

Gordon Research Conference on Inorganic Chemistry, 2002

224th National ACS Meeting, 2002; Symposium on Recent Advances in
Inorganometallic Chemistry
Bradley University, 2002

Peoria Section of the American Chemical Society, 2002

Leadoff Lecturer, Midwest Association of Chemistry Teachers in Liberal Arts Colleges
Meeting, 2002

Indiana University of Pennsylvania, 2002

Spiers Lecture, Faraday Discussion 124 on Quantum Inorganic Chemistry, York
University, UK, 2003

DOE Heavy Element Chemistry Contractors Meeting, Santa Fe, NM, 2003

Los Alamos National Laboratory, 2003

Very Heavy Metals 2003, La Colle-sur-Loup, France, 2003

226th National ACS Meeting, 2003; Symposium on Contemporary Aspects of Chemical
Bonding
University of Georgia, 2003

Emory University, 2003

The Ohio State University, Evans Lectures Mini-Symposium, 2003

University of California, Irvine, 2003

University of California, San Diego, 2003
Indiana University, 2003

Michigan State University, 2004

Joint DOE/NSF Workshop on Actinide Science in the 21st Century, Washington,
DC,
2004

36th International Conference on Coordination Chemistry, Merida, Mexico, 2004;

Symposium on d- and f-Element Coordination Chemistry
228th National ACS Meeting, 2004; Symposium honoring Daryle Busch
University of North Carolina, Chapel Hill, 2004 229th National ACS Meeting,
2005; Symposium in honor of the recipient of the ACS

University of California, Davis, 2004

University of California, Berkeley/Lawrence Berkeley National Laboratory, 2004
Award in Inorganic Chemistry
Actinides 2005 Conference, Manchester, UK, 2005

Publications of Dr. Bruce E. Bursten

Books

T. L. Brown, H. E. LeMay, Jr., and B. E. Bursten, "Chemistry: The Central Science,"
5th Edition, Prentice-Hall: Englewood Cliffs, NJ, 1991.

T. L. Brown, H. E. LeMay, Jr., and B. E. Bursten, "Chemistry: The Central Science,"
6th Edition, Prentice-Hall: Englewood Cliffs, NJ, 1994.

T. L. Brown, H. E. LeMay, Jr., and B. E. Bursten, "Chemistry: The Central Science,"
7th Edition, Prentice-Hall: Upper Saddle River, NJ, 1997.

T. L. Brown, H. E. LeMay, Jr., and B. E. Bursten, "Chemistry: The Central Science,"
8th Edition, Prentice-Hall: Upper Saddle River, NJ, 2000.

T. L. Brown, H. E. LeMay, Jr., B. E. Bursten, and J. R. Burdge, "Chemistry: The
Central Science," 9th Edition, Prentice-Hall: Upper Saddle River, NJ, 2003.

Articles

1. V. L. Goedken, J. J. Pluth, S.-M. Peng, and B. Bursten, "Structure Relationships between the Four-Coordinate S=1, Macrocyclic Complex, [Fe(C₂₂H₂₂N₄)] and the Neutral Ligand, C₂₂H₂₄N₄," *J. Am. Chem. Soc.*, **98**, 8014-8020 (1976).
2. M. C. Weiss, B. Bursten, S.-M. Peng, and V. L. Goedken, "Effects of Peripheral Steric Constraints and Metal Ion Size on the Structure of Three Five-Coordinate Macrocyclic Ligand Complexes of the Type [M(C₂₂H₂₂N₄)X], M = Co(III), Fe(III), Mn(II); X=I, Cl, N(C₂H₅)₃," *J. Am. Chem. Soc.*, **98**, 8021-8031 (1976).

3. P. M. Treichel, H. J. Mueh and B. E. Bursten, "Specific Syntheses and Electrochemistry of Isomeric $[\text{Mn}(\text{CO})_{6-n}(\text{CNMe})_n]^+$ ($n = 3, 4$) Complexes," *J. Organomet. Chem.*, **110**, C49-C52 (1976).
4. B. E. Bursten and R. F. Fenske, "Substituent Effects on the Electronic Structure of Arylisocyanide-Transition Metal Complexes," *Inorg. Chem.*, **16**, 963-964 (1977).
5. P. M. Treichel, H. J. Mueh and B. E. Bursten, "Stereospecific Syntheses of Isomeric $[\text{Mn}(\text{CO})_{6-n}(\text{CNMe})_n]^+$ Complexes and Study of Their Electrochemical Oxidations," *Israel J. Chem.*, **15**, 253-257 (1977).
6. B. E. Bursten and R. F. Fenske, "The LCAO Representation of X-SW Molecular Orbitals," *J. Chem. Phys.*, **67**, 3138-3145 (1977).
7. B. E. Bursten, J. R. Jensen and R. F. Fenske, "An $X\alpha$ Optimized Atomic Orbital Basis," *J. Chem. Phys.*, **68**, 3320-3321 (1978).
8. B. E. Bursten and R. F. Fenske, "Molecular Orbital Studies on Cyclobutadienemetal Complexes: The Concept of Metalloaromaticity," *Inorg. Chem.*, **18**, 1760-1765 (1979).
9. B. E. Bursten, F. A. Cotton, A. H. Cowley, B. E. Hanson, M. Lattman and G. G. Stanley, "Strong Metal-to-Metal Quadruple Bonds in a Series of Five Isostructural Compounds as Indicated by Photoelectron Spectroscopy," *J. Am. Chem. Soc.*, **101**, 6244-6249 (1979).
10. B. E. Bursten, F. A. Cotton, J. C. Green, E. Seddon and G. G. Stanley, "The Electronic Structures and Photoelectron Spectra of the Metal Atom Cluster Species Re_3Cl_9 , Re_3Br_9 and $[\text{Re}_3\text{Cl}_{12}]^+$," *J. Am. Chem. Soc.*, **102**, 955-968 (1980).
11. B. E. Bursten, F. A. Cotton and G. G. Stanley, "Bonding in Metal Atom Cluster Compounds From the d-Orbital Overlap Model to SCF- $X\alpha$ -SW Calculations," *Israel J. Chem.*, **19**, 132-142 (1980).
12. B. E. Bursten, D. G. Freier and R. F. Fenske, " $X\alpha$ -SW Studies of Metal Ligand Backbonding in Metal Carbonyls: 2π or not 2π ?" *Inorg. Chem.*, **19**, 1810-1811 (1980).
13. B. E. Bursten, F. A. Cotton, J. C. Green, E. A. Seddon and G. G. Stanley, "Molecular Orbital and Spectroscopic Studies of Triple Bonds Between Transition Metal Atoms. I. The $d^3-d^3 \text{Mo}_2\text{L}_6$ Compounds ($\text{L} = \text{OR}, \text{NR}_2, \text{CH}_2\text{R}$)," *J. Am. Chem. Soc.*, **102**, 4579-4588 (1980).
14. B. E. Bursten, F. A. Cotton and M. B. Hall, "Dimolybdenum: Nature of the Sextuple Bond," *J. Am. Chem. Soc.*, **102**, 6348-6349 (1980).
15. B. E. Bursten and F. A. Cotton, "Dependence of Stability, Bond Strength and Electronic Structure of Dimetal Units upon Atomic Number, Oxidation Number and Chemical Environment," *Symp. Faraday Soc.*, **14**, 180-193 (1980).
16. D. E. Bergbreiter, B. E. Bursten, M. S. Bursten and F. A. Cotton, "The Crystal Structure of Dichlorobis(triphenylphosphine)(norbornadiene)ruthenium," *J. Organomet. Chem.*, **205**, 407-415 (1981).
17. B. E. Bursten and F. A. Cotton, "Electronic Structure of Phosphine Adducts of Tetrakis(carboxylato)dirhodium (II): The Pronounced Influence of Axial Ligands," *Inorg. Chem.*, **20**, 3042-3048 (1981).
18. B. E. Bursten, J. Robert Jensen, D. J. Gordon, P. M. Treichel and R. F. Fenske, "Electronic Structure of Transition Metal Nitrosyls. $X\alpha$ -SW and Configuration

