#### CURRICULUM VITAE

## JOEL F. LIEBMAN

### Personal Data

Date of Birth: May 6, 1947 Place of Birth: Brooklyn, New York

### Professional Position, Address and Access

Professor of Chemistry, Department of Chemistry and Biochemistry,

University of Maryland, Baltimore County (UMBC), 1000 Hilltop Circle, Baltimore, MD 21250 (USA)

(ph) 410-455-2549 (fx) 410-455-2608 (e-m) jliebman@umbc.edu

Web page http://umbc.edu/chem/general/user/jliebman

### Education

B.S. 1967 Brooklyn College, Chemistry (with honors)

M.A. 1968 Princeton University, Chemistry

Ph.D. 1970 Princeton University, Chemistry (with Prof. Leland C. Allen)

Thesis title: “Bonding in Rare Gas and Fluorine Compounds and Other Quantum Chemical Considerations”

### Appointments in Higher Education

Professor, 1982 – present, University of Maryland, Baltimore County

Associate Professor, 1977 – 1982; Assistant Professor, 1972 – 1977

### Other Affiliations

1979 – 2006, 2012 - 2015 Consultant, contractor, co‑investigator at National Institute of Standards and Technology

1978 (summer) Visiting Associate Professor, University of Utah (invitation of Prof. Jack Simons)

1978 (early summer) Visiting Research Affiliate, Department of Engineering and Applied Science, Yale University (invitation of Prof. Kenneth D. Jordan)

1977 – 1980 Adjunct/Affiliate Faculty (official), University of Maryland, College Park

1976 (early summer) Visiting Assistant Professor, University of Utah (invitation of Prof. Jack Simons)

1975 – 1982 Argonne National Laboratory, Chemistry Division, Guest Scientist

1975 (summer) Visiting Postdoctoral Fellow, Department of Chemistry, University of South Carolina (with Prof. Benjamin M. Gimarc)

1971 – 1972 National Bureau of Standards, NRC ‑ NBS Postdoctoral Associate (with Dr. Thomas D. Coyle)

1970 – 1971 NATO Postdoctoral Fellow, Departments of Theoretical and Physical Chemistry, Cambridge University (with Prof. A. David Buckingham and Prof. John W. Linnett)

### Multiyear Professional Activities

Member, Editorial Advisor Board, 2017 – present, Journal of Chemical Thermodynamics

Member, Editorial Board: 2015 – present, New Frontiers of Chemistry

Member, Editorial Board, 2015 – present, International Journal of Chemical Modeling

### Consulting and Paradigms and Paradoxes Editor: 2010 – present, Structural Chemistry

Associate/Series Editor: 2009 – present, “Patai’s Chemistry of Functional Groups” (a series of research monographs published by Wiley, Chichester, UK). (I have coedited five volumes in this series, and I have contributed chapters to over 30 volumes, other volumes and chapters are in preparation.) I am now also an editor of “e-Patai: Patai’s Chemistry of Functional Groups,” published by Wiley, Chichester, UK. I also coauthored the 2010 “the Patai Series Instructions for Contributors” and the 2010 forward to the series.

### SciFinder, beta version, evaluator: 2009

### Coeditor and cofounder: 1991 – 1998 “SEARCH: Structure, Energetics and Reactivity in Chemistry,” (a series of four research monographs published by Blackie Academic & Professional, an imprint of Chapman & Hall, Inc., London, UK and New York, NY).

Consulting Editor: 1990 – present, Structural Chemistry (ed. I. Hargittai, a journal published by Springer, New York, NY). As part of my role in this journal, I have occasional columns entitled “Paradigms and Paradoxes: A Personal Perspective” and “Community and Commentary”.

Coeditor and cofounder: 1984 – 1991, “Molecular Structure and Energetics,” (a series of 11 research monographs published by VCH Publishers Inc., Deerfield Beach, FL and New York, NY).

Member: 1984 – 2000, International Editorial Advisory Board, “Methods in Stereochemical Analysis” (ed. A.P. Marchand, a series of research monographs published by VCH Publishers Inc., Deerfield Beach, FL and New York, NY).

Member: 1990-1992, Executive Committee, Fluorine Division, American Chemical Society

Memberships: American Chemical Society, American Physical Society, Sigma Xi

### Honors and Fellowships

Certificate of Appreciation, Peer Reviewer, American Chemical Society, 2011

Presidential Research Professor at UMBC, 2006-2009a

UMBC “New Student Book” program, suggested book selected by University committeeb, 2005

American Chemical Society – Slovenian Chemical Society International Activities Travel Award Associate, 2004c

American Chemical Society – Croatian Chemical Society International Activities Travel Award Grantee, 2002d

USM (University System of Maryland) “Regents’ Award for Excellence in Research, Scholarship and Creative Activity,” 2002d

Maryland Chemist of the Year, 1998e

J. William Fulbright Faculty Associate, 1997f

Norwegian-Marshall Fund Faculty Travel Grantee, 1994g

Luso-American Fund for Development (Portugal), Faculty Travel Granteeh, 1992

Norwegian Marshall Fund Faculty Travel Grantee, 1992g

University of Maryland, Baltimore County, “Faculty Distinguished Service Award,” 1985i

University of Maryland, Baltimore County, “Outstanding Young Chemistry Teacher Award,” 1981j

University of Maryland Faculty Research Fellow, 1977

German Academic Exchange Service (DAAD) Faculty Fellow, 1976k

NRC ‑ NBS (National Research Council - National Bureau of Standards) Postdoctoral Fellow, 1971 ‑ 1972

Honorary Ramsay Fellow, 1970 – 1971*l*

NATO Postdoctoral Fellow, 1970 – 1971

Recipient of Osgood Honorarium, 1968 – 1970m

NSF (National Science Foundation) Fellowship, 1968 ‑ 1970:  Traineeship, 1967

Elected to Sigma Xi, 1967

Brooklyn College Chemistry Department Senior & Junior Alumni Awards, 1967 & 1966

NSF-URP Participant, Brooklyn College, 1964n

California State Regents Scholarship, 1963o

aIt is my understanding that I was the first UMBC faculty member to have won all three of these awards, the UMBC Presidential Research Professorship, the USM Regents award (v.i). and the ACS Chemist of the Year award (v.i.).

bBook suggested: K. Brouwer, “The Starship and the Canoe”. (This was the second year of this book program, the first year that selections were solicited from general campus community.)

cSponsor of Dr. Maja Ponikvar (Jožef Stefan Institute, Slovenia).

dAt the Ruđer Bošković Institute (with the invitation and endorsement of Prof. Mirjana Eckert-Maksić and Prof. Zvonimir B. Maksić). Note, I was one of the first two Americans to go to Croatia under the auspicies of this program.

eAwarded by the Maryland Section of the American Chemical Society.

fSponsor of Prof. Ivan Černušák (Comenius University, Slovakia).

gAt the Universities of Tromsø and Trondheim (with the invitation and endorsement of Prof. Anne Skancke and Prof. Marit Trætteberg).

hAt the Instituto Superior Tcnico (with the invitation and endorsement of Prof. Jos A. Martinho Simes).

iGiven by the UMBC Honors Student Association.

jSponsored by the District of Columbia chapter of the American Institute of Chemists.

kAt the Technische Universität der Braunschweig (with the invitation and endorsement of Prof. Reinhard Schmutzler).

*l*English Award.

mPrinceton Award.

nResearch with Prof. Norman Indictor.

oAt UCLA (with the invitation and endorsement of Prof. Donald J. Cram).

**Referee, grant requests:**

US Civilian Research and Development Fund (for the Independent States of the Former Soviet Union), Department of Energy, Finnish National Academy, Israel ‑ US Binational Science Foundation, National Oceanic and Atmospheric Administration, NATO Collaborative “Linkage” Research Grants, National Institutes of Health, National Science Foundation, Natural Sciences and Engineering Research Council (Canada), Office of Standard Reference Data (Nation­al Institute of Standards and Technology), Petroleum Research Fund, Research Corporation (Cottrell College Grants), University of California Energy Institute (Energy Science and Technology Program)

**Referee, journal articles:**

Accounts of Chemical Research, ACS Catalysis, ACS Omega, Acta Aeronautica, Acta Chemica Scandinavica, Advances in Molecular Structure Research, African Journal of Pure and Applied Chemistry, American Chemical Science Journal, American Journal of Physics, American Mineralogist, Analytical Chemistry, Angewandte Chemie International Edition, Australian Journal of Chemistry, Australian Journal of Physics, Biochemical Engineering Journal, Biomedical and Environmental Mass Spectrometry, Biophysical Chemistry, Canadian Journal of Chemistry, Cancer Research, Chemical Educator, Chemical Engineering Communications, Chemical Intelligencer, Chemical Physics, Chemical Physics Letters, Chemical Reviews, Chemistry: An Asian Journal, Chemistry: A European Journal, Chemistry Open, Croatica Chemica Acta, Crystals, Energy and Fuels, Entropy, Environmental Science and Technology, European Journal of Inorganic Chemistry, European Journal of Organic Chemistry, Graphene, Heteroatom Chemistry, Industrial and Engineering Chemistry-Research, Inorganic Chemistry, Inorganic and Nuclear Chemistry Letters, Inorganica Chimica Acta, Inter­national Journal of Chemical Kinetics, Inter­national Journal of Chemical Modeling, Internet Electronic Journal of Molecular Design, Internet Journal of Molecular Sciences, Inorganic Chemistry, International Journal of Mass Spectrometry, Journal of Alloys and Compounds, Journal of the American Chemical Society, Journal of the American Society of Mass Spectrometry, Journal of the Brazilian Chemical Society, Journal of the Chemical Society Chemical Communications, Journal of the Chemical Society Dalton Transactions, Journal of the Chemical Society Perkin Transactions, Journal of Chemical Education, Journal of Chemical and Engineering Data, Journal of Chemical Information and Computer Science/Journal of Chemical Information and Modeling, Journal of the Chemical Society of Pakistan, Journal of Chemical Theory and Computation, Journal of Chemical Thermodynamics, Journal of Computational Chemistry, Journal of the Electrochemical Society, Journal of Energetikc Materials, Journal of Fluorine Chemistry, Journal of Hazardous Materials, Journal of Inorganic Biochemistry, Journal of Inorganic and Nuclear Chemistry, Journal of Macromolecular Science: Pure and Applied Chemistry, Journal of Mass Spectrometry, Journal of the Mexican Chemical Society, Journal of Molecular Modeling, Journal of Molecular Structure, Journal of Organic Chemistry, Journal of Organometallic Chemistry, Journal of Pharmaceutical Science, Journal of Physical and Chemical Reference Data, Journal of Physical Chemistry, Journal of Physical Chemistry A, Journal of Physical Chemistry B, Journal of Physical Organic Chemistry, Journal of Physics and Chemistry of Solids, Journal of Polymer Science Part B: Polymer Physics, Journal of Scientific Exploration, Journal of Sulfur Chemistry, Journal of Theoretical and Computational Chemistry, Letters in Organic Chemistry, Macromolecules, Magnetic Resonance in Chemistry, Mass Spectrometry Reviews, Molecular Pharmacology, Molecular Physics, Molecules, Monatschefte für Chemie (Chedmical Monthly), New Journal of Chemistry, Open Diabetes Journal, Open Structural Biology Journal, Organic and Biomolecular Chemistry, Organic Letters, Organometallics, Philippine Journal of Science, Physical Chemistry Chemical Physics, Polyhedron, Proceedings of the Royal Society A, Propellants, Explosives and Pyrotechnics, Reviews on Chemical Intermediates, Science, Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy, Structural Chemistry, Symmetry, Tetrahedron, Tetrahedron Letters, Theochem, Theoretical Chemistry Accounts and Thermochimica Acta. I am also an “extramural” reviewer for the Washington and Boulder Editorial Review Boards of the National Institute of Standards and Technology.

**External evaluator:**

Air Force Office of Scientific Research, American Society for Engineering Education (for the awarding of National Defense Science and Engineering Graduate Felloahips), the Alcan Award (of the Canadian Society of Chemistry), City University of New York for awarding CUNY Collaborative Incentive Research Grants and CUNY ‑ PSC (Professional Staff Congress) Faculty Fellowships, for the Finnish National Academy (Akademia Suomen) for awarding of research professorships and postdoctoral associates, the Thomas F. and Kate Miller Jeffress Memorial Trust, Killiam Research Fellowships (of the Canada Council/Coun­seil des Artes du Canada), the New Jersey Agricultural Experiment Station, the Polanyi Award (of the Ottawa, Canada, provincial govt.), Poster Presentations – Winter ACS Fluorine Meeting, and for the US State Department for recommenda­tions on a NATO ASI (Advanced Study Institute) program.

**Book reviewer:**

Chemical Intelligencer, Chemistry International, Journal of the American Chemical Society, Molecular Crystals and Liquid Crystals, Structural Chemistry.

I have also evaluated manuscripts for the following book publishers: Academic Press, Chapman & Hall, CRC Press/Taylor & Francis, Freeman, Harper and Row, Kluwer, Plenum, Prentice Hall, Springer-Verlag, Thomson Science, VCH, Wiley, Wiley-VCH and World Scientific.

### University courses taught and/or team-taught include

(Note: \*Graduate course, \*\*Undergraduate course)

Advanced Organic Chemistry\*

Chemical Bonding Theory/Quantum Chemistry\*,\*\*

The Chemical World\*\*

Chemistry of the Main Group Elements\*

Design of a Living Molecule (“minimester”)\*\*

Independent Study and Research\*,\*\*

Inorganic Chemistry\*,\*\*

Introductory Chemistry 1 (regular and “honors”)\*\*

Introductory Chemistry 2 (regular and “honors”)\*\*

Mathematical Chemistry (“minimester”)\*\*

Paradigms and Paradoxes: An Attempt to Understand the Universe (“First Year Seminar”)\*\*

Physical Chemistry 2\*\*

Special Topics in Physical Chemistry\*

### Service to Public Sector (Involvement in middle schools/high schools) include

ACS Winter Fluorine Meeting Student Posters, mentor and judge

Advisor/instructor/mentor of students working at NIST (National Institute of Standards and Technology)

Guest lecturing in schools upon invitation

Guest lecturing in “Gifted and Talented Programs” (Maryland Academy of Science)

1:1 Mentoring

Science Fair Judging

**Departmental and university service includes**

(Note: \*Departmental, \*\*University, italics means I have chaired committee)

Academic Conduct Committee\*\*

Academic Integrity Committee (communications subcommittee\*\* and steering committee\*\*)

Academic Program Review Committee\*\*

Advisement: undergraduate\*,\*\*, graduate\*

Arbitraary and Capricious Grade Review Panel\*\*

Chancellor’s Commission for Affirmative Action\*\*

Chancellor’s Commission for the Status of Women\*\* (member, cochaired *Science Subcommittee*)

Campus-wide Retreat\*,\*\*

Dissertation Committees/External Reader\*,\*\* (at *UMBC*, Bharathidasan University (India), Complutense Universidad (Spain), Indian Institute of Technology – Bombay (India), Saint-Petersburg State Institute of Technology (Russia), University of Münich (Germany), University of New Brunswick (Canada), Waikato University (New Zealand))

Executive Committee*\**

Faculty Marshal, Convocation\*\* and Graduation\*\*

*Faculty Search Committee\**

Governance: executive committee\*, Faculty Senate\*,\*\*

Graduate Council\*\* (general member, course evaluation and *graduate faculty* subcommittees)

Honors and Awards\* (chair dept. committee), \*\*

Honors College Advisory Council\*\*

Honors College Governance Board\*\*

Honors Program\*\*

Honors University Task Force\*\*

Independent Studies Program Coadvisor\*\*, Committee member\*\*

Library Liaison\*,\*\*

McNair Scholar Mentor\*\*

“New Student Book” program: book suggestor\*\*, cofacilitator\*\*

Presidential Professor Advisory Committee\*\*

*Promotion and Tenure*\*,\*\* (including Habilitation evaluator at University of Rostock (Germany) and Ruswe Bošković Institute (Croatia) , Jožef Stefan International Postgraduate School (Slovenia)) and *5-year Post Tenure Review* (UMBC)

Recruitment: *undergraduat*e\*,\*\*, graduate\*,\*\*

Regents award professors nomination

*Research Advisor: undergraduate\*,\*\*, graduate\**

“Research Day” Advisor and Judge\*,\*\*

*Seminar Program\**

Undergraduate Council\*\*

Undergraduate Program Oversight\*,\*\*

Valedictorian Selection Committee\*\*

**Journal Publications**

J362. J.Z. Dávalos, C.F.R.A.C. Lima, L.M.N.B.F. Santos, V.L. Romero and J.F. Liebman, “Thermochemical and Structural Studies of Gallic and Ellagic Acids:, J. Chem. Thermodyn., 129, 108-113 (2019). (This invited, primary research, refereed article is in honor of Gennady Kabo on the occasion of his 80th birthday. This special issue was edited by A. Bazyleva, E. Paulechka and R. Weir.).