Interaction Calculations of the Valence Ionization Potentials of $\text{Co}(\text{CO})_5\text{NO}$ and $\text{Mn}(\text{CO})_4\text{NO}$,” *J. Am. Chem. Soc.*, **103**, 5226-5231 (1981).

11. 19. B. E. Bursten, F. A. Cotton, M. B. Hall, and R. C. Najjar, “A Survey of the Bonding in Several Structural Types of Trinuclear Molybdenum and Tungsten Cluster Compounds,” *Inorg. Chem.*, **21**, 302-307 (1982).
12. 20. B. E. Bursten, “Ligand Additivity: Applications to the Electrochemistry and Photoelectron Spectroscopy of d^1 Octahedral Complexes,” *J. Am. Chem. Soc.*, **104**, 1299-1304 (1982).
13. 21. A. Bino, B. E. Bursten, F. A. Cotton, and A. Fang, “Structural and Bonding Studies of the Hexachlorobis(:-chloro)(:-hydrido)dimolybdenum(III) Ion, $[\text{Mo}_2\text{Cl}_8\text{H}]^3-$,” *Inorg. Chem.*, **21**, 3755-3759 (1982).
14. 22. B. E. Bursten, “On the Stability of Early-Transition-Metal Metallacyclobutadiene Complexes,” *J. Am. Chem. Soc.*, **105**, 121-122 (1983).
15. 23. B. E. Bursten, F. A. Cotton, P. E. Fanwick, G. G. Stanley, and R. A. Walton, “Molecular Orbital and Spectroscopic Studies of Triple Bonds Between Transition-Metal Atoms. 2. The d^5-d^5 $\text{Re}_2\text{Cl}_4(\text{PR})_4$ Compounds,” *J. Am. Chem. Soc.*, **105**, 2606-2611 (1983).
16. 24. B. E. Bursten, F. A. Cotton, P. E. Fanwick, and G. G. Stanley, “A Molecular Orbital Calculation of the $[\text{Re}_2\text{Cl}_8]^-$ Ion by the Relativistic SCF-X α -SW Method; Redetermination and Reassignment of the Electronic Absorption Spectrum,” *J. Am. Chem. Soc.*, **105**, 3082-3087 (1983).
17. 25. B. E. Bursten, F. A. Cotton and A. Fang, “Ground State Electronic Structures and Other Electronic Properties of the Octahedral and Oligooctahedral Ruthenium Complexes. Hexachlororuthenium (III), Nonachlorodiruthenium (III,III) and Dodecachlorotriruthenium (III,II,III),” *Inorg. Chem.*, **22**, 2127-2133 (1983).
18. 26. B. E. Bursten and A. Fang, “Valence Electronic Structures of the Organouranium Complexes $(\eta^5\text{-C}_5\text{H}_5)_2\text{UX}_2$ ($X = \text{Cl}, \text{CH}_3$),” *J. Am. Chem. Soc.*, **105**, 6495-6496 (1983).
19. 27. B. E. Bursten and M. G. Gatter, “Molecular Orbital Studies of Organometallic Hydride Complexes. 1. The Acidic vs. Hydridic Behavior of Some $(\eta^5\text{-C}_5\text{H}_5)\text{ML}_n\text{H}$ Systems,” *J. Am. Chem. Soc.*, **106**, 2554-2558 (1984).
20. 28. B. E. Bursten and M. G. Gatter, “Molecular Orbital Studies of Organometallic Hydride Complexes. 2. The Correlation of Hydrogen Atom Reactivity with Valence Orbital Energetics,” *Organometallics*, **3**, 895-899 (1984).
21. 29. B. E. Bursten and M. G. Gatter, “Molecular Orbital Studies of Organometallic Hydride Complexes. 3. Structural and Electronic Effects on the H Reactivity in $(\eta^5\text{-C}_5\text{H}_5)\text{ML}_2\text{H}$ and $(\eta^5\text{-C}_5\text{H}_5)\text{ML}_3\text{H}$ Systems,” *Organometallics*, **3**, 941-943 (1984).
22. 30. B. E. Bursten and G. A. Ozin, “X α -SW Calculations for Naked Actinide Dimers: On the Existence of φ Bonds Between Metal Atoms,” *Inorg. Chem.*, **23**, 2910-2911 (1984).
23. 31. B. E. Bursten, D. J. Darensbourg, G. E. Kellogg, and D. L. Lichtenberger, “Ligand Additivity in the Valence Photoelectron Spectroscopy of Phosphine-substituted Molybdenum Carbonyls,” *Inorg. Chem.*, **23**, 4361-4365 (1984).
24. 32. P. E. Fanwick, B. E. Bursten, and G. B. Kaufmann, “The Electronic Spectra of the Quadruply Bonded Group VI Metal Dimers of 2-methyl-6-oxopyridine,” *Inorg. Chem.*, **24**, 1165-1169 (1985).
25. 33. P. Legzdins, S. J. Rettig, L. Sánchez, B. E. Bursten, and M. G. Gatter, “Novel Sixteen-Electron Organometallic Complexes of Molybdenum and Tungsten: $(\eta^5\text{-C}_5\text{H}_5)\text{M}(\text{NO})(\text{alkyl})_2$,” *J. Am. Chem. Soc.*, **107**, 1411-1413 (1985).
26. 34. B. E. Bursten, M. Casarin, S. DiBella, A. Fang, and I. Fragalà, “Photoelectron Spectroscopy of f-Element Organometallic Complexes. 6. The Electronic Structure of Tetrakis(cyclopentadienyl)actinide Complexes,” *Inorg. Chem.*, **24**, 2169-2173 (1985).