J361. D.Z. Spera and J.F. Liebman, “Paradigms And Paradoxes. Hess’ Law and the Thermodynamic Validity of Jolly’s Method for Estimating Bond Dissociation Energies”, Struct. Chem., 29, 1589-1591 (2018).

J360. D. Pavlović, M. Ponikvar-Svet and J.F.Liebman,”[Paradoxes and Paradigms: Observations On Pyrohydrolysis, Oxygen Bomb Combustion, and Alkaline Carbonate Fusion, Most Frequently Used Decomposition Methods for Subsequent Determination of Fluorine and Accompanying Thermochemistry](https://scifinder.cas.org/scifinder/references/answers/1F2317E5X86F350AFX1E995A4D41BE845057:1F23774FX86F350AFX7B36BE62591BF578F5/2.html?nav=eNpb85aBtYSBMbGEQcXQzcjY3NzELcLCzM3Y1MDRLcLcydjMydXMyNTS0MnN1NzCzRSoNKm4iEEwK7EsUS8nMS9dzzOvJDU9tUjo0YIl3xvbLZgYGD0ZWMsSc0pTK4oYBBDq_Epzk1KL2tZMleWe8qCbiYGhooCBgYEZaGBGCYO0Y2iIh39QvKdfmKtfCJDh5x_vHuQfGuDp517CwJmZW5BfVAI0obiQoY6BGaiPASianVsQlFqIIgoATN47aQ&key=caplus_2018:1231423&title=UGFyYWRveGVzIGFuZCBwYXJhZGlnbXM6IG9ic2VydmF0aW9ucyBvbiBweXJvaHlkcm9seXNpcywgb3h5Z2VuIGJvbWIgY29tYnVzdGlvbiwgYW5kIGFsa2FsaW5lIGNhcmJvbmF0ZSBmdXNpb24sIG1vc3QgZnJlcXVlbnRseSB1c2VkIGRlY29tcG9zaXRpb24gbWV0aG9kcyBmb3Igc3Vic2VxdWVudCBkZXRlcm1pbmF0aW9uIG9mIGZsdW9yaW5lIGFuZCBhY2NvbXBhbnlpbmcgdGhlcm1vY2hlbWlzdHJ5&launchSrc=reflist&pageNum=1&sortKey=ACCESSION_NUMBER&sortOrder=DESCENDING)”, Struct. Chem., 29, 1247-54 (2018).

J359. Y.P. Ortiz, D.J. Klein and J.F. Liebman, “Paradigms and Paradoxes: Tetrahedral Units: Dodecahedral Super-structures,” Struct. Chem., 29, 78-96 (2018).

J358 V.L.S. Freitas, J R.B. Gomes, J.F. Liebman and M. D. M. Ribeiro Da Silva,, “[Energetic and Reactivity Properties of 9,​10-​Dihydroacridine And Diphenylamine: A Comparative Overview](https://scifinder.cas.org/scifinder/references/answers/1F2317E5X86F350AFX1E995A4D41BE845057:1F23774FX86F350AFX7B36BE62591BF578F5/6.html?nav=eNpb85aBtYSBMbGEQcXQzcjY3NzELcLCzM3Y1MDRLcLcydjMydXMyNTS0MnN1NzCzRSoNKm4iEEwK7EsUS8nMS9dzzOvJDU9tUjo0YIl3xvbLZgYGD0ZWMsSc0pTK4oYBBDq_Epzk1KL2tZMleWe8qCbiYGhooCBgYEZaGBGCYO0Y2iIh39QvKdfmKtfCJDh5x_vHuQfGuDp517CwJmZW5BfVAI0obiQoY6BGaiPASianVsQlFqIIgoATN47aQ&key=caplus_2017:1552602&title=RW5lcmdldGljIGFuZCByZWFjdGl2aXR5IHByb3BlcnRpZXMgb2YgOSwxMC1kaWh5ZHJvYWNyaWRpbmUgYW5kIGRpcGhlbnlsYW1pbmU6IEEgY29tcGFyYXRpdmUgb3ZlcnZpZXc&launchSrc=reflist&pageNum=1&sortKey=ACCESSION_NUMBER&sortOrder=DESCENDING)”,  J. Chem. Thermodynam., 115, 276-284 (2017).

J357. I. Abramova, B. Rudhsteiyn, A. Greer and J.F. Liebman, “Computed Regioselectivity and Conjectured Biological Activity of Ene Reactions of Singlet Oxygen with the Prenylnatural Product Hyperforin?”, Photochem. Photobiol., 93, 626-631 (2017).

J356 C.A. Deakyne, A.M. Abele and J.F. Liebman, “Bond Dissociation Enthalpy Ratios Involving Pentaatomic 16-Valence Electron Anions,” (a primary research article appearing in C.A. Deakyne and J.F. Liebman (eds.), “Special Issue Dedicated to and in Honor and Memory of Professor Henry A. Bent” Intl. J. Chem. Model., 8, 293-304 (2016).)

J355. C. A. Deakyne, K.F. Edwards, M. Ponikvar-Svet, H.A. Bent and J F. Liebman, “The Existence of Argon Difluoride: Is There Any Reason for Optimism?” (a primary research article appearing in C.A. Deakyne and J.F. Liebman (eds.), “Special Issue Dedicated to and in Honor and Memory of Professor Henry A. Bent” Intl. J. Chem. Model., 8, 257-64 (2016).)

J354. B.R. Duncan and J.F. Liebman, “Inhaled Anesthetic Potency Results from Charge Delocalization and Stability of a Charge Transfer Complex at an Electron-Transfer Site in Microtubules: A Unitary Theory of General Anesthesia,” (A primary research article appearing in “Special Issue Dedicated to and in Honor and Memory of Leland C. Allen”,) C.A. Deakyne and J.F. Liebman (eds.)), Intl. J. Chem. Model,, 8. 199-243 (2016).)

J352. J.F. Liebman and L.C. Allen, “Finding Patterns in the Periodic Table: Summing Configuration Energies,” (A primary research article appearing in “Special Issue Dedicated to and in Honor and Memory of Leland C. Allen”, C.A. Deakyne and J.F. Liebman (eds.)), Intl. J. Chem. Model,, 8, 43-7 (2016).)

.

## J351. Y, Ortiz, D. J. Klein and J. F. Liebman, [Tetrahedral Units: for Dodecahedral Super-​Structures](https://scifinder.cas.org/scifinder/references/answers/87808E58X86F3514BX44B25B45436F677081:8780E69DX86F3514BX71C72C3C4494ED6717/1.html?nav=eNpb85aBtYSBMbGEQcXC3MLA1czSJcLCzM3Y1NDEKcLc0NncyNnY2cTE0sTVxczc0ByoNKm4iEEwK7EsUS8nMS9dzzOvJDU9tUjo0YIl3xvbLZgYGD0ZWMsSc0pTK4oYBBDq_Epzk1KL2tZMleWe8qCbiYGhooCBgYEZaGBGCYO0Y2iIh39QvKdfmKtfCJDh5x_vHuQfGuDp517CwJmZW5BfVAI0obiQoY6BGaiPASianVsQlFqIIgoAOsw7TQ&key=caplus_2016:1076091&title=VGV0cmFoZWRyYWwgdW5pdHM6IGZvciBkb2RlY2FoZWRyYWwgc3VwZXItc3RydWN0dXJlcw&launchSrc=reflist&pageNum=1&sortKey=ACCESSION_NUMBER&sortOrder=DESCENDING),

arXiv.org, e-Print Archive, Physics, 1-12.(2016).

## J350. Á.Vegas, J.F. Liebman and H.D.B. Jenkins, “Unique Thermodynamic Relations for ΔfH⁰ and ΔfG⁰ for Crystalline Inorganic Salts. I. Predicting the Existence and Possible Synthesis of Na2SO2 and Na2SeO2 Addendum” Acta Cryst., B72, 927 (2016).

## J349. D.J.R. Duarte, M.S. Miranda, J. C.G. Esteves da Silva and J. F. Liebman, A Theoretical Study of the Strong Interactions Between Carbon Dioxide and OH+ and NH2+ Products Resulting from Protonation of 1,2-Dioxirane-3-one and 1,2-Oxaziridine- 3-one Respectively, Struct. Chem., 27, 1743-1751 (2016).

J348. Y. Ortiz, D. Bhattachrya, D.J. Klein and J.F. Liebman, “Supermolecules’ a primary, invited, refereed research article in honor of A.T. Balaban on the Occasion of his 85th Birthday), Rev. Roum. Chim. 61, 269-276 (2016).

J347. D.J.R. Duarte, M.S. Miranda, J.C.G. Esteves da Silva and J.F. Liebman, “Theoretical Characterization of the Chemical Bonds of Some Three-Membered Ring Compounds Through QTAIM Theory,” Struct. Chem., 27, 663-670 (2016).

J346. M.S, Miranda, D.J.R. Duarte and J.F. Liebman, “What is the Enthalpy of Formation of Pyrazine-2-carboxylic Acid,” J. Chem. Thermodynam., 97, 261-263 (2016).

J345. V.L.S. Freitas, M.D.M.C. Ribeiro da Silva and J.F. Liebman, “The Enthalpy of Formation of the Isomeric 2,3- and 2,5-Dihydrofuran,” J. Chem. Thermodynam., 97, 135-136 (2016).

J344. M. Ponikvar-Svet, D.N. Zeiger and J.F. Liebman, “Which Halogen is the Strongest Oxidant? A Study with Systematics and Surprises,” Struct. Chem., 26, 1621-1628 (2015). (This invited, primary research, refereed article is in honor of Magdolna Hargittai. This special issue was edited by A. Kovács and L. Nyulászi.)

J343. M.S. Miranda, D.J.R. Duarte, J.C.G. Esteves da Silva and J.F. Liebman, “Protonated Heterocyclic Derivatives of Cyclopropane and Cyclopropanone: Classical Species, Alternate Sites and Ring Fragmentation,” Canad. J. Chem., 93, 708-714 (2015).

J342. M.J.S. Monte, A.R.R.P. Almeida and J.F. Liebman, “Prediction of Enthalpy and Standard Gibbs Energy of Vaporization of Haloaromatics from Atomic Properties,” Chemosphere, 138, 478-485, (2015).

J341. M. Ponikvar-Svet and J.F. Liebman, “Some Systematics and Surprises in the Energetics and Structural Preferences of ‘Few-Boron Species’ and Related Compounds with Carbon and Nitrogen,” New Front. Chem., 24, 27-36 (2015). (This invited primary research, refereed article is part of an inaugural set of issues for this journal).

J340. A. Fattahi, J.F. Liebman, M.S. Miranda, V.M.F. Morais, M.A.R. Matos, L. Lis and S.R. Kass, “[Indenone and Cyclopentadienone Energetics via Mass Spectrometry and Computations: Are These Species Antiaromatic or ‘Merely’ Nonaromatic?](https://scifinder.cas.org/scifinder/references/answers/6F11B489X86F3514CX71B6AAD511599A5FAF:6F121B73X86F3514CX5B566BFD25AC068F2B/1.html?nav=eNpb85aBtYSBMbGEQcXMzdDI0MncOMLCzM3Y1NDEOcLUydTMzMnNxcjU0dnAzMLNyAmoNKm4iEEwK7EsUS8nMS9dzzOvJDU9tUjo0YIl3xvbLZgYGD0ZWMsSc0pTK4oYBBDq_Epzk1KL2tZMleWe8qCbiYGhooCBgYEZaGBGCYO0Y2iIh39QvKdfmKtfCJDh5x_vHuQfGuDp517CwJmZW5BfVAI0obiQoY6BGaiPASianVsQlFqIIgoARxM7Yg&key=caplus_2014:1103049&title=SW5kZW5vbmUgYW5kIGN5Y2xvcGVudGFkaWVub25lIGVuZXJnZXRpY3MgdmlhIG1hc3Mgc3BlY3Ryb21ldHJ5IGFuZCBjb21wdXRhdGlvbnM6IEFyZSB0aGVzZSBzcGVjaWVzIGFudGlhcm9tYXRpYyBvciAibWVyZWx5IiBub25hcm9tYXRpYz8&launchSrc=reflist&pageNum=1&sortKey=ACCESSION_NUMBER&sortOrder=DESCENDING),” Intl. J. Mass Spectrom., 378, 175–179 (2015) (This paper is a reprint of paper J337 cited below, now appearing in a special issue dedicated to Veronica M. Bierbaum.)

J339. M.S. Miranda, P.J.O. Ferreira, J.C.G. Esteves da Silva and J.F. Liebman, “Three-Membered Ring Amides: A Calculational and Conceptual Study of the Structure and Energetics of 1,2-Oxaziridine-3-one and Aziridine-2,3-dione,” Canad. J. Chem., 93, 406-413 (2015). (This invited primary research, refereed article is in honor of R. Stan Brown. This special issue was edited by W. Leigh and V. Snieckus.)

J338. M.S. Miranda, J.C.G. Esteves da Silva and J.F. Liebman, “Gas-phase Thermochemical Properties of Some Tri-substituted Phenols: A Density Functional Theory Study,” J. Chem. Thermodyn., 80, 65-72 (2015).

## J337. A. Fattahi, J.F. Liebman, M.S. Miranda, V.M.F. Morais, M.A.R. Matos, L. Lis and S.R. Kass, “[Indenone and Cyclopentadienone Energetics via Mass Spectrometry and Computations: Are These Species Antiaromatic or ‘Merely’ Nonaromatic?](https://scifinder.cas.org/scifinder/references/answers/6F11B489X86F3514CX71B6AAD511599A5FAF:6F121B73X86F3514CX5B566BFD25AC068F2B/1.html?nav=eNpb85aBtYSBMbGEQcXMzdDI0MncOMLCzM3Y1NDEOcLUydTMzMnNxcjU0dnAzMLNyAmoNKm4iEEwK7EsUS8nMS9dzzOvJDU9tUjo0YIl3xvbLZgYGD0ZWMsSc0pTK4oYBBDq_Epzk1KL2tZMleWe8qCbiYGhooCBgYEZaGBGCYO0Y2iIh39QvKdfmKtfCJDh5x_vHuQfGuDp517CwJmZW5BfVAI0obiQoY6BGaiPASianVsQlFqIIgoARxM7Yg&key=caplus_2014:1103049&title=SW5kZW5vbmUgYW5kIGN5Y2xvcGVudGFkaWVub25lIGVuZXJnZXRpY3MgdmlhIG1hc3Mgc3BlY3Ryb21ldHJ5IGFuZCBjb21wdXRhdGlvbnM6IEFyZSB0aGVzZSBzcGVjaWVzIGFudGlhcm9tYXRpYyBvciAibWVyZWx5IiBub25hcm9tYXRpYz8&launchSrc=reflist&pageNum=1&sortKey=ACCESSION_NUMBER&sortOrder=DESCENDING),” Intl. J. Mass Spectrom., 369, 87-91 (2014).