27. 35. M. D. Braydich, B. E. Bursten, M. H. Chisholm, and D. L. Clark, "Comparative Studies on the Electronic Structures of $W_2(O_2CH)_4$ and $W_2(O_2CH)_4(CH_3)_2$ by the Relativistic $X\alpha$ -SW Method: A d^3-d^3 Metal Dimer with a Quadruple Metal-Metal Bond?", *J. Am. Chem. Soc.*, **107**, 4459-4465 (1985).
28. 36. J. P. Blaha, B. E. Bursten, J. C. Dewan, R. B. Frankel, C. L. Randolph, B. A. Wilson, and M. S. Wrighton, "A Dinuclear, Eighteen-Electron Species Having a Triplet Ground State: Isolation, Characterization, and Crystal Structure of Photogenerated $(\eta^5-C_5Me_5)_2Fe_2(\mu-CO)_3$ ", *J. Am. Chem. Soc.*, **107**, 4561-4562 (1985).
29. 37. B. E. Bursten and A. Fang, "The Quasi-relativistic $X\alpha$ -SW Molecular Orbital Method in Organo-f-element Chemistry: Applications to UCl_4 , $(\eta^5-C_5H_5)_4U$, and $(\eta^5-C_5H_5)_2UCl_2$ ", *Inorg. Chim. Acta*, **110**, 153-160 (1985).
30. 38. B. E. Bursten, M. R. Green, V. Katovif, J. R. Kirk, and D. Lightner, Jr., "Electrochemistry of Niobium(IV) and Tantalum(IV) Complexes: Ligand Additivity in d^1 Octahedral Complexes", *Inorg. Chem.*, **25**, 831-834 (1986).
31. 39. B. E. Bursten, M. Casarin, D. E. Ellis, I. Fragalà, and T. J. Marks, "Combined He-I/He-II Photoelectron Spectroscopic and Hartree-Fock-Slater Investigation of Electronic Structure and Bonding in Uranium Hexamethoxide", *Inorg. Chem.*, **25**, 1257-1261 (1986).
32. 40. B. E. Bursten and R. H. Cayton, "On the Bonding of Methyl Groups in Dinuclear Complexes: Terminal, Symmetrically Bridging, or Asymmetrically Bridging?", *Organometallics*, **5**, 1051-1053 (1986).
33. 41. A. D. Hunter, P. Legzdins, F. W. B. Einstein, A. C. Willis, B. E. Bursten, and M. G. Gatter, "Structural and Electronic Consequences of Coordinating Butadienes to $(\eta^5-C_5H_5)Mo(NO)$ ", *J. Am. Chem. Soc.*, **108**, 3843-3844 (1986).
34. 42. B. E. Bursten and R. H. Cayton, "Electronic Structure of Piano-Stool Dimers. 3. Relationships Between the Bonding and Reactivity of the Organically-Bridged Iron Dimers $[CpFe(CO)]_2(\mu-CO)(\mu-L)$ ($L = CO, CH_2, C=CH_2, CH^+$)", *J. Am. Chem. Soc.*, **108**, 8241-8249 (1986).
35. 43. L. B. Anderson, T. J. Barder, D. Esjornson, R. A. Walton, and B. E. Bursten, "Reactions of the Dirhenium (II) Complexes $Re_2X_4(dppm)_2$ ($X = Cl$ or Br ; $dppm = Ph_2PCH_2PPh_2$) with Isocyanides. Part 3. The A-Frame-Like Monoisocyanide Species $[Re_2(\mu-X)(\mu-dppm)_2X_3(CNR)]^+$ ($R = Me, t-Bu, \text{ or } Xylyl$; $n = 0$ or 1)", *J. Chem. Soc., Dalton Trans.*, 2607-2612 (1986).
36. 44. B. E. Bursten and K. J. Novo-Gradac, "Metal-Metal Bonds Involving the f-Elements. 2. The Nature of the Bonding in $(\eta^5-C_5H_5)(I)M-Ru(\eta^5-C_5H_5)(CO)_2$ ($M = Zr, Th$) Complexes", *J. Am. Chem. Soc.*, **109**, 904-905 (1987).
37. 45. B. E. Bursten and D. L. Clark, "Theoretical Description of Metal-Metal Multiple Bonds in $M_2(O_2CH)_4$ Compounds Using the $X\alpha$ -SW MO Method", *Polyhedron*, **6**, 695-704 (1987).
38. 46. M. R. Green, N. Jubran, B. E. Bursten, and D. H. Busch, "Transition Metal Complexes of Dithiooxamide Ligands. Vibrational Fine Structure in the Electronic Spectra of Symmetrically N,N'-Disubstituted Dithiooxamides and Their Divalent Nickel Ion Complexes", *Inorg. Chem.*, **26**, 2326-2332 (1987).
39. 47. B. E. Bursten and R. H. Cayton, "Electronic Connections Between Exceptional Low Valent and High Valent Organometallic Compounds: The Case of $CpM(L)R_3$ ($M = W, Re$; $L = NO, O$; $R = Alkyl$)", *Organometallics*, **6**, 2004-2005 (1987).
40. 48. B. E. Bursten and R. H. Cayton, "Electronic Structure of Piano Stool Dimers. 4. Electronically Induced Changes in the Electrophilic and Nucleophilic Reactions and the Conformations of a Series of Isovalent Hydrocarbyl-Bridged Complexes", *J. Am. Chem. Soc.*, **109**, 6053-6059 (1987).
40. 49. B. E. Bursten and R. J. Strittmatter, "f-Orbital to Carbonyl 2B Backbonding.

The Electronic Structures of $(\eta^5\text{-C}_5\text{H}_5)_3\text{U-CO}$ and $(\eta^5\text{-C}_5\text{H}_5)_3\text{U-OC}$,” *J. Am. Chem. Soc.*, **109**, 6606-6608 (1987).

41. 50. M. H. Chisholm, D. L. Clark, J. C. Huffman, W. G. Van Der Sluys, E. M. Kober, D. L. Lichtenberger, and B. E. Bursten, “Bisalkyltetracarboxylates of Dimolybdenum and Ditungsten. Triple Bonds Between Metal Atoms with the Valence MO Description $\pi^4\delta^2$,” *J. Am. Chem. Soc.*, **109**, 6796-6816 (1987).