## 

## J336. J.Z. Dávalos, R. Herrero, J.C.S. Costa, L.M.N.B.F. Santos and J.F. Liebman, “[Energetic and Structural Study of Bisphenols](https://scifinder.cas.org/scifinder/references/answers/6F11B489X86F3514CX71B6AAD511599A5FAF:6F121B73X86F3514CX5B566BFD25AC068F2B/3.html?nav=eNpb85aBtYSBMbGEQcXMzdDI0MncOMLCzM3Y1NDEOcLUydTMzMnNxcjU0dnAzMLNyAmoNKm4iEEwK7EsUS8nMS9dzzOvJDU9tUjo0YIl3xvbLZgYGD0ZWMsSc0pTK4oYBBDq_Epzk1KL2tZMleWe8qCbiYGhooCBgYEZaGBGCYO0Y2iIh39QvKdfmKtfCJDh5x_vHuQfGuDp517CwJmZW5BfVAI0obiQoY6BGaiPASianVsQlFqIIgoARxM7Yg&key=caplus_2014:722576&title=RW5lcmdldGljIGFuZCBTdHJ1Y3R1cmFsIFN0dWR5IG9mIEJpc3BoZW5vbHM&launchSrc=reflist&pageNum=1&sortKey=ACCESSION_NUMBER&sortOrder=DESCENDING),” J. Phys. Chem. A., 118, 3705-9 (2014).

J335. C.M. Mayhan, H. Kumari, E.M. McClure, J.F. Liebman and C.A.Deakyne, “Gas-phase Basicity of Hydroxyquinol: A Computational Study,” J. Chem. Thermodyn., 73, 171-7 (2014). (This primary research, refereed article is in memory of Manuel A.V. Ribeiro da Silva. This special issue was edited by R.D. Weir, J.A. Martinho Simões, J.F. Liebman and M.J.S. Monte).

## J334. R. Notario, J.S. Chickos and J.F. Liebman, [“The Enthalpy of Formation of Selenocysteine: A G3 and G4 Quantum Chemical Study](https://scifinder.cas.org/scifinder/references/answers/6F11B489X86F3514CX71B6AAD511599A5FAF:6F121B73X86F3514CX5B566BFD25AC068F2B/9.html?nav=eNpb85aBtYSBMbGEQcXMzdDI0MncOMLCzM3Y1NDEOcLUydTMzMnNxcjU0dnAzMLNyAmoNKm4iEEwK7EsUS8nMS9dzzOvJDU9tUjo0YIl3xvbLZgYGD0ZWMsSc0pTK4oYBBDq_Epzk1KL2tZMleWe8qCbiYGhooCBgYEZaGBGCYO0Y2iIh39QvKdfmKtfCJDh5x_vHuQfGuDp517CwJmZW5BfVAI0obiQoY6BGaiPASianVsQlFqIIgoARxM7Yg&key=caplus_2013:1970875&title=VGhlIGVudGhhbHB5IG9mIGZvcm1hdGlvbiBvZiBzZWxlbm9jeXN0ZWluZTogQSBHMyBhbmQgRzQgcXVhbnR1bSBjaGVtaWNhbCBzdHVkeQ&launchSrc=reflist&pageNum=1&sortKey=ACCESSION_NUMBER&sortOrder=DESCENDING),” J. Chem. Thermodyn., 73, 134-9 (2014). (This primary research, refereed article is in memory of Manuel A.V. Ribeiro da Silva. This special issue was edited by R.D. Weir, J.A. Martinho Simões, J.F. Liebman and M.J.S. Monte)..)

J333.M.S. Miranda, J.S. Chickos, J.C.G. Esteves da Silva and J.F. Liebman, “Feeling and Investigating Blue: On the Enthalpy of Formation of Indigo,” J. Chem. Thermodyn., 73, 69-75 (2014). (This primary research, refereed article is in memory of Manuel A.V. Ribeiro da Silva. This special issue was edited by R.D. Weir, J.A. Martinho Simões, J.F. Liebman and M.J.S. Monte).

J332. B. Rudshteyn, A. Castillo, A.A. Ghogare, J.F. Liebman and A. Greer, “Theoretical Study of the Reaction Fomalhydrazone with Singlet Oxygen. Fragmentation of the C=N Bond, Ene Reaction and Other Processes,” Photochem. Photobiol., 90, 431-8 (2014). (This primary research, refereed article is in memory of Nicholas J. Turro. This special issue was edited by G.B. Schuster.)

J331. K.F. Edwards, E. Lewars and J.F. Liebman, “On the Existence and Energetics of o- and p-Benzoquinone and Their Derivatives: Additional Understanding from the Vantage Point of the Conceptual Trichotomy of Convenience, Anthropocentrism and Folksonomy,” Intl. J. Chem. Model., 5, 327-334 (2013). (This primary research, refereed article is in honor of Alexandru T. Balaban on the happy occasion of his 50th anniversary of his Romanian Academy membership. This special issue was edited by M.V.Putz.) This paper was reproduced in slightly modified form as “On the Existence and Energetics of o- and p-Benzoquinone and Their Derivatives: Additional Understanding from the Vantage Point of the Conceptual Trichotomy of Convenience, Anthropocentrism and Folksonomy,” Intl. J. Chem. Model., 5, 327-334 (2015).

J330. M. Ponikvar-Svet, A.T. Thomas, B.J. Dodson, B.M. Henegar, M.W. Brewster, N.K. Neerchal and J.F. Liebman, “Linear Model for Estimating the Entropy of Formation of Aqueous Anions,” Struct. Chem., 24, 2069-2082 (2013). (This primary research, refereed article is in honor of Maria Victoria Roux on the occasion of her retirement. This special issue was edited by J.F. Liebman, J.S. Chickos and R. Notario.)

J329. J.E. Bartmess and J. Liebman, “Pushing and Pulling Electrons: The Effect on the Heat of Formation of Trifluoromethyl Compounds,” Struct. Chem. 24, 2035 – 2045 (2013). (This primary research, refereed article is in honor of Maria Victoria Roux on the occasion of her retirement. This special issue was edited by J.F. Liebman, J.S. Chickos and R. Notario.)

J328. J.Z. Dávalos, P. Jiménez, M.V. Roux, M.T. Molina, T. Filipova, E. Lewars and J.F. Liebman, “Thermochemical and Structural Properties of Anthraquinones,” Struct. Chem., 24, 2027 – 2034 (2013). (This primary research, refereed article is in honor of Maria Victoria Roux on the occasion of her retirement. This special issue was edited by J.F. Liebman, J.S. Chickos and R. Notario.)

J327. S. Perisanu, I. Contineanu, A. Neacsu, N.P. Rath, J.S. Chickos, R. Notario and J.F. Liebman, “Thermochemical and Structural Study of a Dibenzocycloheptane Cyanoenamine” Struct. Chem. 24, 1975 – 1980 (2013). (This primary research, refereed article is in honor of Maria Victoria Roux on the occasion of her retirement. This special issue was edited by J.F. Liebman, J.S. Chickos and R. Notario.)

J326. M.S. Miranda, J.C.G. Esteves da Silva, C. Hon, S.J. McKerrall and J.F. Liebman, “The Structure and Energetics of Pyrrolidinones, Tetrahydrofuranones, Piperidinones and Tetrahydropyranones: A Computational Study,” Struct. Chem., 24, 1829-1839 (2013). (This primary research, refereed article is in honor of Maria Victoria Roux on the occasion of her retirement. This special issue was edited by J.F. Liebman, J.S. Chickos and R. Notario.)

J325. R. Notario, T.M. Klapötke and J.F. Liebman, “The Gas Phase Enthalpies of Formation of Hydrazine, its Methylated Derivatives, and the Corresponding Values for Ammonia and its Methylated Derivatives,” Struct. Chem., 24, 1817-1819 (2013). (This primary research, refereed article is in honor of Maria Victoria Roux on the occasion of her retirement. This special issue was edited by J.F. Liebman, J.S. Chickos and R. Notario.)

J324. M.S. Miranda, J.C.G. Esteves da Silva, A. Castillo, A.T. Frank, A. Greer, J.A. Brown, B.C. Davis and J.F. Liebman, “Amino, Ammonio and Aminioethenes: A Theoretical Study of their Structure and Energetics,” J. Phys. Org. Chem., 26, 613-625 (2013). (A figure from our article was chosen as the cover design of the issue.)

J323. K.F. Edwards, S. Perişanu and J.F. Liebman, “The Aromaticity of Benzene and the Lack of Aromaticity of Cyclooctatetraene: Is Our Calorimetric Perspective a Manifestation of Convenience, Anthropocentrism, or Folksonomy?,” Intl. J. Chem. Model., 5, 51 – 65 (2013). (This paper was reproduced in slightly modified form as K.F. Edwards, S. Perişanu and J.F. Liebman, “The Aromaticity of Benzene and the Lack of Aromaticity of Cyclooctatetraene: Is Our Calorimetric Perspective a Manifestation of Convenience, Anthropocentrism, or Folksonomy?,” Advances in Molecular Modeling, 5, 417 – 432 (2015) (ed. M. V. Putz, Nova Science Publishers, Hauppage, 2015).

J322. K.F. Edwards, J.C. Williams and J.F. Liebman, “Organizing Principles and Gaps in the Periodic Table: Do We Find Manifestations of Convenience, Anthropocentrism, or Folksonomy?,” Intl. J. Chem. Model, 4, 391 – 404 (2013). (This paper was reproduced in slightly modified form as K.F. Edwards, J.C. Williams and J.F. Liebman, “Organizing Principles and Gaps in the Periodic Table: Do We Find Manifestations of Convenience, Anthropocentrism, or Folksonomy?,” Advances in Molecular Modeling, 4, 525 – 538 (2013) (ed. M. V. Putz, Nova Science Publishers, Hauppage).

J321. E. Lewars and J.F. Liebman, “What is the Enthalpy of Formation and Stabilization Energy of Acrolein?,” Struct. Chem., 24, 741 – 744 (2013). (This primary research, refereed article is in honor of Aldo Domenicano. This paper is part of a special issue edited by Anna Rita Campanelli.)

J320. M. Maatallah, M. Guo, D. Cherqaoui, A. Jarid and J.F. Liebman, “Aluminium Clusters for Molecular Hydrogen Storage and the Corresponding Alanes as Fuel Alternatives: A Structural and Energetic Analysis,” Intl. J. Hydrog. Energ., 38, 5758-5767 (2013).

J319. Á.Vegas, R. Notario, E. Chamorro, P. Perez and J.F. Liebman, “Isoelectronic and Isolobal O, CH2, CH3+ and BH3 as Electron Pairs. Similarities between Molecular and Solid State Chemistry,” Acta Cryst. B, 69, 163 – 175 (2013).

J318. R. Notario, V. Emel´yanenko, M.V. Roux, F. Ros, S.P. Verevkin, J.S. Chickos and J.F. Liebman, "Thermochemistry of Uracils. Experimental and Computational Enthalpies of Formation of 5,6-Dimethyl-, 1,3,5-Trimethyl-, and 1,3,5,6-Tetramethyluracils,” J. Phys. Chem. A, 117, 244-251 (2013).

J317. S.P. Verevkin, V.N. Emel’yanenko, M.V. Roux, R. Notario, J.S. Chickos, J.F. Liebman, “Rediscovering the Wheel. Thermochemical Analysis of Energetics of the Aromatic Diazines," J. Phys. Chem. Lett., 3, 3454-3459 (2012).

J316. M.V. Roux, R. Notario, M. Segura, J.S. Chickos and J.F. Liebman, “The Enthalpy of Formation of Methionine Revisited,” J. Phys. Org. Chem., 25, 916 – 924 (2012).

J315. Á.Vegas, J.F. Liebman and H.D.B. Jenkins, “Unique Thermodynamic Relations for ΔfH⁰ and ΔfG⁰ for Crystalline Inorganic Salts. I. Predicting the Existence and Possible Synthesis of Na2SO2 and Na2SeO2” Acta Cryst., B68, 511-527 (2012).

J314. M.S. Miranda, M.A.R. Matos, V.M.F. Morais and J.F. Liebman, “Paradigms and Paradoxes: En Route to the Understanding of the Aromaticity of ‘Iso-Species’ Isobenzofuran, Anthranil, Benzofurazan and 2,1,3-benzothiadiazole,” Struct. Chem. 23, 1241 – 1243 (2012).

J313. M. Maatallah, D. Cherqaoui, A. Jarid and J.F. Liebman, “Large Gallanes and the PSEPT Theory: A Theoretical Study of GanHn+2 Clusters (n=7-9),” J. Mol. Model., 18, 3321 – 3328 (2012).

J312. A. Kayembe, E. Lewars and J.F. Liebman, “The Quinones of Bicyclo[3.1.0]hexatriene: A

Computational Study of Their Chemistry and Thermochemistry,” J. Chem. Thermodyn., 52, 43 – 56 (2012) (this invited, primary, refereed research article appears in the special issue entitled “Biothermodynamics” edited by Robert N. Goldberg)

J311. R. Notario, M. Temprado, M.V. Roux and J.F. Liebman, “Substituent Effects on the Thermochemistry of Thiophenes, A Theoretical (G3(MP2)//B3LYP and G3) Study,” J. Phys. Chem. A., 116, 4363 – 4370 (2012).

J310. M.S. Miranda, M.A.R. Matos, V.M.F. Morais and J.F. Liebman, “2,1,3-benzothiadiazole: Study of Its Structure, Energetics and Aromaticity,” J. Chem. Thermodyn., 50, 30-36 (2012).

J309. J. Morgan, A. Greenberg and J.F. Liebman, “Paradigms and Paradoxes: O- and N-Protonated Amides, Stabilization Energy and Resonance Energy," Struct. Chem., 23, 197-199 (2012).

J308. M.V. Roux, M. Temprado, P. Jiménez, R. Notario, A.R. Parameswar, A.V. Demchenko, J.S. Chickos, C.A. Deakyne and J.F. Liebman, “Knowledge of a Molecule: An Experimental and Theoretical Study of the Structure and Enthalpy of Formation of Tetrahydro-2*H*-1,3-oxazine-2-thione,” J. Chem. Eng. Data,56, 4725 – 4532 (2011). (This primary, invited, refereed research paper is in honor of Kenneth D. Marsh).

J307. M.S. Miranda, M.A.R. Matos, V.M.F. Morais and J.F. Liebman, “Energetics of Quinazoline-2,4(1*H*,3*H*)-dione: An Experimental and Computational Study,”J. Chem. Eng. Data**.,** 56, 4516-4523 (2011). (This primary, invited, research paper is in honor of Kenneth D. Marsh).

J306. M.S. Miranda, M.A.R. Matos, V.M.F. Morais and J.F. Liebman, “Paradigms and Paradoxes: The Aromaticity of 6:6 Fused Carbocycles and Heterocycles as an Extension of a Study of Indane and Indene Derivatives,” Struct. Chem., 22, 1221 ─ 1224 (2011).

J305. K.F. Edwards and J.F. Liebman, “Amphoteric, Amphihydric and Ambisaline: Are These Descriptive Concepts Manifestations of Convenience, Anthropocentrism, or Folksonomy?” Int. J. Chem. Model., 3, 213 – 226 (2011). (This invited, refereed, primary research paper is in honor of Eduardo A. Castro on the occasion of his 65th birthday). (This paper was reproduced in slightly modified form as K.F. Edwards and J.F. Liebman, “Amphoteric, Amphihydric and Ambisaline: Are These Descriptive Concepts Manifestations of Convenience, Anthropocentrism, or Folksonomy?” in Advances in Molecular Modeling, Vol. 3, 67-77 (2012) (ed. M. V. Putz, Nova Science Publishers, New York, 2012).

J304. M.S. Miranda, M.A.R. Matos, V.M.F. Morais and J.F. Liebman, “Study of Energetics and Structure of 1,2,3-Benzotriazin-4(3*H*)-one and its 1*H* and Enol Tautomers,” J. Phys. Chem. B, 115, 6616-6622 (2011).

J303. M.V. Roux, G. Martín-Valcarcel, R. Notario, S. Kini, J.S. Chickos and J.F. Liebman “The Joining of Measurement and Prediction: The Enthalpy of Formation of 1,4-Cubanedicarboxylic Acid, J. Chem. Eng. Data, 56, 1220 – 1228 (2011). (This primary, invited, refereed research paper is in honor of John M. Prausnitz.)

J302. M. Maatallah, D. Cheraqaoui, A. Jarid and J.F. Liebman, “Are Closed Clusters Expected from the (n+1) Skeletal Electron Pairs Rule in Alanes and Gallanes? A DFT Structural Study of AnHn+2 (A = Al, Ga, and n = 4–6),” Polyhedron, 30, 1080 - 1084 (2011).

J301. H.A. Bent and J.F. Liebman, “Paradigms and Paradoxes: The Weak Bonds in Elemental Halogens, Peroxides, Disulfides, Interhalogens, Noble Gas Monohalide Cations and Isoelectronic Species,” Struct. Chem., 22, 371 – 372 (2011) (this invited, refereed, primary research paper appears in a special issue devoted to Lev Vilkov.)

J300. M.A.R. Matos, V.M.F. Morais, M.S. Miranda and J.F. Liebman, “Combined Experimental and Computational Study on the Energetics of 1,2-Benzisothiazol-3(2*H*)-one and 1,4-Benzothiazin-3(2*H*, 4*H*)-one,” J. Chem. Thermodyn., 43, 635 – 644 (2011).

J299. T.M. Klapötke, C.A. Deakyne and J.F. Liebman, “Paradigms and Paradoxes: Why is the Electron Affinity of the Azide Radical, N3, So Large?” Struct. Chem., 22, 189 – 191 (2011). (This research paper is in honor of H. Donald B. Jenkins.)

J298. S. Perişanu, I. Contineanu, A. Neacşu, R. Notario, M.V. Roux, J.F. Liebman and B.J. Dodson, “Thermochemistry and Quantum Chemical Calculations of Two Dibenzocycloalkane Nitriles,” Struct. Chem, 22, 89 – 94 (2011).

J297. M.A.R. Matos, M.S. Miranda, V.M.F. Morais and J.F. Liebman, “Experimental and Computational Study on the Energetics of 10,11-Dihydro-5H-dibenzo[a,d]cycloheptene (Dibenzosuberane),” J. Chem. Thermodyn., 43, 364 – 370 (2011).

J296.C.A. Deakyne, A.K. Ludden, M.V. Roux, R. Notario, A.V. Demchenko, J.S. Chickos and J.F. Liebman, “Energetics of the Lighter Chalcogen Analogues of Carboxylic Acid Esters,” J. Phys. Chem. B, 114, 16253 – 16262 (2010). (This invited, refereed, primary research paper is in honor of Robert A. Alberty.)

J295. H.D.B. Jenkins, L. Glasser and J.F. Liebman, “The Thermodynamic Hydrate Difference Rule Applied to Salts of Carbon-Containing Oxyacid Salts and Their Hydrates: Materials at the Inorganic/Organic Interface,” J. Chem. Eng. Data, 55, 4369 − 4371 (2010). (This invited, refereed, primary research paper is in honor of John S. Rowlinson.)

J294. T.M. Klapötke and J.F. Liebman, “Paradigms and Paradoxes: A Comparison of the Enthalpies of Formation of Trinitromethyl and Trimethylmethyl (t-Butyl) Containing Species,” Struct. Chem., 21, 1051 − 1052 (2010).

J293. A. Guermoune, D. Cherqaoui, A. Jarid and J.F. Liebman, “Structure and Decomposition of [HFe(CO)4(B2H5)], a Revised Behavior of an Old Uncharacterized Complex,” J. Organomet. Chem. 695, 1715 – 1721 (2010).

J292. M.A.R. Matos, M.S. Miranda, V.M.F. Morais and J.F. Liebman, “Experimental and Computational Thermochemical Study of Oxindole,” J. Chem. Thermodyn., 42, 1101 – 1106 (2010).

J291. M.S. Miranda, V.M.F. Morais, M.A.R. Matos and J.F. Liebman, “Standard Molar Enthalpy of Formation of 1-Benzosuberone: An Experimental and Computational Study,” J. Chem. Thermodyn., 42, 1094 – 1100 (2010).

J290. M.V. Roux, M. Temprado, P. Jiménez, C. Foces-Foces, R. Notario, A.R. Parameswar, A.V. Demchenko, J.S. Chickos, C.A. Deakyne and J.F. Liebman, “Experimental and Theoretical Study of the Structures and Enthalpies of Formation of 3H-1,3-Benzoxazole-2-thione, 3H-1,3-Benzothiazole-2-thione, and Their Tautomers,” J. Phys. Chem. A, 114, 6336 – 6341 (2010).

J289. R. Notario, M.V. Roux and J.F. Liebman, “What is the Enthalpy of Formation of Acrylonitrile?” Struct. Chem., 21, 481 – 484 (2010).

J288. D. Lipkind, J.S. Chickos and J.F. Liebman,”Study of the Anomalous Behavior of 1,2-Diazines by Correlation – Gas Chromatography,” J. Chem. Eng. Data, 55, 1628 – 1635 (2009).

J287. J.S. Chickos and J.F. Liebman, “Paradigms and Paradoxes: Properties of Ideal Gases for Large and Small Species,” Struct. Chem., 20, 1077 – 1078 (2009).

J286. M.V. Roux, M. Temprado, P. Jiménez, C. Foces-Foces, R. Notario, A.R. Parameswar, A.V. Demchenko, J.S. Chickos, C.A. Deakyne, A.K. Ludden and J.F. Liebman, “An Experimental and Theoretical Study of the Structures and Enthalpies of Formation of the Synthetic Reagents, 1,3-Thiazolidine-2-thione and 1,3-Oxazolidine-2-thione,” J. Phys. Chem. A, 113, 10772 – 10778 (2009).

J285. C.A. Deakyne, H.M. Thomas and J.F. Liebman. “The Structure and Energetics of Triplet [B, C, F, H2],” J. Fluor. Chem., 130, 836 – 845 (2009). (This primary, invited, refereed, research paper is in honor of Henry Selig on the occasion of his winning the 2008 Award for Creative Work in Fluorine Chemistry given by the American Chemical Society.)

J284. Z. Mazej, M. Ponikvar-Svet, J.F. Liebman, J. Passmore and H.D.B. Jenkins, “Nitrosyl and Dioxygenyl Cations and Their Salts – Similar but Further Investigation Needed,” J. Fluor. Chem., 130, 788 – 791 (2009). (This primary, invited, refereed, research paper is in honor of Henry Selig on the occasion of his winning the 2008 Award for “Creative Work in Fluorine Chemistry” given by the American Chemical Society.)

J283. H.D.B. Jenkins, M. Ponikvar-Svet and J.F. Liebman, "Relative Packing Efficiency in Hydrates," J. Chem. Eng. Data, 54, 2722 – 2728 (2009). (This invited, refereed, primary research paper is in honor of William A. Wakeham on the occasion of his retirement.)

J282. E. Golas, E.G. Lewars and J.F. Liebman, “The Quinones of Benzocyclobutadiene: a Computational Study,” J. Phys. Chem. A, 113, 9485 – 9500 (2009).

J281. J.F. Liebman and Z.S. Herman, “On the Angular Independence of Sets of Atomic Orbitals,” Croat. Chim. Acta, 82, 261 – 265 (2009). (This invited, refereed, primary, research paper is in honor of Zvonimir B. Maksić on the occasion of his 70th birthday.)

J280. C.A. Deakyne, L.H. Warfel IV, H.M. Thomas, D. Nauduri, T.E.A. Ajibowo, N.J. Carbonaro, A.G. Simpson and J. F. Liebman, “The Energetics of Halogenated Ethylenes (Ethynes) and 1,3-Butadienes (Butadiynes): A Computational and Conceptual Study of Substituent Effects and ‘Dimerization’,” Croat. Chim. Acta, 82, 165 – 172 (2009). (This invited, refereed, primary,research paper is in honor of Zvonimir B. Maksić on the occasion of his 70th birthday.)

J279. M.A.R. Matos, C.C.S. Sousa, M.S. Miranda, V.M.F. Morais and J.F. Liebman, “Energetics of Coumarin and Chromone,” J. Phys. Chem. B, 113, 11216 – 11221 (2009).

J278. M. Ponikvar-Svet and J.F. Liebman, “Paradoxes and Paradigms: Influence of the Power of z on the Estimation of Entropies of Formation of Aqueous Anions Using Simple Parameters,” Struct. Chem., 20, 757 – 765 (2009).

J277. R.S. Hosmane and J.F. Liebman, “Paradoxes and Paradigms: Why is Quinoline Less Basic Than Pyridine or Isoquinoline? A Classical Organic Chemical Perspective,” Struct. Chem., 20, 693 – 697 (2009).

J276. J.F. Liebman, D. Lipkind and J.S. Chickos, “Chemistry, Commentary and Community: Discussion of ‘An Examination of the Vaporization Enthalpies and Vapor Pressures of Pyrazine, Pyrimidine, Pyridazine, and 1,3,5-Triazine’ by Lipkind and Chickos,” Struct. Chem., 20, 617 – 618 (2009).

J275. H.D.B. Jenkins, J.F. Liebman, M. Ponikvar and S. Scheiner, “The Heat Capacities and Standard Entropies of Corresponding Potassium and Ammonium Ion Species: Is There a Constant Difference?,” Struct. Chem., 20, 31 – 35 (2009) (this primary, invited, refereed, research paper is to celebrate the 20th Anniversary of the journal “Structural Chemistry”.)

J274. H.D.B. Jenkins and J.F. Liebman, “Extensions and Corollaries of the Thermodynamic Solvate Difference Rule,” J. Chem. Eng. Data, 54, 351 – 358 (2009) (this invited, refereed, primary research paper is in honor of Robin H. Stokes on the occasion of his 90th birthday).

J273. H. Brand, J.F. Liebman and A. Schulz, “Cyano-, Nitro- and Nitrosomethane Derivatives: Structure and Gas-phase-Acidity,” Eur. J. Org. Chem., 4665 – 4675 (2008).

J272. A. Greer and J.F. Liebman, “Paradigms and Paradoxes: Energetics of the Oxidative Cleavage of Azo Compounds (Diazenes),” Struct. Chem., 19, 817 – 818 (2008).

J271. M.A.R. Matos, M.S. Miranda, D.A.P. Fonesca, V.M.F. Morais and J.F. Liebman, "Calorimetric and Computational Thermochemical Study of 3,3-tetramethyleneglutaric acid, 3,3-tetramethyleneglutaric Anhydride and 3,3-tetramethyleneglutarimide," J. Phys. Chem. A, 112, 10053 – 10058 (2008).

J270. D. Roy, C. Patel, J.F. Liebman and R.B. Sunoj, “Probing Intramolecular Interactions in Arylselenides Using a Property Descriptor Based Approach,” J. Phys. Chem. A, 112, 8797 – 8803 (2008).

J269. S.W. Slayden and J.F. Liebman, “Paradigms and Paradoxes: Organic Thermochemistry Without Hydrogen: Carbon Oxides and Nitrides,” Struct. Chem., 19, 683 – 687 (2008).

J268. A. Schulz and J.F. Liebman, "Paradoxes and Paradigms: High Oxidation States and Neighboring Rows in the Periodic Table - Lanthanides, Actinides, Exotica and Explosives," Struct. Chem., 19, 633 –655 (2008).

J267. C.A. Deakyne, J.F. Liebman, E.A. Vlasov and Y.E. Zevatsky, “Paradigms and Paradoxes: Analysis of the Site of Protonation of Bifunctional Organic Compounds with the Protonation Energy/Volume Computation Method,” Struct. Chem., 19, 609 – 611 (2008).

J266. M. Ponikvar and J.F. Liebman, “Paradoxes and Paradigms: Patterns and Estimation of the Entropy of Formation of Some Aqueous Complex Anions," Struct. Chem., 18, 501-508 (2008).

J265. A. Castillo, J.F. Liebman and A. Greer, “Monoradicals and Diradicals From 3- and 4-Mercaptocatechol, and 3,4-Bismercaptocatechol: A Computational Study,” J. Sulfur Chem., 29, 445-457 (2008).

J264. D. Ponomarev, V. Takhistov, S. Slayden and J. Liebman, “Thermochemistry of Organic, Elementorganic and Inorganic Species. Part XXI: Enthalpies of Formation for Bi- and Triradicals of Main Group Elements' Halogenides,” J. Mol. Struct., 876, 34-55 (2008).

J263. D. Ponomarev, V. Takhistov, S. Slayden and J. Liebman, “Thermochemistry of Organic, Elementorganic and Inorganic Species. Part XX: Enthalpies of Formation for Free Radicals of Main Group Elements' Halogenides,” J. Mol. Struct., 876, 15-33 (2008).

J262. Y.B. Tewari, D.J. Vanderah, M.M. Schantz, R.N. Goldberg, J.D. Rozzell, J.F. Liebman, R.W.-M. Hui, Y. Nissenbaum, and A.R. Parniani, “A Thermodynamic Study of Ketoreductase-Catalyzed Reactions 5. Reduction of Substituted Ketones in n-Hexane,” J. Chem.Thermodynam., 40, 661-670 (2008).

J261. M. Temprado, M.V. Roux, A.R. Parameswar, A.V. Demchenko, J.S. Chickos and J.F. Liebman, “Thermophysical Properties in Medium Temperature Range of Several Thio and Dithiocarbamates,” J. Therm. Anal. Calorim., 91, 471-475 (2008).

J260. M. Ponikvar, H.D.B. Jenkins and J.F. Liebman, “Patterns and Estimation of the Entropies of Formation of Fluorine Containing Aqueous Anions,” Struct. Chem., 18, 883-889 (2007). (This primary, invited, research paper is in honor of Neil Bartlett on the occasion of his 75th birthday.)

J259. M.A.R. Matos, V.M.F. Morais, C.C.S. Sousa, M.V. Roux, R. Notario and J.F. Liebman, “The Energetics of Naphthalene Derivatives, IV: A Calorimetric and Calculational Thermochemical Study of the Isomeric Naphthalenemethanols,” Mol. Phys., 105, 1789-1796 (2007).

J258. M.A.R. Matos, M.S. Miranda, M.J.S. Monte, L.M.N.B.F. Santos, V.M.F. Morais, J.S. Chickos, P. Umnahanant and J.F. Liebman, “Calorimetric and Computational Study of Indanones,” J. Phys. Chem. A, 111, 11152-11159 (2007).

J257. C.A. Deakyne, L.K. Norton, A.M. Abele, A.K. Ludden and J.F. Liebman, “Thermochemical Considerations and Bond Enthalpy Ratios Involving Triatomic 16-Valence Electron Neutrals and Ions and Some Isoelectronically Related Pentaatomics,” Intl. J. Mass Spectry., 267, 324-337 (2007). (This primary, invited, refereed, research paper is in a volume in memory of Sharon G. Lias, edited by John E. Bartmess and Karl K. Irikura.)

J256. M.A.R. Matos, M.S. Miranda, S.M.M. Pereira, V.M.F. Morais and J.F. Liebman, “The Experimental and Calculational Thermochemistry of 1,2,4,5-Benzenetetracarboxylic Dianhydride: Is This 10 π Multiring Species Aromatic?,” J. Phys. Chem. A, 111, 7181-7188 (2007).

J255. M. Ponikvar and J.F. Liebman, “Paradigms and Paradoxes: Patterns and Estimation of the Entropy of Formation of Hydrogen Containing Aqueous Polynuclear Oxyanions,” Struct. Chem., 19, 409-413 (2007).

J254. R. Notario, M.V. Roux, D.A. Bors and J.F. Liebman, “What is the Enthalpy of Formation of Acrylic Acid?” Struct. Chem., 18, 395-398 (2007).

J253. J.F. Liebman, Z. Varga and M. Hargittai, “Chemistry, Commentary and Community: Discussion of ‘The NaDyBr4 Complex: Its Molecular Structure and Thermodynamic Properties’ by Varga and Hargittai,” Struct. Chem., 18, 269-271 (2007).

J252. I. Hargittai and J.F. Liebman, “Editorial Commentary: Announcement of a New Column for Structural Chemistry: Chemistry, Commentary and Community,” Struct. Chem., 18, 267 (2007).