42. 51. B. E. Bursten, M. H. Chisholm, and D. L. Clark, “Electronic Structure and Bonding in Halide- and Alkoxide-Supported Tetranuclear Molybdenum Clusters,” *Inorg. Chem.*, **27**, 2084-2096 (1988).

43. 52. B. E. Bursten and M. R. Green, “Ligand Additivity in the Vibrational Spectroscopy, Electrochemistry, and Photoelectron Spectroscopy of Metal Carbonyl Derivatives,” *Prog. Inorg. Chem.*, **36**, 393-485 (1988).

44. 53. B. E. Bursten, R. H. Cayton, and M. G. Gatter, “Electronic Structure of Piano-Stool Dimers. 5. Relationships Between the π -Acidity and Electrochemistry in a Series of Isoelectronic Compounds of the Type $\text{Cp}_2\text{M}_2\text{L}_4$ (L = CO, NO),” *Organometallics*, **7**, 1342-1348 (1988).

45. 54. B. E. Bursten and R. H. Cayton, “Electronic Structure of Piano-Stool Dimers. 6. Bimetallic Transition Metal Hydrides of the Type $\text{Cp}_2\text{M}_2\text{H}_n\text{L}_{6-n}$,” *Organometallics*, **7**, 1349-1356 (1988).

46. 55. B. E. Bursten and R. H. Cayton, “Electronic Structure of Piano-Stool Dimers - VII. Interrelationships Among the Electronic Structure, Reactivity, and Conformational Preferences of Hydrocarbyl-Bridged Piano-Stool Dimers,” *Polyhedron*, **7**, 943-954 (1988).

47. 56. B. E. Bursten and R. H. Cayton, “Electronic Structure of Piano-Stool Dimers. 8. Electronically Induced Conformational Changes in High-Valent Bimetallic Chalcogen Complexes of the Type, $[\text{CpML}](\mu\text{-L})_2$ (M = Mo, Re; L = S, O),” *Inorg. Chem.*, **28**, 2846-2853 (1989).

2

1. 57. B. E. Bursten, L. F. Rhodes, and R. J. Strittmatter, “Bonding in $\text{Tris}(\eta^5\text{-cyclopentadienyl})$ Actinide Complexes. 2. On the Ground Electronic Configurations of Cp_3An Complexes (An = Th, Pa, U, Np, Pu),” *J. Am. Chem. Soc.*, **111**, 2756-2758 (1989).

2. 58. P. DeShong, G. A. Slough, D. R. Sidler, W. von Philipsborn, R. W. Kunz, B. E. Bursten, and T.

W. Clayton, Jr., “Probing the Chemistry of Organomanganese Complexes. Correlation of Chemical Reactivity, Manganese-55 NMR Chemical Shifts, and Molecular Orbital Studies of Organomanganese Pentacarbonyl Complexes. Aromaticity of an Organomanganese Complex,” *Organometallics*, **8**, 1381-1388 (1989).

1. 59. B. E. Bursten, L. F. Rhodes, and R. J. Strittmatter, “Bonding in $\text{Tris}(\eta^5\text{-cyclopentadienyl})$ Actinide Complexes. 3. The Interaction of π -Neutral, π -Acidic, and π -Basic Ligands with $(\eta^5\text{-C}_5\text{H}_5)_3\text{U}$,” *J. Am. Chem. Soc.*, **111**, 2758-2766 (1989).

.60. B. E. Bursten, L. F. Rhodes, and R. J. Strittmatter, “The Bonding in $\text{Tris}(\eta^5\text{-cyclopentadienyl})$ Actinide Complexes. 4. Electronic Structural Effects in AnCl_3 and $(\eta^5\text{-C}_5\text{H}_5)_3\text{An}$ (An = Th through Cf) Complexes,” *J. Less-Common Met.*, **149**, 207-211 (1989).

2. 61. D. S. Yang, G. M. Bancroft, R. J. Puddephatt, B. E. Bursten, and S. D. McKee, “The Electronic Structure of $(\eta^5\text{-C}_5\text{H}_5)\text{Pt}(\text{CH}_3)_3$ and $(\eta^5\text{-C}_5\text{Me}_5)\text{Pt}(\text{CH}_3)_3$ from UV Photoelectron Spectra,” *Inorg. Chem.*, **28**, 872-877 (1989).

3. 62. S. D. Loren, B. K. Campion, R. H. Heyn, T. D. Tilley, B. E. Bursten, and K. W. Luth, "Alkoxy and Aryloxy Derivatives of (Pentamethylcyclopentadienyl)ruthenium. X-ray Crystal Structures of $[(\eta^5\text{-C}_5\text{Me}_5)\text{Ru}(\mu\text{-OMe})]_2$, $[(\eta^5\text{-C}_5\text{Me}_5)(\text{CO})\text{Ru}(\mu\text{-OEt})]_2$, and $(\eta^5\text{-C}_5\text{Me}_5)\text{Ru}(\eta^5\text{-2,6-Bu}_2\text{C}_6\text{H}_3\text{O})$, and Molecular Orbital Analysis of $[(\eta^5\text{-C}_5\text{H}_5)\text{Ru}(\mu\text{-OMe})]_2$," *J. Am. Chem. Soc.*, **111**, 4712-4718 (1989).
4. 63. B. E. Bursten, S. D. McKee, and M. S. Platz, "Photochemical Insertion of Alkynes into $\text{Cp}_2\text{Fe}_2(\text{CO})_2(\mu\text{-CO})_2$: A Mechanistic Study by Laser Flash Photolysis," *J. Am. Chem. Soc.*, **111**, 3428-3429 (1989).
5. 64. B. E. Bursten and W. F. Schneider, "The Electronic Structure of Asymmetric Metal-Metal Bonds: The $d^2\text{-}d^6$ Complexes $\text{X}_4\text{Mo-Mo}(\text{PH}_3)_4$ (X = OH, Cl)," *Inorg. Chem.*, **28**, 3292-3296 (1989).
6. 65. C. J. Burns and B. E. Bursten, "Covalency in f-Element Organometallic Complexes: Theory and Experiment," *Comm. Inorg. Chem.*, **9**, 61-93 (1989).
7. 66. B. E. Bursten and W. F. Schneider, "Theoretical Studies of Dinuclear Compounds with Multiple Metal-Metal Bonds," in *Metal-Metal Bonds and Clusters in Chemistry and Catalysis*, J. P. Fackler, Editor, Plenum: New York, P. 19-39 (1990).
8. 67. B. E. Bursten, M. G. Gatter, and K. I. Goldberg, "On the Scarcity of Two-Legged Piano-Stool Complexes," *Polyhedron*, **9**, 2001-2011 (1990).
9. 68. M. Pepper and B. E. Bursten, "Ab Initio Studies of the Electronic Structure of the Diuranium Molecule," *J. Am. Chem. Soc.*, **112**, 7803-7804 (1990).
10. 69. R. J. Strittmatter and B. E. Bursten, "The Bonding in $\text{Tris}(\eta^5\text{-cyclopentadienyl})$ Actinide Complexes. 5. A Comparison of the Bonding in Np, Pu, and Transplutonium Compounds with that in Lanthanide Compounds and a Transition Metal Analogue," *J. Am. Chem. Soc.*, **113**, 5525-5529 (1991).
11. 70. S. D. McKee and B. E. Bursten, "Photochemistry of a μ -Alkylidene Piano-Stool Dimer," *J. Am. Chem. Soc.*, **113**, 1210-1217 (1991).
12. 71. W. F. Schneider, R. J. Strittmatter, B. E. Bursten, and D. E. Ellis, "Relativistic DV-X α Studies of Three-Coordinate Actinide Complexes," in *Density Functional Methods in Chemistry*, J. K. Labanowski and J. W. Andzelm, Editors, Springer-Verlag: New York, 1991, P. 247-260.
13. 72. B. E. Bursten and R. J. Strittmatter, "Cyclopentadienyl-Actinide Complexes: Bonding and Electronic Structure," *Angew. Chem.*, **103**, 1085-1103 (1991); *Angew. Chem. Int. Ed. Engl.*, **30**, 1069-1085 (1991).
14. 73. B. E. Bursten, "Some Comments on Approximate Molecular Orbital Theory in Organometallic Chemistry: Getting More by Doing Less?" *Pure & Appl. Chem.*, **63**, 839-844 (1991).
15. 74. R. H. Cayton, K. J. Novo-Gradac, and B. E. Bursten, "Metal-Metal Bonds Involving the f-Elements. 4. Molecular Orbital Studies of Metal-Metal and Metal-Ligand Interactions in Dinuclear U(V) Systems," *Inorg. Chem.*, **30**, 2265-2272 (1991).
16. 75. M. Pepper and B. E. Bursten, "The Electronic Structure of Actinide-containing Molecules: A Challenge to Applied Quantum Chemistry," *Chem. Rev.*, **91**, 719-741 (1991).
17. 76. T. W. Clayton, Jr. and B. E. Bursten, "On the Correlation of ^{55}Mn NMR Chemical Shifts with Atomic Orbital Populations," *New J. Chem.*, **15**, 713-716 (1991).
18. 77. W. F. Schneider, C. K. Narula, H. Nöth, and B. E. Bursten, "Structure and Bonding Trends in Two- and Three-Coordinate Boron Cations," *Inorg. Chem.*, **30**, 3919-3927 (1991).
19. 78. H. B. Abrahamson, G. P. Nicolai, D. M. Heinekey, C. P. Casey, and B. E. Bursten, "The Electronic Structure of $[(\eta^5\text{-C}_5\text{H}_5)\text{Co}]_2$: A Comment on the Existence of a Complex with an Unsupported Co-Co Double Bond," *Angew. Chem.*, **104**, 464-466 (1992); *Angew. Chem., Int. Ed. Engl.*, **31**, 471-473 (1992).
20. 79. B. E. Bursten, M. R. Callstrom, C. A. Jolly, L. A. Paquette, M. R. Sivik, R. S.

- Tucker, and C. A. Wartchow, "Importance of Steric Requirements Relative to Electronic Contributions in Bicycloalkyl Substituted Titanocene Dichlorides," *Organometallics*, **13**, 127-133 (1994).
21. 80. B. E. Bursten and T. W. Clayton, Jr., "A Simplified View of the δ σ δ^* Transition Energies in Compounds with Multiple Metal-Metal Bonds: The Isolated δ σ δ^* Manifold Model," *J. Cluster Science*, **5**, 157-171 (1994).
22. 81. B. E. Bursten, J. C. Green, and N. Kaltsoyannis, "Theoretical Investigation of the Effects of Spin-Orbit Coupling on the Valence Photoelectron Spectrum of OsO_4 ," *Inorg. Chem.*, **33**, 2315-2316 (1994).
23. 82. S. D. McKee, J. A. Krause, D. M. Lunder, and B. E. Bursten, "On the Mechanism of Photochemical Alkyne Insertion into Cyclopentadienylironcarbonyl Dimer: Alkyne Addition to a 'Tied-Back' Cp-Fe Dimer," *J. Coord. Chem.*, **32**, 249-259 (1994).
24. 83. T. A. Barckholtz, B. E. Bursten, G. P. Niccolai, and C. P. Casey, "An Analysis of the Metal-Metal Bonding in Organodirhenium Complexes with Re-Re Double Bonds," *J. Organomet. Chem.*, **478**, 153-160 (1994).
25. 84. B. E. Bursten, J. C. Green, N. Kaltsoyannis, M. A. MacDonald, K. H. Sze, and J. S. Tse, "Variable Photon Energy Photoelectron Spectroscopic and Theoretical Investigations of the Electronic Structure of TiCl_4 ," *Inorg. Chem.*, **33**, 5086-5093 (1994).
26. 85. C. S. Nash and B. E. Bursten, "Metalloaromaticity in Metallocarbohedrenes: The Electronic Structures of C_{20} and TiC_{12} ," in *Proc. - Electrochem. Soc.*, 94-24 (Recent Advances in the Chemistry and Physics of Fullerenes and Related Materials), 384-396 (1994).
27. 86. F. A. Kvietok and B. E. Bursten, "Stepwise Photochemical CO Loss from $\text{Cp}_2\text{Fe}_2(\text{CO})_2(\mu\text{-CO})_2$ in Low-Temperature Matrices: Evidence for an Unsupported Fe-Fe Triple Bond," *J. Am. Chem. Soc.*, **116**, 9807-9808 (1994).
28. 87. T. L. Gustafson, M. Vitale, K. K. Lee, and B. E. Bursten, "Resonance Raman Spectra of Dinuclear Metal Carbonyls," in *Proceedings of the Fourteenth International Conference on Raman Spectroscopy*, N.-T. Yu and X.-Y. Li, Editors, Wiley: New York, P. 548-549 (1994).
29. 88. M. A. Lynn and B. E. Bursten, "An Analysis of the Bonding in Some 'Nonclassical' d^0 and d^{10} Metal Carbonyl Complexes," *Inorg. Chim. Acta*, **229**, 437-443 (1995).
30. 89. N. Kaltsoyannis and B. E. Bursten, "The Electronic Structure of f^1 Actinide Complexes. 1. Nonrelativistic and Relativistic Calculations of the Optical Spectra of AnX_6^q Complexes," *Inorg. Chem.*, **34**, 2735-2744 (1995).
31. 90. M. Vitale, K. K. Lee, C. F. Hemann, R. Hille, T. L. Gustafson, and B. E. Bursten, "Resonance Raman Studies of $[\text{CpFe}(\text{CO})_2]_2$ and $[\text{Cp}^*\text{Fe}(\text{CO})_2]_2$: A Probe of Photoreactive States and Intermediates," *J. Am. Chem. Soc.*, **117**, 2286-2296 (1995).
32. 91. C. S. Nash and B. E. Bursten, "Comparisons Among Transition Metal, Actinide, and Transactinide Complexes: The Relativistic Electronic Structures of $\text{Cr}(\text{CO})_6$, $\text{W}(\text{CO})_6$, $\text{U}(\text{CO})_6$, and $\text{Sg}(\text{CO})_6$," *New J. Chem.*, **19**, 669-675 (1995).
33. 92. F. A. Kvietok and B. E. Bursten, "Matrix Photochemistry of $\text{Mn}_2(\text{CO})_{10}$: Reversible Formation of $\text{Mn}_2(\text{CO})_8$ from $\text{Mn}_2(\text{CO})_8(\mu\text{-}\eta^1\text{:}\eta^2\text{-CO})$," *Organometallics*, **14**, 2395-2399 (1995).
34. 93. Y. H. Spooner, E. M. Mitchell, and B. E. Bursten, "Matrix Photochemistry of *trans*- $[\text{Cp}^*\text{Fe}(\text{CO})]_2(\mu\text{-CO})(\mu\text{-CH}_2)$: Generation of the *cis* Isomer and of a Double-CO-Loss Photoproduct," *Organometallics*, **14**, 5251-5257 (1995).
35. 94. E. M. Mitchell, T. A. Barckholtz, and B. E. Bursten, "Experimental and Theoretical Studies of the Single- and Double-CO Loss Photoproducts of $[\text{CpCo}(\text{CO})]_2(\mu\text{-CH}_2)$," *Inorg. Chim. Acta*, **252**, 405-412 (1996).
36. 95. N. Kaltsoyannis and B. E. Bursten, "The Electronic Structure of f^1 Actinide