J251. Y.B. Tewari, J.F. Liebman, J.D. Rozzell, D.J. Vanderah and M.M. Schanze, “A Thermodynamic Study of Ketoreductase-Catalyzed Reactions 4. Reduction of 2-Substituted Cyclohexanones in n-Hexane,” J. Chem. Thermodynam., 39, 1090-1097 (2007).

J250. O.R. Wauchope, S. Shayka, N. Sawwan, J.F. Liebman and A. Greer, “Photocleavage of Plasmid DNA by Dibenzothiophene S-Oxide Under Anaerobic Conditions,” J. Sulfur Chem., 28, 11-16 (2007).

J249. I. Černušák, M. Čukovičová, A.A. Asiama, S.K. Gregurick, P.A. Hoover, S.C. Tsay and J.F. Liebman, “The Absolute Entropies of Alkali Metal Borides. Simple Patterns and High Level Calculations,” Coll. Czech. Chem. Commun., 72, 269-277 (2007). (This primary, invited, refereed, research paper is in honor of Jaroslav Koutecký on the occasion of his 75th birthday.)

J248. A.T. Frank, A. Adenike, D. Aebisher, A. Greer, R. Gao and J.F. Liebman, “Paradigms and Paradoxes: Energetics of the Oxidative Cleavage of Indigo and of Other Olefins,“ Struct. Chem., 18, 71-74 (2007).

J247. J.R.B. Gomes, J.F. Liebman and M.A.V. Ribeiro da Silva, “The Thermodynamics of the Isomerization of Cyanophenol and Cyanothiophenol Compounds,” Struct. Chem., 18, 15-23 (2007).

J246. M. Ponikvar and J.F. Liebman, “Paradigms and Paradoxes: Patterns and Estimation of the Entropy of Formation of Aqueous Polynuclear Oxyanions,” Struct. Chem., 17, 623-629 (2006).

J245. M.V. Roux, M. Temprado, P. Jiménez, C. Foces-Foces, R. Notario, S.P. Verevkin and J.F. Liebman “Thermochemistry of 2,5-Thiophenedicarboxylic Acid,” J. Phys. Chem. A, 110, 12477-12483 (2006).

J244. C.A. Deakyne, A.K. Corum, H.M. Thomas and J.F. Liebman, “The Structure and Energetics of [B, C, F, H2]: Simplicity Resulting in Diversity,” J. Fluor. Chem., 127, 1355-1367 (2006). (This primary, invited, refereed, research paper is in honor of Boris Žemva on the occasion of his winning the 2006 Award for Creative Work in Fluorine Chemistry given by the American Chemical Society.)

J243. I. Alkorta, J. Elguero and J.F. Liebman, “The Annular Tautomerism of Imidazoles and Pyrazoles: The Possible Existence of Non-aromatic Forms,” Struct. Chem., 17, 439-444 (2006).

J242. D. Lenoir, C. Wattenbach and J.F. Liebman, “Tetra-tert-butylethylene: Fantasy, Fake, or Reality?” Struct. Chem., 17, 419-422 (2006).

J241. A. Greer, O.R. Wauchope, N.S. Farina, P. Haberfield and J.F. Liebman, “Paradigms and Paradoxes: Mechanisms for Possible Enhanced Biological Activity of Bilaterally Symmetrical Chemicals,” Struct. Chem., 17, 347-350 (2006).

J240. H. Brand, J.F. Liebman, A. Schulz, P. Mayer and A. Villinger, “Nonlinear, Resonance-Stabilized Pseudohalides: From Alkali Methanides to Ionic Liquids of Methanides,” Eur. J. Inorg. Chem., 4294-4308 (2006).

J239. M.A.R. Matos, M.S. Miranda, V.M.F. Morais and J.F. Liebman, “Benzanilide: On the Crossroads of Calorimetry, Computations and Concepts,” Mol. Phys., 104, 2855-2860 (2006).

J238. N. Gandra, A. T. Frank, O. Le Gendre, N. Sawwan, D. Aebisher, J. F. Liebman, K. N. Houk, A. Greer and R. Gao, “Singlet Oxygen Generation from the Photolysis of Indigo Dyes in Methanol, DMSO, Water and an Ionic Liquid (1-Butyl-3-methylimidazolium—BF4), “ Tetrahedron, 62, 10771-10776 (2006). (This primary, invited, refereed, research paper is part of a special symposium-in-print on advances in singlet oxygen chemistry.)

# J237. E. Taskinen, T. Alanko and J.F. Liebman, “Relative Thermodynamic Stabilities of the Isomeric Dihydrofurans and Isomeric Dihydropyrans. An Experimental and DFT Study,” Struct. Chem., 17, 323-326 (2006).

J236. J.F. Liebman, “Paradigms and Paradoxes: A Semi-Quantitative Thermochemical Analysis of a Dearomatizing Reaction of a [1*H*-Imidazole into a Related 2*H*-Imidazole](http://newfirstsearch.oclc.org/WebZ/FSFETCH?fetchtype=fullrecord:sessionid=sp05sw09-38766-ei8xv7ot-ecrn34:entitypagenum=12:0:recno=1:resultset=10:format=FI:next=html/record.html:bad=error/badfetch.html:entitytoprecno=1:entitycurrecno=1:numrecs=1),” Struct. Chem., 17, 127-129 (2006).

J235. M. Ponikvar and J.F. Liebman, "Paradoxes and Paradigms: Observations on Pyrohydrolytic Decomposition of Fluorine-Containg Materials and Accompanying Thermochemistry,” Struct. Chem., 17, 75-78 (2006).

J234. M.A.R. Matos, M.S. Miranda, V.M.F. Morais and J.F. Liebman, “Calorimetric and Computational Study of 2*H*-1,4-Benzoxazin-3(4H)-one and of Related Species,” Mol. Phys., 104, 1833-1841 (2006).

J233. K.K. Bhasin, M.-J. Crawford, H.D.B. Jenkins, T.M. Klapötke and J.F. Liebman, “The Volume-Based Thermodynamics (VBT) and Attempted Preparation of an Isomeric Salt, Nitryl Chlorate: [NO2] [ClO3],” Z. Anorg. Allgem. Chem., 632, 697-700 (2006).

J232. Y.B. Tewari, K.W. Phinney and J.F. Liebman, “A Thermodynamic Study of Ketoreductase-Catalyzed Reactions 2. Reduction of Cycloalkanones in Non-aqueous Solvents,” J. Chem. Thermodyn., 38, 388-395 (2006).

J231. V.M.F. Morais, M.S. Miranda, M.A.R. Matos and J.F. Liebman, “Experimental and Computational Thermochemistry of Three Nitrogen-containing Heterocycles: 2-Benzimidazolinone, 2-Benzoxazolinone and 3-Indazolinone," Mol. Phys., 104, 325-334 (2006).

J230. M. Ponikvar and J.F. Liebman, “Paradoxes and Paradigms: When Do Alkali Metal (Na) and Alkaline Earth (Mg, Ca) Halides (F, Cl) Completely Dissociate? A Combined Analytical and Thermo-Chemical Approach,” Struct. Chem., 16, 587-591 (2005).

J229. A.L.L. East, K.L. Grittner, A.I. Afzal, A.G. Simpson and J.F. Liebman, “Length and Substituent-Scrambling Energies of Parent and Halogen-Substituted Conjugated Polyynes,” J. Phys. Chem. A, 109, 11424-11428 (2005). (This primary, invited, refereed, research paper is in honor of Jack Simons on the occasion of his 60th birthday.)

J228. J.F. Liebman and M. Ponikvar, “Ion Selective Electrode Determination of Free versus Total Fluoride Ion in Simple and Fluoroligand Coordinated Hexafluoropnictate (PnF6–, Pn = P, As, Sb, Bi) Salts,” Struct. Chem., 16, 521-528 (2005).

J227. H.D.B. Jenkins and J.F. Liebman, “Volume of Solid State Ions and Their Estimation,” Inorg. Chem., 44, 6359-6372 (2005).

J226. M.V. Roux, J.Z. Dávalos, P. Jiménez, R. Notario, O. Castaño, J.S. Chickos, W. Hanshaw, H. Zhao, N. Rath, J.F. Liebman, B.S. Farivar and A. Bashir-Hashemi, “Cubane, Cuneane and Their Carboxylates: A Calorimetric, Crystallographic, Calculational and Conceptual Coinvestigation,” J. Org. Chem., 70, 5461-5470 (2005).

J225. M.A.R. Matos, M.S. Miranda, N.A.B. Pinto, V.M.F. Morais, N. Dhananjaya and J.F. Liebman, “Thermochemistry of Diphenic Anhydride. A Combined Experimental and Theoretical Study,” Mol. Phys., 103, 1885-1894 (2005).

J224. A.D. Gudmundsdottir and J.F. Liebman, “The Energetics of N-Acylimines,” Struct. Chem., 16, 155-157 (2005).

J223. A. Fattahi, S.R. Kass, J.F. Liebman, M.A.R. Matos, M.S. Miranda and V.M.F. Morais, “The Enthalpies of Formation of *o*-, *m*-and *p*-Benzoquinone: Gas-Phase Ion Energetics, Combustion Calorimetry and Quantum Chemical Computations Combined,” J. Am. Chem. Soc., 127, 6116-6122 (2005).

J222. M.V. Roux, P.J. Smith and J.F. Liebman, “Thoughts on the Enthalpy of Formation of Guanidine and its Monosubstituted Derivatives,” Struct. Chem., 16, 73-75 (2005).

J221. M.A.R. Matos, M.S. Miranda, V.M.F. Morais and J.F. Liebman, “Saccharin: A Combined Experimental and Computational Thermochemical Investigation of a Sweetener and Sulfonamide,” Mol. Phys., 103, 221-228 (2005). (This primary, invited, research paper is in honor of Nicholas D. Handy on the occasion of his 65th birthday.)

J220. Z.S. Herman and J.F. Liebman, “Where are the Angles? Angular Dependence (and Independence) of Orbitals and Functions,” Intl. J. Quantum Chem., 101, 283-286 (2005).

J219. A. Bashir-Hashemi,J.S. Chickos, W. Hanshaw, H. Zhao, B.S. Farivar and J.F. Liebman, “The Enthalpy of Sublimation of Cubane,” Thermochim. Acta, 424, 91-97 (2004).

J218. R. Vianello, J.F. Liebman and Z.B. Maksić, “In Search of Ultrastrong Brønsted Neutral Organic Superacids – A DFT Study of Some Cyclopentadiene Derivatives,” Eur. Chem. J., 10, 5751-5760 (2004).

J217. D.W. Rogers, N. Matsunaga,F.J. McLafferty, A.A. Zavitsas and J.F. Liebman, “On the Lack of Conjugation Stabilization in Polyalkynes,” J. Org. Chem., 69, 7143-7147 (2004).

J216. H.D.B. Jenkins, L. Glasser, T.M. Klapötke, M.-J. Crawford, K.K. Bhasin, J. Lee, G.J. Schrobilgen, L.S. Sunderlin and J.F. Liebman, “The Ionic Isomegethic Rule and Additivity Relationships: Estimation of Ion Volumes — A Route to the Energetics and Entropics of New, Traditional, Hypothetical and Counterintuitive Ionic Materials,” Inorg. Chem., 43, 6238-6248 (2004).

J215. M. Ponikvar and J.F. Liebman, “Aqueous Polynuclear Oxyanions of Sulfur and Homologous Series,” Struct. Chem., 15, 539-542 (2004).

J214. M. Ponikvar,J.F. Liebman and H.D.B. Jenkins, “The Redox Chemistry of SbF6– Ion,” Eur. J. Inorg. Chem., 3273-3276 (2004).

J213. B.L. Kormos, J.F. Liebman and C.J. Cramer,“298 K Enthalpies of Formation of Monofluorinated Alkanes: Theoretical Predictions for Methyl, Ethyl, Isopropyl and *tert*–Butyl Fluoride,” J. Phys. Org. Chem., 17, 656-664 (2004).

J212. M.A.R. Matos, M.S. Miranda, V.M.F. Morais and J.F. Liebman, “Aspects of the Aromaticity of Anthranil,” Eur. J. Org. Chem., 3340-3345 (2004).

J211. V.M.F. Morais, M.A.R. Matos, M.S. Miranda and J.F. Liebman, “The Energetics of Isomeric Benzoxazine Diones: Isatoic Anhydride Revisited,” Org. Biomol. Chem., 2, 1647-1650 (2004).

J210. R. Notario, M.V. Roux and J.F. Liebman, “The Energetics of the Isomeric Anthrols,” Mol. Phys., 102, 623-625 (2004).

J209. V.M.F. Morais, M.A.R. Matos, M.S. Miranda and J.F. Liebman, “Surprises with Strain Energy and Sulpholane (Tetrahydrothiophene 1,1-Dioxide): A Combined Experimental and Theoretical Investigation,” Mol. Phys., 102, 525-530 (2004).

J208. M.A.R. Matos, M.S. Miranda, D.V.S.S. Martins, N.A.B. Pinto, V.M.F. Morais and J.F. Liebman, “Thermochemistry of Biphenylcarboxylic and Dicarboxylic Acids. A Combined Experimental and Theoretical Study,” Org. Biomol. Chem., 2, 1353-1358 (2004).

J207. M. Ponikvar, B. Sedej and J.F. Liebman, “The Solid-State Lanthanoid Assisted Hydrolysis of the Solvolytically ‘Inert’ AsF6– Ion,” Eur. J. Inorg. Chem., 1349-1352 (2004).

J206. I. Černušák, S.K. Gregurick, M. Roswell, C.A. Deakyne, H.D.B. Jenkins and J.F. Liebman, “Additivity of Absolute Entropies,” Coll. Czech. Chem. Commun., 69, 213-230 (2004). (This primary, invited, refereed research paper is in honor of Rudolf Zharadnik on the occasion of his 75th birthday.)

J205. R.S. Hosmane and J.F. Liebman, “Resonance Stabilization in Diazophenoxides (Quinone Diazides),” Struct. Chem., 15, 253-255 (2004).

J204. J.F. Liebman, “The Solubility of AgCl in Water: Some Thermochemical Issues of Aqueous Ag+  Ion,” Struct. Chem., 15, 165-168 (2004).

J203. M.V. Roux, M. Temprado, R. Notario, S.P. Verevkin, V.N. Emel’yanenko, D.E. DeMasters and J.F. Liebman, “The Energetics of Naphthalene Derivatives, III: Phenylacetic Acid and the Isomeric 1- and 2-Naphthylacetic Acids,” Mol. Phys., 102, 1909-1917 (2004).

J202. S.P. Verevkin, M.V. Roux, R. Notario, D.E. DeMasters and J.F. Liebman, “The Energetics of Naphthalene Derivatives, II: The Isomeric 1- and 2-Naphthyl Acetates,” Mol. Phys., 101, 3231–3237 (2003).

J201. M. Mahavadi, D.N. Zeiger, D. Naqib, M.V. Roux, R. Notario and J.F. Liebman, “The Strain Energy of Perchlorocyclopropane is Small: It Might Even Be Negative. A Density Functional Theory Study of Perhalocycloalkanes,” Intl. J. Quantum Chem., 95, 784-790 (2003). (This primary, invited, research paper is in honor of Leland C. Allen on the occasion of his 75th birthday.)

J200. C.A. Deakyne, L. Li, W. Zheng, D. Xu and J.F. Liebman, “Regularities in the Bond Dissociation Enthalpies of Molecules of Type AB and BAB: Energetics of 10- and 16-Valence Electron Ions of Groups 13, 15 and 16,” Intl. J. Quantum Chem., 95, 713-718 (2003). (This primary, invited, research paper is in honor of Leland C. Allen on the occasion of his 75th birthday.)

J199. M. Ponikvar, B. Žemva and J.F. Liebman, “The Analytical and Descriptive Inorganic Chemistry of the Hydrolysis of Hexafluoropnictate Ions, PnF6– (Pn = P, As, Sb, Bi),” J. Fluor. Chem., 123, 217-220 (2003).