Complexes. 2. Nonrelativistic and Relativistic Calculations of the Ground State Electronic Structures and Optical Transition Energies of $[\text{Ce}(\eta\text{-C}_5\text{H}_5)_3]$, $[\text{Th}(\eta\text{-C}_5\text{H}_5)]$, and $[\text{Pa}(\eta\text{-C}_8\text{H}_8)_2]$,” *J. Organomet.*

3

Chem., **528**, 19-33 (1997).

1. 96. C. S. Nash, B. E. Bursten, and W. C. Ermler, “*Ab Initio* Relativistic Effective Potentials with Spin-Orbit Operators. VII. Am through Element 118,” *J. Chem. Phys.*, **106**, 5133-5142 (1997); erratum *J. Chem. Phys.*, **111**, 2347 (1999).
2. 97. T. L. Gustafson, H. B. Lavender, M. Vitale, F. A. Kvietok, B. E. Bursten, T. Yuzawa, and H. Hamaguchi, “The Photochemistry of Dinuclear Organometallic Compounds: Ground State Resonance Raman and Time-Resolved Infrared Studies of $\text{Mn}_2(\text{CO})_{10}$,” in *Time-Resolved Vibrational Spectroscopy VII*, R. B. Dyer, M. A. D. Martinez, A. Shreve, and W. H. Woodruff, Editors (Los Alamos Conference Proceedings, LA-13290), Springer-Verlag: Berlin, 1997, p. 215216.
3. 98. J. Li and B. E. Bursten, “Density Functional Theoretical Studies of Cycloheptatrienyl Sandwich Compounds of Actinides: $\text{An}(\eta^7\text{-C}_7\text{H}_7)_2$ ($\text{An} = \text{Th}, \text{Pa}, \text{U}, \text{Np}, \text{Pu}, \text{Am}$),” *J. Am. Chem. Soc.*, **119**, 9021-9032 (1997).
4. 99. M. Vitale, M. E. Shapiro, and B. E. Bursten, “Theoretical and Experimental Studies of the Spin-Dependent Structure of the Double-CO-Loss Product of $\text{Cp}_2\text{Fe}_2(\text{CO})_4$,” *J. Chem. Soc., Chem.*

Commun., 179-180 (1998).

100. T. A. Barckholtz and B. E. Bursten, “On the Possible Structures of $\text{Mn}_2(\text{CO})_8$: Theoretical Support for an Unprecedented Asymmetric Unbridged Isomer,” *J. Am. Chem. Soc.*, **120**, 19261927 (1998).
101. J. Li and B. E. Bursten, “Relativistic Density Functional Study of the Geometry, Electronic Transitions, Ionization Energies, and Vibrational Frequencies of Protactinocene, $\text{Pa}(\eta^8\text{-C}_8\text{H}_8)_2$,” *J. Am. Chem. Soc.*, **120**, 11456-11466 (1998).
102. G. Rodriguez, J. P. Graham, W. D. Cotter, C. K. Sperry, G. C. Bazan, and B. E. Bursten, “Binding Preferences of the Tribenzylidenemethane Ligand in High-Oxidation State Tantalum Complexes,” *J. Am. Chem. Soc.*, **120**, 12512-12523 (1998).
103. C. S. Nash and B. E. Bursten, “Spin-Orbit Effects, VSEPR Theory, and the Electronic Structures of Heavy and Superheavy Group IVA Hydrides and Group VIIIA Tetrafluorides. A Partial Role Reversal for Elements 114 and 118,” *J. Phys. Chem. A*, **103**, 402-410 (1999).
104. C. S. Nash and B. E. Bursten, “Spin-Orbit Coupling vs. the VSEPR Method: On the Possibility of a Nonplanar Structure for the Super-Heavy Noble-Gas Tetrafluoride $[\text{118}]\text{F}_4$,” *Angew. Chem.*, **111**, 115-117 (1999); *Angew. Chem. Int. Ed. Engl.*, **38**, 151-153 (1999).
105. T. A. Barckholtz, D. E. Powers, T. A. Miller, and B. E. Bursten, “ZEKE Spectroscopy