J198. M.A.R. Matos, M.S. Miranda, V.M.F. Morais and J.F. Liebman, “Thermochemistry of (E)- and (Z)-Alkene Species: A Combined Experimental and Theoretical Investigation on the Isomeric Dimethyl Fumarate and Dimethyl Maleate,” J. Org. Biomol. Chem., 1, 2930–2934 (2003).

J197. M.A.R. Matos, M.S. Miranda, V.M.F. Morais and J.F. Liebman, “Are Isatin and Isatoic Anhydride Antiaromatic and Aromatic Respectively? A Combined Experimental and Theoretical Investigation,” J. Org. Biomol. Chem., 1, 2566-2571 (2003).

J196. J.S. Chickos, D.M. Hillesheim, S.P. Verevkin, M.V. Roux, M. Temprado, M. Segura, R. Notario, D.E. DeMasters and J.F. Liebman, “The Energetics of the Isomeric 1- and 2-Naphthoic Acids: Context, Quantum Chemical Calculations and Thermochemical Measurements,” Mol. Phys., 101, 1311-1318 (2003). (This primary research, refereed, invited article is in honor of W.G. Richards.)

J195. M.V. Roux, P.Jiménez, J.Z. Dávalos, M. Temprado and J.F. Liebman, “Destabilization in the Isomeric Nitrobenzonitriles: An Experimental Thermochemical Study,” J. Chem. Thermodyn., 35, 803-811 (2003).

J194. D.W. Rogers, N. Matsunaga, A. A. Zavitsas, F. J. McLafferty and J.F. Liebman, “The Conjugation Stabilization of 1,3-Butadiyne is Zero,” Org. Lett., 5, 2373-2375 (2003).

J193. H.M. Perks and J.F. Liebman, “Accidental Degeneracies, II: Suppose the 3p and 3d Orbitals Were Closer in Energy: How Would Biochemistry be Different?” Struct. Chem., 14, 421-423 (2003).

J192. H.M. Perks and J.F. Liebman, “Accidental Degeneracies, I: Suppose the 2s and 2p Orbitals Were Closer in Energy: How Would Organic Chemistry be Different?” Struct. Chem., 14, 417-419 (2003).

J191. C.A. Deakyne, L. Li and J.F. Liebman, “The Structure and Energetics of [B, C, F, H3]+: Quantum Chemistry Shows Multiple Minima,” Intl. J. Mass Spectry., Ion Proc., 227, 555-561 (2003). (This invited, refereed, research article is in a special issue of this journal entitled “Thermochemistry and Solvation of Gas Phase Ions” edited by T.B. McMahon.)

J190. S. Perişanu, J. Constantineau, M.D. Banciu, J.F. Liebman, B.S. Farivar, M.A. Mullan, J.S. Chickos, N. Rath and D.M. Hillesheim, “The Enthalpies of Formation of Two Dibenzocyclooctadienones,” Thermochim. Acta, 400, 109-120 (2003).

J189. J.P.Toscano, C.A. Deakyne and J.F. Liebman, “Energetics of Aqueous Oxyanions of Nonmetals and Metalloids,” Struct. Chem., 14, 315-320 (2003).

J188. I. Fishtik, R. Datta and J.F. Liebman, “Group Additivity Methods in Terms of Response Reactions,” J. Phys. Chem. A, 107, 2334-2342 (2003).

J187. I. Fishtik, R. Datta and J.F. Liebman, “Response Reactions: A Mathematical Well-Defined Way to Obtain Accurate Thermochemistry from Ab Initio Calculations,” J. Phys. Chem. A, 107, 695-705 (2003).

J186. R.S. Hosmane and J.F. Liebman, “Diazomethane and Ethyl Diazoacetate: The Role of Substituent

Effects on Stability,” Struct. Chem., 13, 501-503 (2002).

J185. B. Kovačević, J.F. Liebman and Z.B. Maksić, “Nibbering’s C7H7N: An Ab Initio Study of the Structure and Electronic Properties of Benzaldimine and its Protonated Ion,” J. Chem. Soc., Perkin Trans. 2, 1544-1548 (2002).

J184. E.D. Balighian and J.F. Liebman, “How Anomalous are the Anomalous Properties of Fluorine? Ionization Energy and Electron Affinity Revisited,” J. Fluor. Chem., 116, 35-39 (2002).

J183. M.V. Roux, M. Temprado, J.Z. Dávalos, P. Jiménez, R.S. Hosmane and J.F. Liebman, “Enthalpy of Formation of Methyl Benzoate: Calorimetry and Consequences,” Phys. Chem. Chem. Phys., 4, 3611-3613 (2002).

J182. C.A. Deakyne, L. Li, W. Zheng, D. Xu and J.F. Liebman, “Regularities in the Bond Dissociation Enthalpies of Molecules of Type AB and BAB Energetics of Compounds of Groups 14 and 16,” J. Chem. Thermodyn., 34, 185-192 (2002). (This invited, refereed, research article is in honor of Patrick A.G. O’Hare on the occasion of his 65th birthday. A poem of mine, “Ode to Pat O’Hare” also appeared in the frontsmatter of this journal issue.)

J181. H.P. Diogo, T. Kiyobayashi, M.E. Minas da Piedade, N. Burlak, D.W. Rogers, D. McMasters, G. Persy, J. Wirz and J.F. Liebman, “The Aromaticity of Pyracylene: An Experimental and Computational Study of the Energetics of the Hydrogenation of Acenaphthylene and Pyracylene,” J. Am. Chem. Soc., 124, 2065-2075 (2002).

J180. S. Parthiban, J.M.L. Martin and J.F. Liebman, “The Heat of Formation of the Haloacetylenes XCCY [X, Y = H, F, Cl]: Basis Set Limit Ab Initio Results and Thermochemical Analyses,” Mol. Phys., 100, 453-464 (2002). (This invited, refereed, research article is in honor of Ernest R. Davidson on the occasion of his 65th birthday.)

J179. M.V. Roux, R. Notario, D.N. Zeiger and J.F. Liebman, “Strainless Reference States for Poly- and Perfluorocycloalkanes: The Ultradiagonal Strain Energy Approach,” J. Fluor. Chem., 112, 91-94 (2001). (This invited, refereed, research article is part of the special issue of selected talks from the 15th Winter Fluorine Meeting, special editors G.B. Hammond and E. Winiarz.)

J178. M.A.V. Ribeiro da Silva, M.D.M.C. Ribeiro da Silva, L.C.M. da Silva, F. Dietze, E. Hoyer, L. Beyer, B. Schröder, A.M. Damas and J.F. Liebman, “Synthesis, Characterization and Thermochemical Properties of N-acyl-N’,N’-diethylthioureas,” J. Chem. Soc., Perkin Trans. 2, 2174-2178 (2001).

J177. G. DeOliveira, J.M.L. Martin, I.K.C. Silwal and J.F. Liebman, “Definitive Heat of Formation of Methylenimine, CH2NH and of Methylenimmonium Ion, CH2NH2+ by Means of W2 Theory.,” J. Comput. Chem., 22, 1297-1305 (2001). (This invited, refereed, research article is in honor of Paul v.R. Schleyer on the occasion of his 70th birthday.)

J176. H.M. Perks and J.F. Liebman, “Common and Maximum Accessible Oxidation States of the Elements,” Struct. Chem., 12, 197-199 (2001).

J175. J.F. Liebman, I. Černušák and A. Miková, “Divalent Boron and Phosphorus: HBCN- and HPCN- Case Study,” Intl. J. Quantum Chem., 84, 140-148 (2001).

J174. A. Skancke and J.F. Liebman, “Tetrazines and Tetraphosphorins, Tetrazoles and Tetraphospholes: A Density Functional Theory Study,” J. Mol. Struct., 567/568, 59-65 (2001). (This invited, refereed, research article is in honor of Marit Trætteberg on the occasion of her 70th birthday.)

J173. M. Trætteberg, L.S. Khaikin, O.E. Grikina, J.F. Liebman and M. Hulce, “Structure, Spectra and Intramolecular Motions of 1,4-Bis(trimethylsilyl)-1,3-butadiyne: An Electron Diffraction Study Using the Results of Spectral Analysis Based on Scaled Quantum-Chemical Force Field for Calculating Vibrational Effects,” J. Mol. Struct. 559, 295-313 (2001).

J172. H.M. Perks and J.F. Liebman, “Electronegativity and Bond Energies - Living Legacies of Linus and Lee,” Struct. Chem., 11, 375-378 (2000).

J171. D.N. Zeiger and J.F. Liebman, “The Strain Energy of Fluorinated Cyclopropanes: Quantum Chemical Realization of Homodesmotic, Diagonal and Ultradiagonal Approaches,” J. Mol. Struct., 556, 83-94 (2000). (This invited, refereed, research article is in honor of N.L. (“Lou”) Allinger on the occasion of his 70th birthday.)

J170. H.M. Perks and J.F. Liebman, “Estimation of the Enthalpies of Formation of Some Common, Solid-Phase Compounds of Considerable Theoretical Importance,” Struct. Chem., 11, 325-329 (2000).

J169. H.M. Perks and J.F. Liebman, “Aspects of the Energetics of Carboxylic Acids and their Anhydrides,” Struct. Chem., 11, 265-269 (2000).

J168. J.F. Liebman, “Exothermicity of Some Reactions Involving the Noble Gas Fluorides and Oxides,” Struct. Chem., 11, 261-263 (2000).

J167. P.S. Woodcock and J.F. Liebman, “Energy Levels and Orbitals of the Simplest Clusters in N-Dimensions,” Struct. Chem., 11, 173-176 (2000). (This invited, refereed, research article is for a special issue of this journal on the occasion of Lev Vilkov’s 70th birthday and the 70th anniversary of electron diffraction.)

J166. M.V. Roux, P. Jiménez, J.Z. Dávalos, M.A. Martin-Luengo, V.M. Rotello, A.O. Cuello and J.F. Liebman, “The Plausible Aromaticity of 1,8-Naphthalimides: The Enthalpy of Formation of N-Methyl-1,8-Naphthalimide,” Struct. Chem., 11, 1-7 (2000).

J165. A. Pappová, I. Černušák, M. Urban and J.F. Liebman, “MBPT and DFT Study of Hydrogen Cyanide Borane(1) Oligomers and Dehydrogenated Analogs,” J. Phys. Chem. A., 104, 5810-5816 (2000).

J164. M.-J. Crawford, T. M. Klapötke and J.F. Liebman, “The Isomers and Energetics of the Nitrosamines F2N2O, H2N2O: A Computational and Conceptual Study, J. Fluor. Chem., 102, 119-124 (2000). (This primary research, invited, refereed, research article is in honor of Paul Tarrant on the occasion of his 85th birthday.)

J163. J.Z. Dávalos, H. Flores, P. Jiménez, R. Notario, M.V. Roux, E. Juaristi, R.S. Hosmane and J.F. Liebman, “Calorimetric, Computational (G2(MP2) and G3) and Conceptual Study of the Energetics of the Isomeric 1,3- and 1,4-Dithianes,” J. Org. Chem., 64, 9328-9336 (1999).

J162. O. Mó, M. Yáñez, M.V. Roux, P. Jiménez, J.Z. Dávalos, M.A.V. Ribeiro da Silva, M.D.M.C. Ribeiro da Silva, M.A.R. Matos, L.M.P.F. Amaral, A. Sánchez-Migallón, P. Cabildo, R. Claramunt, J. Elguero and J.F. Liebman, “Enthalpies of Formation of N-Substituted Pyrazoles and Imidazoles,” J. Phys. Chem., A103, 9336-9344 (1999). (Errata: J. Phys. Chem. A117, 10569 (2013).)

J161. J.F. Liebman, K. Nyman-Petersen and P.N. Skancke, “Computational Study of Ring Strain in 1,3,2-Dioxathiolane, its 2-Oxide and its 2,2-Dioxide,” Acta Chem. Scand., 53, 1003-1008 (1999).

J160. J.F. Liebman and S. Scheiner, “Does Thermochemical Mimicry Extend to Gibbs Energies? The Differences of K+ and NH4+ and of Na+ and H3O+,” Struct. Chem., 10, 391-392 (1999).

J159. J.F. Liebman, “Are Acyl Azides Resonance Stabilized?” Struct. Chem., 10, 327-329 (1999).

J158. C.A. Deakyne, D.M. Knuth, M. Meot-Ner (Mautner), C.M. Breneman and J.F. Liebman, “Experimental and Theoretical Study of the Energetics of Trialkylsulfonium Ions,” J. Mol. Struct., 485/486, 33-41 (1999). (This invited, refereed, research article is in honor of Lawrence S. Bartell on the occasion of his 75th birthday.)

J157. A. Skancke and J.F. Liebman, “The Energetics of Cyclopropene, I,4-Cyclohexadiene and Some of Their Hetero- and/or Exocyclic Derivatives,” J. Org. Chem., 64, 6361-6365 (1999).

J156. M. Adamczeski, Z. Zhang, K. Tomioka, K. Byrne and J.F. Liebman, “Exact Computer Solutions to Derive the Hydration Equilibria Constants and Molar Refractions of Carbonyl Compounds from Refractive Index and Density Measurements: A Thermochemical Study, Part 2,” American Laboratory, 31 (6) 38, 40, 42, 44, 46, 48, 50, 52 (1999).

J155. M. Adamczeski, Z. Zhang, K. Tomioka, K. Byrne and J.F. Liebman, “Exact Computer Solutions to Derive the Hydration Equilibria Constants and Molar Refractions of Carbonyl Compounds from Refractive Index and Density Measurements: A Thermochemical Study, Part 1,” American Laboratory, 31 (5), 76C, 78C, 80C, 82C, 84C, 86C, 87C, 89C (1999).

J154. A. Skancke, S.W. Slayden and J.F. Liebman, “Thermodynamic Reference States and Thermochemical Preference States: What do We Choose for Sulfur and Phosphorus?” Struct. Chem., 9, 429-430 (1998).

J153. D.W. Rogers, Y. Zhao, M. Trætteberg, M. Hulce and J. Liebman, “Enthalpies of Hydrogenation and Formation of Enones: Resonance Energies of 2-Cyclopentenone and 2-Cyclohexenone,” J. Chem. Thermodyn., 30, 1393-1400 (1998).

J152. E.P. Hunter, S.G. Lias, C.M. Rooney, J.L. Winstead and J.F. Liebman, “The ‘Thermochemical Mimicry’ of Phenyl and Vinyl Groups: Can It Be Extended to Charged Species?” Intl. J. Mass Spectry. Ion Proc., 179/180, 261-266 (1998). (This invited, refereed, research article is in homage of Fulvio Cacace.)

J151. J.F. Liebman, H.L. Paige and J. Passmore, “Why Aren’t There Any Trioxygenyl or Ozonium Salts? Or, Why Does Our Reaction of O3 and PtF6 Give O2PtF6?” Struct. Chem., 9, 315-317 (1998).

J150. A. Skancke, R.S. Hosmane and J.F. Liebman, “Unification of Some Literature Models of Aromaticity: A Calculational and Conceptual Study of a Set of One-Ring Species,” Acta Chem. Scand., 52, 967-974 (1998).

J149. J.F. Liebman and S.T. Purrington, “Some Thoughts on Hydrogen Fluoride Traps in Fluorine Bomb Calorimetry,” Struct. Chem., 9, 237-238 (1998).

J148. I. Černušák and J.F. Liebman, “Calculational and Conceptual Study of Cyano Derivatives of Diborane and Their Iso-analogs,” Mol. Phys., 94, 147-155 (1998).

J147. A. Skancke and J.F. Liebman, “Structures and Energies of Isomers of Si2BH5 - a Computational Study,” J. Mol. Struct., 445, 29-34 (1998). (This invited, refereed, research article is in memory of O. Bastiansen.)

J146. M.V. Roux, P. Jiménez, J.Z. Dávalos, C. Turrión, H.Y. Afeefy and J.F. Liebman, “Enthalpies of Formation of Methyl Benzenecarboxylates,” J. Chem. Soc. Faraday Trans., 94, 887-890 (1998).

J145. M. Trætteberg, J.F. Liebman, M. Hulce, A.A. Bohn and D.W. Rogers, “Extended Conjugation in Enynones, Dienones and Related Species. A Theoretical and Experimental Study. The Molecular Structures of 2-Methyl-3-ethynyl-2-cyclopentenone, 2-Methyl-3-ethenyl-2-cyclopentenone and 2-Methyl-3-ethyl-2-cyclopentenone, as Studied by Gas Electron Diffraction,” J. Chem. Soc. Perkin Trans., 2, 1925-1932 (1997).

J144. R.A. Caldwell, J.F. Liebman, D.W. Rogers and D.J. Unett, “Enthalpies of Hydrogenation and of Formation of 1-Phenylcycloalkenes,” J. Mol. Struct., 413/414, 575-578 (1997). (This primary research, invited, refereed article is in honor of K. Kuchitsu on the occasion of his 70th birthday. This special issue was edited by J. Laane).

J143. J.F. Liebman, “Some Thoughts on the Solubility of Carbon Dioxide and Silicon Dioxide in Water,” Struct. Chem., 8, 379-381 (1997).

J142. J.F. Liebman, “Existence and Estimated Enthalpies of Formation of Ammonium Hydroxide, Hydronium Amide and Some Related Species,” Struct. Chem., 8, 313-315 (1997).

J141. J.F. Liebman and A. Skancke, “The Energetics and Structures of Some Highly Unsaturated Alicyclic Hydrocarbons and their Derivatives,” Mol. Phys., 91, 471-482 (1997). (This invited, refereed, research article is in honor of J.A. Pople on the occasion of his 70th birthday).

J140. M.V. Roux, P. Jiménez, M.A. Martin-Luengo, J.Z. Dávalos, Z. Sun, R.S. Hosmane and J.F. Liebman, “The Elusive Antiaromaticity of Maleimides and Maleic Anhydride: Enthalpies of Formation of N-Methylmaleimide, N-Methylsuccinimide, N-Methylphthalimide and N-Benzoyl-N-methylbenzamide,” J. Org. Chem., 62, 2732-2737 (1997).

J139. K.-H. Su, C.A. Deakyne and J.F. Liebman, “G2 Prediction of the Enthalpies of Formation for Some Diatomic Cations and Neutrals,” Chin. J. At. Mol. Phys., 14, 136-140 (1997).

J138. J.F. Liebman, “The Difference of the Enthalpies of Formation of Disulfides and Corresponding Monosulfides,” Struct. Chem., 8, 85-89 (1997).

J137. J.S. Chickos, R. Sabbah, S. Hosseini and J.F. Liebman, “The Sublimation Enthalpy of Dimethyl

Oxalate,” Struct. Chem., 7, 391-395 (1996). (This special issue was edited by M.V. Roux, P. Jiménez and D.R. Kirklin).

J136. M.A.V. Ribeiro da Silva, M.D.M.C. Ribeiro da Silva, M.F.B.M. Monteiro, M.L.A.C.N. Gomes, J.S. Chickos, A.P. Smith and J.F. Liebman, “Thermochemical Studies for Determination of the Molar Enthalpy of Formation of Aniline Derivatives,” Struct. Chem., 7, 367-373 (1996). (This special issue was edited by M.V. Roux, P. Jiménez and D.R. Kirklin.)

J135. D.R. Kirklin, J.S. Chickos and J.F. Liebman, “Enthalpy of Formation of Triphenylphosphine Sulfide,” Struct. Chem., 7, 355-361 (1996). (This special issue was edited by M.V. Roux, P. Jiménez and D.R. Kirklin.)

J134. K.-H. Su, C.A. Deakyne and J.F. Liebman, “Systematic Discrepancy of the Enthalpies of Formation Between the G2 Theoretical and the Experimental Values for O2+, Cl2+, HF+, ClF+, ClO+, PS, SF and ClF Diatomic Species,” Chin. J. At. Mol. Phys., 13, 522-526 (1996).

J133. A. Pappová, C.A. Deakyne, A. Skancke, I. Černušák and J.F. Liebman, “Complexes of Borane (1) [BH] and HBCN-, HBCO, HBCF+: A Calculational and Conceptual Study,” Mol. Phys., 89, 247-265 (1996). (This invited, refereed, research article is in honor of A. David Buckingham on the occasion of his 65th birthday.)

J132. J.F. Liebman, “Problems in the Measurement of the Enthalpies of Formation of Organic and Organometallic Compounds: Does Fluorine Bomb Calorimetry Provide an Answer?” Struct. Chem., 7, 301-302 (1996).

J131. J.F. Liebman and P.N. Skancke, “Evaluation of Strain in Heterosiliranes: Systematics, Surprises and Problems,” Intl. J. Quantum Chem., 58, 707-715 (1996). (This invited, refereed, research article is in honor of J.P. Dahl on the occasion of his 60th birthday. This special issue was edited by J. Avery.)

J130. M. Meot-Ner (Mautner), L.W. Sieck, J.F. Liebman and S. Scheiner, “Complexing of the Ammonium Ion by Polyethers. Comparative Complexing Thermochemistry of the Ammonium, Hydronium and Alkali Ions,” J. Phys. Chem., 100, 6445-6450 (1996).

J129. K.K. Irikura, M. Meot-Ner (Mautner), L.W. Sieck, A.D. Fant and J.F. Liebman, “Protonated Para-Benzoquinone,” J. Org. Chem., 61, 3167-3171 (1996) (+ 15 Supplemental sheets).

J128. A. Skancke, D. Van Vechten, J.F. Liebman and P. Skancke, “Strain Energy of Three-Membered Rings: A New Ultradiagonal Definition as Applied to Silicon and Carbon-Containing Species,” J. Mol. Struct., 376, 461-468 (1996). (This invited, refereed, research article is in honor of James E. Boggs on the occasion of his 75th birthday. This special issue was edited by J.R. Durig, A.J. Barnes and W.J. Orville-Thomas.)

J127. C.S. Weisbecker and J.F. Liebman, “How Many Bonds are There in Diatomic Fluorine and Chlorine?” Struct. Chem., 7, 85-86 (1996).

J126. Z. Zhang, P.S. Monks, L.J. Stief, J.F. Liebman, R.E. Huie, S.-C. Kuo and R.B. Klemm, “Experimental Determination of the Ionization Energy of IO(X2Π3/2) and Estimations of ΔfHo0(IO+) and PA(IO),” J. Phys. Chem., 100, 63-68 (1996).

J125. K.-H. Su, C.A. Deakyne and J.F. Liebman, “G2 Calculations and Assessment of the Atomization Energies, Electronic Affinities and Ionization Potentials for Some Small Molecules,” Wuli Huexue Xuebao, (Acta Physico-Chimica Sinica), 11, 865-869 (1995).

J124. P.S. Monks, L.J. Stief, D.C. Tardy, J.F. Liebman, Z. Zhang, S.-C. Kuo and R.B. Klemm, “A Discharge Flow-Photoionization Mass Spectrometric Study of HOI: Photoionization Efficiency and Ionization Energy,” J. Phys. Chem., 99, 16566-16570 (1995).

J123. T. Su, G.B. Hammond, R.A. Morris, A.A. Viggiano, J.F. Paulson, J.F. Liebman and A.C.L. Su, “Gaseous Ion-Molecule Reactions of F-, CF3-, C2F5-, CF3+ and C2F5+ with Hexafluoropropene Oxide,” J. Fluor. Chem., 74, 149-157 (1995).

J122. A. Greenberg, H.-J. Hsing and J.F. Liebman, “Aziridinone and 2-Azetidinone and their Protonated Structures: An Ab Initio Molecular Orbital Study Making Comparisons with Bridgehead Bicyclic Lactams and Acetamide,” J. Mol. Struct. (Theochem), 338, 83-100 (1995). (This invited, refereed, research article commemorates the 120th anniversary of the tetrahedral carbon atom. This special issue was edited by Z. Maksić and W.J. Orville-Thomas.)

J121. D.J. Berger, P.P. Gaspar and J.F. Liebman, “π-Overlap, Pyramidalization and Protonation of Group 15 Heterocycles: The Basicity of the ‘Higher Pyridines’,” J. Mol. Struct. (Theochem), 338, 51-70 (1995). (Thisinvited, refereed, research article commemorates the 120th anniversary of the tetrahedral carbon atom. A poem of mine, “Ode to Van’t Hoff and LeBel” appeared in the frontsmatter of this special journal issue. This special issue was edited by Z. Maksić and W.J. Orville-Thomas.)

J120. J.S. Chickos, D.G. Hesse, S. Hosseini, J.F. Liebman, G.D. Mendenhall, S.P. Verevkin, K. Rakus, H.-D. Beckhaus and C. Rüchardt, “Vaporization Enthalpies of Some Highly Branched Hydrocarbons,” J. Chem. Thermodyn., 27, 693-705 (1995).

J119. J.F. Liebman and E.H. Mørkved, “Resonance in Aromatic and Heteroaromatic o-Dicarboxylic Acids, Their Anhydrides and Imides,” Struct. Chem., 6, 207-209 (1995).

J118. R.A. Morris, A.A. Viggiano, S.T. Arnold, J.F. Paulson and J.F. Liebman, “Reactions of Atmospheric Ions with Selected Hydrofluorocarbons,” J. Phys. Chem., 99, 5992-5999 (1995).

J117. M. Trætteberg, P. Bakken, J.F. Liebman and M. Hulce, “The Interaction between Silyl Groups and Acetylenes,” J. Mol. Struct., 346, 101-109 (1995). (This primary research, invited, refereed article is in honor of K. Hedberg on the occasion of his 75th birthday.)

J116. J.-L.M. Abboud, P. Jiménez, M.V. Roux, C. Turrión, C. Lopez-Mardomingo, A. Podosenin, D.W. Rogers and J.F. Liebman, “Interrelations of the Energetics of Amides and Olefins: The Enthalpies of Formation of N,N-Dimethyl Derivatives of Pivalamide, 1-Adamantylcarboxamide and Benzamide and of Styrene and Its α-, Trans-β- and β,β-Methylated Derivatives,” J. Phys. Org. Chem., 8, 15-25 (1995).

J115. J.F. Liebman, J.A. Martinho Simes and S.W. Slayden, “The Enthalpy of Formation of Methyl Fluoride,” Struct. Chem., 6, 65-69 (1995).

J114. A. Skancke and J.F. Liebman, “Carbonyl Compounds of Boron and Their Isomers,” J. Phys. Chem., 98, 13215-13220 (1994).

J113. A.S. Hyman, L.H. Ladon and J.F. Liebman, “The Entropy Term in Isodesmic, Association and Conformational Equilibration Reactions,” Struct. Chem., 5, 399-401 (1994).

J112. J.F. Liebman, D. Van Vechten and A. Haaland, “The Energetics of Ions, Atoms and Salts: Sodium

and Its Chloride,” Struct. Chem., 5, 341-343 (1994).

J111. J.F. Liebman, “When is Oxygen a Metal?,” Struct. Chem., 5, 205-206 (1994).

J110. S.-C. Kuo, Z. Zhang, R.B. Klemm, J.F. Liebman, L.J. Stief and F.L. Nesbitt, “Photoionization of Hydroxymethyl (CD2OH and CD2OD) and Methoxy (CD3O) Radicals: Photoion Efficiency Spectra, Ionization Energies and Thermochemistry,” J. Phys. Chem., 94, 4023-4026 (1994).

J109. M. Colomina, C. Turrión, P. Jiménez, M.V. Roux and J.F. Liebman, “What are the Relative Steric Demands of Carboxyl and Methyl Groups?,” Struct. Chem., 5, 141-143 (1994).

J108. D.L. Kunkel, A.D. Fant and J.F. Liebman, “The Energetics of Fluorinated Species, Estimation, Enthalpies of Formation and Electronegativity,” J. Mol Struct., 300, 509-517 (1993).

J107. C.L. Bumgardner and J.F. Liebman, “Considerations of the Mechanism of Reductive Deamination of Primary Amines with HNF2,” J. Fluor. Chem., 65, 7-9 (1993).

J106. J.S. Chickos, S. Hosseini and J.F. Liebman, “A Group Additivity Approach for the Estimation of Vapor Pressures of Liquid Hydrocarbons from 298 to 500 K, J. Org. Chem., 58, 5345-5350 (1993) (+ 22 Supplemental sheets).

J105. J.S. Chickos, S. Hosseini, D.G. Hesse and J.F. Liebman, “Heat Capacity Corrections to a Standard State. A Comparison of New and Some Literature Methods for Organic Liquids and Solids,” Struct. Chem., 4, 271-278 (1993).

J104. J.S. Chickos, D.G. Hesse and J.F. Liebman, “A Group Additivity Approach for the Estimation of Heat Capacities of Organic Liquids and Solids at 298K,” Struct. Chem., 4, 261-269 (1993).

J103. D.W. Rogers, A. Pododensin and J.F. Liebman, “Stabilization in Ground State Tropilidine and Tropone,” J. Org. Chem., 58, 2589-2592 (1993).

J102. A. Skancke and J.F. Liebman, “The Isomeric Structures of B3H5 and Derived All-Boron Containing Group Increments,” J. Mol. Struct. (Theochem), 280, 75-82 (1993).

J101. J.F. Liebman and A. Skancke, “B4H62− New Low Symmetry Structures for Triborylborane Dianion,” J. Mol. Struct. (Theochem), 280, 67-73 (1993).

J100. J.F. Liebman, “The Relative Conjugation Energies of Dienes and α-Diketones,” Struct. Chem., 3, 449-450 (1992).

J99. C.A. Deakyne, K.K. Brown, C.S. Pacini, D.C. Pohlman, D.N. Gray and J.F. Liebman, “Isoelectronic and Isogyric Reactions. II. Diatomic Oxides and Sulfides,” J. Mol. Struct. (Theochem), 260, 395-418 (1992). (This invited, refereed, research article is part of the special issue “Valence and the Chemical Bond” in homage to C.A. Coulson, special editors R.B. Mallion, R. McWeeny and W.J. Orville-Thomas.)

J98. A. Skancke and J.F. Liebman, “Boron Versus Carbon: Conjugation, Hyperconjugation and Rotational Barriers in the 'Neoclassical' Boron Hydride, Triborylborane [B(BH2)3] and its Dianion,” J. Mol. Struct. (Theochem), 259, 411-429 (1992). (This invited, refereed, research article is part of the special issue “Valence and the Chemical Bond” in homage to Charles A. Coulson, special editors R.B. Mallion, R. McWeeny and W.J. Orville-Thomas.)

J97. S. Eldin, J.F. Liebman, L.D. Reynolds and P. Dowd, “Design of Molecules with High π-Orbital Degeneracies,” Tetrahedron Lett., 33, 4525-4528 (1992).

J96. R.S. Hosmane and J.F. Liebman, “Aromaticity of Five-Membered Heterocycles: An Experimentally Convenient Theoretical Model for Prediction of Relative Aromaticity,” Tetrahedron Lett., 33, 2303-2306 (1992).

J95. J.S. Chickos, D.G. Hesse, S.Y. Panshin, D.W. Rogers, M. Saunders, P.M. Uffer and J.F. Liebman, “The Strain Energy of Cyclotetradecane is Small,” J. Org. Chem., 57, 1897-1899 (1992) (+ 24 supplemental sheets).

J94. C.A. Deakyne and J.F. Liebman, “The Relative Lewis Acidities of BF3 and SO 3: The Enthalpies of Complexation with the Anionic Bases F−, OH−, NH2−, CH3− and CF3−,” J. Mol. Struct. (Theochem), 234, 343-355 (1991). (This primary research, invited, refereed, research article is part of the special issue “Forty Years of Computational Quantum Chemistry,” in honor of G.G. Hall and C.C.J. Roothaan, special editors Z.B. Maksić and W.J. Orville-Thomas.)

J93. R.S. Hosmane and J.F. Liebman, “Aromaticity of Heterocycles: Experimental Realization of Dewar-Breslow Definition of Aromaticity,” Tetrahedron Lett., 32, 3949-3952 (1991).