- of the Organometallic Radicals MgCH_3 and ZnCH_3 : Construction of a High-Resolution ‘Experimental’ Molecular Orbital Diagram,” *J. Am. Chem. Soc.*, **121**, 2576-2584 (1999).
106. J. P. Graham, A. Wojcicki, and B. E. Bursten, “A Molecular Orbital Description of the Platinum η^3 -Propargyl Complex $[(\eta^3\text{-CH}_2\text{CCPh})\text{Pt}(\text{PPh}_3)]^+$,” *Organometallics*, **18**, 837-842 (1999).
107. C. S. Nash and B. E. Bursten, “Spin-Orbit Effects on the Electronic Structure of Heavy and Superheavy Hydrogen Halides: Prediction of an Anomalously Strong Bond in $\text{H}[117]$,” *J. Phys. Chem. A*, **103**, 632-636 (1999).
108. J.-P. Blaudeau, S. A. Zygmunt, L. A. Curtiss, D. T. Reed, and B. E. Bursten, “Density Functional Investigation of $\text{Pu}(\text{H}_2\text{O})_n^{3+}$ Clusters,” *Chem. Phys. Lett.*, **310**, 347-354 (1999).
109. M. Zhou, L. Andrews, J. Li, and B. E. Bursten, “Reaction of Laser-Ablated Uranium Atoms with CO: Infrared Spectra of CUO , CUO , OUCCO , $(\text{C}_2)\text{UO}_2$, and $\text{U}(\text{CO})_x$ ($x = 1-6$) Molecules in Solid Neon,” *J. Am. Chem. Soc.*, **121**, 9712-9721 (1999).
110. J. Li and B. E. Bursten, “Bis(arene) Actinide Sandwich Complexes, $(\eta^6\text{-C}_6\text{H}_3\text{R}_3)_2\text{An}$: Linear or Bent?,” *J. Am. Chem. Soc.*, **121**, 10243-10244 (1999).
111. C. S. Nash and B. E. Bursten, “Prediction of the Bond Lengths, Vibrational Frequencies, and Bond Dissociation Energy of Octahedral Seaborgium Hexacarbonyl, $\text{Sg}(\text{CO})_6$,” *J. Am. Chem. Soc.*, **121**, 10830-10831 (1999).
112. M. Zhou, L. Andrews, J. Li, and B. E. Bursten, “Reactions of Th atoms with CO: The First Thorium Carbonyl Complex and an Unprecedented Bent Triplet Insertion Product,” *J. Am. Chem. Soc.*, **121**, 12188-12189 (1999).
113. T. A. Barckholtz and B. E. Bursten, “Density Functional Calculations of Dinuclear Organometallic Complexes. I. Metal-Metal and Metal-CO Bond Energies,” *J. Organomet. Chem.*, **596**, 212-220 (2000).
114. L. Andrews, M. Zhou, B. Liang, J. Li, and B. E. Bursten, “Reactions of Laser-Ablated U and Th with CO_2 : Neon Matrix Infrared Spectra and Density Functional Calculations of OUCO , OThCO and Other Products,” *J. Am. Chem. Soc.*, **122**, 11440-11449 (2000).
115. L. Andrews, B. Liang, J. Li, and B. E. Bursten, “Ground State Reversal via Matrix Interaction: Electronic States and Vibrational Frequencies of CUO in Solid Argon and Neon,” *Angew. Chem. Int. Ed. Engl.*, **39**, 4565-4567 (2000).
116. M. R. Antonio, L. Soderholm, C. W. Williams, J.-P. Blaudeau, and B. E. Bursten, “Neptunium Redox Speciation,” *Radiochim. Acta*, **89**, 17-26 (2001).
117. P. M. Bradley, B. E. Bursten, and C. Turro, “Excited State Properties of $\text{Rh}_2(\text{O}_2\text{CCH}_3)_4(\text{L})_2$ ($\text{L} = \text{CH}_3\text{OH}$, py , PPh_3 , THF),” *Inorg. Chem.*, **40**, 1376-1379 (2001).

118. J. Li and B. E. Bursten, "The Electronic Structure of Organoactinide Complexes via Relativistic Density Functional Theory: Applications to the Actinocene Complexes $An(\eta^8-C_8H_8)_2$ ($An = Th-Am$)," in *Computational Organometallic Chemistry*, T. R. Cundari, Editor, Marcel Dekker: New York, 2001, P. 345-379.
119. C. W. Williams, J.-P. Blaudeau, J. C. Sullivan, Mark R. Antonio, B. Bursten, and L. Soderholm, "The Coordination Geometry of Np(VII) in Alkaline Solution," *J. Am. Chem. Soc.*, **123**, 43464347 (2001).
120. J. Li, B. E. Bursten, M. Zhou, and L. Andrews, "A Combined Theoretical and Experimental Study of the Reaction Products of Laser-Ablated Thorium Atoms with CO: First Identification of the CThO, CThO⁻, OThCCO, OTh(η^3 -CCO) and Th(CO)_n (n = 1 - 6) Molecules," *Inorg. Chem.*, **40**, 5448-5460 (2001).
121. B. E. Bursten, M. H. Chisholm, C. M. Hadad, J. Li, and P. J. Wilson, "M₂ δ -to-Oxalate π^* Conjugation in Oxalate-Bridged Complexes Containing M-M Quadruple Bonds," *J. Chem. Soc., Chem. Commun.*, 2382-2383 (2001).
122. B. E. Bursten, M. H. Chisholm, C. M. Hadad, J. Li, and P. J. Wilson, "Electronic Coupling in Quadruple Bonds Between Molybdenum and Tungsten Atoms in Molecular Squares and Extended Chains Linked by Oxalate, Acetylenedicarboxylate and Perfluoroterephthalate Bridges," *Israel J. Chem.*, **41**, 187-195 (2001). (Special issue in honor of F. Albert Cotton)
123. J. Li, B. E. Bursten, B. Liang, and L. Andrews, "Noble Gas-Actinide Compounds: Complexation of the CUO Molecule by Ar, Kr, and Xe Atoms in Noble-Gas Matrices," *Science*, **295**, 2242-2245 (2002).
124. B. E. Bursten, M. H. Chisholm, R. J. H. Clark, S. Firth, C. M. Hadad, A. M. MacIntosh, P. J. Wilson, P. M. Woodward, and J. M. Zaleski, "Oxalate Bridged Molybdenum and Tungsten Quadruply Bonded Complexes Supported by Pivalate Ligands: $(BuCO_2)_3M_2(\mu-O_2C_2O_2)_2M_2(O_2C^iBu)_3$. Electronic, Raman, Resonance Raman Spectra and Electronic Structure Calculations Employing Density Functional Theory," *J. Am. Chem. Soc.*, **124**, 3050-3063 (2002).
125. B. Liang, L. Andrews, J. Li, and B. E. Bursten, "The First Experimental and Theoretical Studies of the Reaction Products of Laser-Ablated Thorium Atoms with H₂O in Excess Argon," *J. Am. Chem. Soc.*, **124**, 6723-6733 (2002).
126. P. M. Bradley, M. L. Drummond, C. Turro, and B. E. Bursten, "Observation of the Photogenerated CO-Loss Intermediate from $[CpFe(CO)]_2(\mu-CO)(\mu-CHCH_3)$ Via Time-Resolved IR Spectroscopy," *Inorg. Chim. Acta*, **334**, 371-375 (2002). (Special issue in honor of Andrew Wojcicki)
127. B. Liang, L. Andrews, J. Li, and B. E. Bursten, "Noble Gas-Actinide Compounds: Evidence for the Formation of Distinct CUO(Ar)_{4n} (Xe)_n and CUO(Ar)_{4n} (Kr)_n (n = 1, 2, 3, 4) Complexes," *J. Am. Chem. Soc.*, **124**, 9016-9017 (2002).
128. B. E. Bursten, M. H. Chisholm, R. J. H. Clark, S. Firth, C. M. Hadad, P. J. Wilson, P. M. Woodward, and J. M. Zaleski, "Perfluoroterephthalate Bridged Complexes with

- M-M Quadruple Bonds: $(\text{BuCO}_2)_3\text{M}_2(\mu\text{-O}_2\text{CCF}_6\text{CO}_2)_2\text{M}_2(\text{O}_2\text{C}^t\text{Bu})_3$, Where M = Mo or W. Studies of Solid-State, Molecular, and Electronic Structure and Correlations with Electronic and Raman Spectral Data,” *J. Am. Chem. Soc.*, **124**, 12244-12254 (2002).
129. B. E. Bursten, M. H. Chisholm, M. L. Drummond, J. C. Gallucci, and C. B. Hollandsworth, “Cyclooctatetraene ditungsten alkoxides: $\text{W}_2(\mu\text{-}\eta^5, \eta^5\text{-COT})(\text{OR})_4$, where R = CH_2^tBu , *i*Pr, and *t*Bu,” *J. Chem. Soc., Dalton Trans.*, 4077-4083 (2002).
 130. L. Andrews, B. Liang, J. Li, and B. E. Bursten, “Noble Gas-Actinide Complexes of the CUO Molecule with Multiple Ar, Kr, and Xe Atoms in Noble-Gas Matrices,” *J. Am. Chem. Soc.*, **125**, 3126-3139 (2003).
 131. B. Liang, L. Andrews, J. Li, and B. E. Bursten, “Bonding of Multiple Noble-Gas Atoms to CUO in Solid Neon: $\text{CUO}(\text{Ng})_n$ (Ng = Ar, Kr, Xe; n = 1, 2, 3, 4) Complexes and the Singlet-Triplet Crossover Point,” *Chem. European J.*, **9**, 4781-4788 (2003).
 132. B. E. Bursten, M. L. Drummond, and J. Li, “Spiers Memorial Lecture: The Quantum Chemistry of d- and f-Element Complexes: From an Approximate Existence to Functional Happiness,” *Faraday Disc. Chem. Soc.*, **124**, 1-24 (2003).
 133. L. Andrews, B. Liang, J. Li, and B. E. Bursten, “Noble Gas-Uranium Coordination and Intersystem Crossing for the $\text{CUO}(\text{Ne})_x(\text{Ng})_n$ (Ng = Ar, Kr, Xe) Complexes in Solid Neon,” *New J. Chem.*, **28**, 289-294 (2004).
 134. B. Liang, L. Andrews, J. Li, and B. E. Bursten, “On the Noble-Gas Induced Intersystem Crossing for the CUO Molecule: Experimental and Theoretical Investigations of $\text{CUO}(\text{Ng})_n$ (Ng = Ar, Kr, Xe; n = 1, 2, 3, 4) Complexes in Solid Neon,” *Inorg. Chem.*, **43**, 882-894 (2004).
 135. J. Li, B. E. Bursten, L. Andrews, and C. J. Marsden, “On The Electronic Structure of Molecular UO_2 in the Presence of Ar Atoms: Evidence for Direct U-Ar Bonding,” *J. Am. Chem. Soc.*, **126**, 3424-3425 (2004).
 136. W. Wang, L. Andrews, J. Li, and B. E. Bursten, “Robust Bonds between Uranium and Noble-Gas Atoms: Coordination of the UO_2^+ Cation by Ne, Ar, Kr, and Xe Atoms,” *Angew. Chem. Int. Ed.*, **43**, 2554-2557 (2004).
 137. M. P. Neu, J. L. Sonnenberg, and B. E. Bursten, “Homoleptic Nine-Coordinate An(III) and Ln(III) Complexes: Classic High-Symmetry Species that Advance our Understanding of f-Element Structure, Bonding, and Dynamics,” *Los Alamos National Laboratory-Actinide Research Quarterly*, 1st Quarter, LALP-04-060, 7-10 (2004).
 138. S. N. Collins, C. M. Brett, and B. E. Bursten, “Density Functional Theory and Low-Temperature Matrix Investigations of CO-Loss Photochemistry from $[(\text{C}_5\text{R}_5)\text{Ru}(\text{CO})_2]_2$ (R=H, Me) Complexes,” *J. Cluster Sci.*, in press. (Special issue in honor of R. A. Walton)

139. C. M. Brett and B. E. Bursten, "Theoretical Studies of 18-electron $M(CH_n)(C_{10-n}H_{10-n})$ ($M = Fe, Ru, Os; n = 3, 4, 5$) Sandwich Complexes," *Polyhedron*, in press. (Special issue in honor of M. L. H. Green)
140. N. Kaltsoyannis, P. J. Hay, J. Li, J.-P. Blaudeau, and B. E. Bursten, "Theoretical Studies of the Electronic Structure of Compounds of the Actinide Elements," in *Chemistry of the Actinide and Transactinide Elements, 3rd Ed.*, J. J. Katz, L. R. Morss, N. Edelstein, and J. Fuger, Editors, Kluwer: Dordrecht, The Netherlands, 2005, in press.
141. J. L. Sonnenberg, P. J. Hay, R. L. Martin, and B. E. Bursten, "Theoretical Investigations of Uranyl-Ligand Bonding: DFT Studies of Four- and Five-Coordinate Uranyl Cyanide, Isocyanide, Carbonyl, and Hydroxide Complexes," submitted for publication.
142. B. Liang, R. D. Hunt, G. P. Kushko, L. Andrews, J. Li, and B. E. Bursten, "Reactions of Laser-Ablated Uranium Atoms with H_2O in Argon Matrices: A Combined Experimental and Theoretical Study," submitted for publication.