J92. J.F. Liebman and A. Skancke, “Three-Membered Rings: Strain vs Aromaticity and Carbon vs Boron,” Struct. Chem., 2, 201-202 (1991). (This primary research, invited, refereed, research article is part of a special issue of Structural Chemistry, entitled “Strained Organic Molecules” edited by E. Lee-Ruff and paginated therein pp. 113-114.)

J91. A. Greenberg, Y.-Y. Chiu, J.L. Johnson and J.F. Liebman, “The Resonance Energy of Amides, The Structure of Aziridinone and Its Relationship to Other Strained Lactams,” Struct. Chem., 2, 117-126 (1991). (This primary research, invited, refereed, research article is part of a special issue of Structural Chemistry, entitled “Strained Organic Molecules” edited by E. Lee-Ruff and paginated therein pp. 29-38.)

J90. J.F. Liebman, M.J. Romm, M. Meot-Ner (Mautner), S.M. Cybulski and S. Scheiner, “Isotropy in Ionic Interactions II: How Spherical is the Ammonium Ion? Comparison of the Gas-Phase Clustering Energies and Condensed-Phase Thermochemistry of K+ and NH4+,” J. Phys. Chem., 95, 1112-1119 (1991). (Paper J71 has been renamed paper I of this series.)

J89. J.F. Liebman, M.J. Crockett and T.C. Dymski, “How Much is Out There? Some Thoughts on Atomic Orbitals and Electron Densities,” Struct. Chem., 2, 81-83 (1991).

J88. J.S. Chickos, C.M. Braton, D.G. Hesse and J.F. Liebman, “Estimating Entropies and Enthalpies of Fusion of Organic Compounds,” J. Org. Chem., 56, 927-938 (1991) (+ 44 supplemental sheets).

J87. R.A.L. Peerboom, S. Ingemann, N.M.M. Nibbering and J.F. Liebman, Proton Affinities and Heats of Formation of the Imines CH2=NH, CH2=NCH3 and C6H5CH=NH, J. Chem. Soc., Perkin Trans. 2, 1825-1828 (1990).

J86. J.F. Liebman and J.S. Chickos, “The Heat of Vaporization of Acyl Derivatives: When are Carboxylic Acid Esters α-Oxaketones or Acylethers?” Struct. Chem. 1, 501-502 (1990).

J85. D.W. Rogers, S.A. Loggins, S.D. Samuel, M.A. Finnerty and J.F. Liebman, “Homoaromaticity and Homoconjugation in the Quinacenes:  Biquinacene, Triquinacene and Hexaquinacene,” Struct. Chem., 1, 481-489 (1990).

J84. J.F. Liebman, “The Lewis Acidity of the Boron Trihalides,” Struct. Chem. 1, 395-397 (1990).

J83. N.J.S. Peters and J.F. Liebman, “Fluorine and Hydrogen Nitrate:  Rotational Barriers and Resonance Structures,” J. Fluor. Chem., 48, 378-393 (1990). (This primary research, invited, refereed article is part of the special issue devoted to the memory of Charles B. Colburn.)

J82. J.S. Chickos, D.G. Hesse and J.F. Liebman, “Estimating Entropies and Enthalpies of Fusion of Hydrocarbons,” J. Org. Chem., 55, 3833-3840 (1990) (+ 21 Supplemental pages).

J81. C.A. Deakyne, J.F. Liebman, G. Frenking and W. Koch, “A Comparative Study of Isoelectronic and Isogyric Reactions.  Molecular Orbital Calculations of Diatomic Hydrides and Halides,” J. Phys. Chem., 94, 2306‑2312 (1990).

J80. S.A. Kafafi, M. Meot‑Ner (Mautner) and J.F. Liebman, “The Proton Affinities of Styrene, Trans‑β‑Methylstyrene and Indene: A Theoret­ical and Experimental Study,” Struct. Chem., 1, 101‑105 (1990).

J79. J.S. Chickos, D.G. Hesse and J.F. Liebman, “Estimating Vaporization Enthalpies of Organic Compounds with Single and Multiple Substitution,” J. Org. Chem., 54, 5250‑5256 (1989) (+ 31 Supplemental pages).

J78. G. Frenking, W. Koch, D. Cremer, J. Gauss and J.F. Liebman, “Helium Bonding in Singly and Doubly Charged First‑Row Diatomic Cations HeXn+ (X = Li ‑ Ne, n = 1,2),” J. Phys. Chem., 93, 3397‑3410 (1989).

J77. G. Frenking, W. Koch, D. Cremer, J. Gauss and J.F. Liebman, “Neon and Argon Bonding in First‑Row Cations NeX+ and ArX+,” J. Phys. Chem., 93, 3410‑3418 (1989).

J76. C.M. Hadad, J.R. Damewood, Jr. and J.F. Liebman, “Interrelationships Among Heats of Formation and Molecular Mechanics Steric Energies,” Tetrahedron, 45, 1623‑1632 (1989).

J75. J.F. Liebman, J.M. Richter, M.J. Bienlein and S.S. Kalkarni, “Square Spirals, Dimensionality and Biopolymers,” Comput. Math Applns., 17, 595‑611 (1989). This volume has been reprinted as “Symmetry Unifying Human Understand­ing,” Vol. 2, (ed. I. Hargittai), Pergamon Press, Oxford (1989).

J74. G. Frenking, W. Koch, C.A. Deakyne, J.F. Liebman and N. Bartlett, “The ArF+ Cation. Is it Stable Enough to be Isolated in a Salt?,” J. Am. Chem. Soc., 111, 31‑33 (1989).

J73. M. Meot‑Ner (Mautner), J.F. Liebman and S.A. Kafafi, “Ionic Probes of Aromaticity in Annelated Rings,” J. Am. Chem. Soc., 110, 5937‑5941 (1988).

J72. J.S. Chickos, D.G. Hesse, J.F. Liebman and S.Y. Panshin, “Estimations of the Heats of Vaporization of Simple Hydrocarbon Derivatives,” J. Org. Chem., 53, 3424‑3429 (1988) (+ 33 Supplemental sheets).

J71. M. Meot‑Ner (Mautner), S.M. Cybulski, S. Scheiner and J.F. Liebman, “Is CN− Significantly Anisotropic? Comparison of CN‑ vs Cl‑: Cluster­ing with HCN and Condensed Phase Thermochemistry” J. Phys. Chem., 92, 2738‑2745 (1988).

J70. A. Greenberg, H.‑T.E. Chen, P.‑C. Lyu and J.F. Liebman, “Substi­tuent Effects on the Geometries of Prismanes,” J. Mol. Struct. Theo­chem., 163, 89‑99 (1988). (This invited, refereed, primary research article is part of the special issue devoted to Michael J.S. Dewar.)

J69. J.F. Liebman and J.E. Huheey, Comments on “Introduction to the Chem­istry of Fractionally Charged Atoms: Electronegativity,” Phys. Rev. D., 36, 1559‑1561 (1987).

J68. J.F. Liebman, L.A. Paquette, J.R. Peterson and D.W. Rogers, Is Triquin­acene Homoaromatic? A Thermochemical Answer in the Affirmative.” J. Am. Chem. Soc., 108, 8267‑8268 (1986).

J67. J.S. Chickos, R. Annunziata, L.H. Ladon, A.S. Hyman and J.F. Liebman, “Estimating Heats of Sublimation of Hydrocarbons: A Semiempirical Approach,” J. Org. Chem., 51, 4311‑4314 (1986) (+ 4 Supplemental sheets).

J66. J.F. Liebman, W.R. Dolbier, Jr. and A. Greenberg, “Hexafluorocyclopropane and Octafluorocyclobutane: A Study of the Strain Energies,” J. Phys. Chem., 90, 394‑397 (1986). (This primary research, invited, refereed article is part of the special issue devoted to Sidney W. Benson.)

J65. J.E. Del Bene, J.F. Liebman and M. Meot‑Ner (Mautner), “The Proton Affinities of the Azoles, Theoretical and Experimental Studies,” J. Org. Chem., 51, 1105‑1110 (1986) (+ 34 Supplemental sheets).

J64. J.F. Liebman, D. Van Vechten, K.D. Donnelly and W.E. Fristad, “Non­periodic Trends in the Oxidation of Transition Metals by Manganese(III) Acetate,” Inorg. Chim. Acta., 115, 37‑50 (1986).

J63. S.G. Lias, Z. Karpas and J.F. Liebman, “Halomethylenes: Effects of Halogen Substitution on Absolute Heats of Formation,” J. Am. Chem. Soc., 107, 6089‑6096 (1985).

J62. T.J. Buckley, L.W. Sieck, R. Metz, S.G. Lias and J.F. Liebman, “Consec­utive Ion‑Molecule Condensation Reactions and Photodissociation Mechanisms of Condensa­tion Ions in Polyacetylenic Compounds,” Intl. J. Mass Spectry. Ion Proc., 65, 181‑196 (1985).

J61. D. Van Vechten and J.F. Liebman, “Considerations on the Selection of Artificial Tunneling Barriers,” J. Vac. Soc. Techn. A., 3, 1881-­1883 (1985).

J60. S.G. Lias, J.A. Jackson, H. Argentar and J.F. Liebman, “Substituted N,N‑Dialkyl Anilines: Relative Ionization Energies and Proton Affinities through Determinations of Ion‑Molecule Reaction Equilibrium Constant,” J. Org. Chem., 50, 333‑338 (1985).

J59. W.V. Steele, B.E. Gammon, N.K. Smith, J.S. Chickos, A. Greenberg and J.F. Liebman, “The Standard Enthalpy of Formation of 2,3-Diphenylcycloprop-2-en‑1‑one,” J. Chem. Thermodyn., 17, 505‑511 (1985).

J58. J.F. Liebman, “Elimination vs Displacement Reactions: An Alternative Interpretation of `The Anomalous Reactions of F‑Propene Dimers with Thiolate Ions',” J. Fluor. Chem., 25, 481‑486 (1984).

J57. A.S. Hyman, S.I. Yaniger, I. Kramer, L.J. Bartolotti and J.F. Liebman, “Interrelationships Among X‑Ray Scattering, Electron Densities and Ionization Poten­tials, II: Upper Bound Results,” J. Chem. Phys., 81, 575‑576 (1984).

J56. A. Mavridis, J.F. Harrison and J.F. Liebman, “Electron­ic Structure of CNa and CNa2 in their Electronic Ground States,” J. Phys. Chem., 88, 4973‑4988 (1984).

J55. R. Schmutzler, O. Steltzer and J.F. Liebman, “Catalytic and Autocat­alytic Disproportionation Reactions of Fluorophosphines and Related Lower Valence Nonmetal Fluorides,” J. Fluor. Chem., 25, 289‑299 (1984).

J54. W.H. Koppenol and J.F. Liebman, “The Oxidizing Nature of the Hydroxyl Radical. A Comparison with the Ferryl Ion (FeO2+),” J. Phys. Chem., 88, 99‑101 (1984).

J53. J.F. Liebman and J.S. Valentine, “Concerning the Radical Character of Superoxide,” Isr. J. Chem., (symposium‑in‑print on oxygen species), 23, 439‑441 (1983).

J52. A. Greenberg, R.P.T. Tomkins, M. Dobrovolny and J.F. Liebman, “The Strain Energy of Diphenylcyclopropenone: A Reexamination,” J. Am. Chem. Soc., 105, 6855‑6858 (1983).

J51. R.L. DeKock, C.P. Jasperse, D.T. Dao, J.R. Bieda and J.F. Liebman, “Quantum Chemical Calculations on the Structure of (Cl2F+) Ion and Related Molecules,” J. Fluor. Chem., 22, 575‑583 (1983).

J50. J.A. Davies and J.F. Liebman, “Cyano and Halo‑Bridged Transition Metal Complexes: Structural Comparison of Neutral and Cationic Oligomers,” J. Chem. Soc. Dalton Transactions, 1793‑1795 (1983).

J49. A. Greenberg, J.F. Liebman, W.R. Dolbier, Jr., K.S. Medinger and A. Skancke, “Strain Energies of Gem‑Di­fluorocyclopropanes and Related Molecules,” Tetrahed­ron, 39, 1533‑1538 (1983).

J48. D.S. Marynick, D.C. Rosen and J.F. Liebman, “On the Electronic Struc­ture of Planar Amines and Phosphines,” J. Mol. Struct. Theochem., 94, 47‑50 (1983).

J47. J.F. Liebman and E.D. Yorke, “Are There Bound States to the 1/rn Potential?” Am. J. Phys., 51, 274 (1983).

J46. J.F. Liebman and J.S. Vincent, “Li12Si7: Theoretical Interest Aroused,” Angew. Chem., 94, 649 (1982); Angew. Chem. Intl. Ed., 21, 632‑633 (1982); Supplement, S1424‑S1428 (1982).

J45. W.R. Dolbier, Jr., K.S. Medinger, A. Greenberg and J.F. Liebman, “The Thermodynamic Effect of Fluorine as a Substituent: Vinylic CF2 and Allylic CF2C,” Tetra­hedron, 38, 2415‑2420 (1982).

J44. A. Greenberg and J.F. Liebman, “Proton Affinities of Substituted Benzaldehydes, 2‑Phenylpropenes (α‑Methyl­styrenes) and Related Mole­cules: Calculational Studies and Comparison with Experimental Data,” J. Org. Chem., 47, 2084‑2088 (1982).

J43. A. Greenberg, R. Winkler, B.M. Smith and J.F. Liebman, “The Negatively Charged Nitrogen in Ammonium Ion and Derived Concepts of Acidity, Basicity, Proton Affinity and Ion Energetics,” J. Chem. Ed., 59, 367‑370 (1982).

J42. D. Van Vechten and J.F. Liebman, “Number and Novelty in Approaches to the Calculation of Strainless Group Increments,” Isr. J. Chem. 21, 105‑110 (1981) (This primary research, invited, refereed article is part of symposium-in-print on small ring species),.

J41. J.S. Chickos, A.S. Hyman, L.H. Ladon and J.F. Liebman, “Measurement and Estimation of the Heat of Vaporization of Hydrocarbons,” J. Org. Chem., 46, 4294‑4296 (1981) (+ 5 supplementary pages).

J40. P.H. Mueller, N.G. Rondan, K.N. Houk, J.F. Harrison, D. Hooper, B.H. Willen and J.F. Liebman, “Carbene Singlet‑Triplet Gaps: Linear Correlations with Substituent π‑Donation,” J. Am. Chem. Soc., 103, 5049‑5052 (1981).

J39. A. Greenberg and J.F. Liebman, “3,3'‑bicyclopropenyl: Evidence for Novel Long‑Range Conjugation of π‑Orbi­tals,” J. Am. Chem. Soc., 103, 44‑48 (1981).

J38. A. Greenberg, J.F. Liebman and D. Van Vechten, “On the Nature of the Perfluoroalkyl (Rf) effect,” Tetrahedron, 36, 1161‑1166 (1980).

J37. A. Greenberg and J.F. Liebman, “Relative Energies of Substituted Benzene Valence Isomers,” Tetrahedron, 35, 2623‑2627 (1979).

J36. J.F. Harrison, R.C. Liedtke and J.F. Liebman, “The Multiplicity of Substituted Acyclic Carbenes and Related Molecules,” J. Am. Chem. Soc., 101, 7162‑7168 (1979).

J35. J.D. Dill, A. Greenberg and J.F. Liebman, “Substituent Effects on Strain Energies,” J. Am. Chem. Soc., 101, 6814‑6826 (1979) (+ 13 supplementary pages).

J34. K.D. Jordan and J.F. Liebman, “Binding of an Electron to a Molecular Quadrupole: (BeO)2−,” Chem. Phys. Lett., 62, 143‑147 (1979).

J33. A.S. Hyman, S.I. Yaniger and J.F. Liebman, “Relation­ships among X‑Ray Scattering, Electron Densities and Ionization Potentials,” Intl. J. Quantum Chem., 14, 757‑766 (1978).

J32. J.F. Liebman, “Conceptual Problems in Noble Gas and Fluorine Chemistry, VII: On the Possible Existence of Einsteinium and Protactinium Hexafluoride,” Inorg. Nucl. Chem. Lett., 14, 245‑247 (1978).

J31. B.M. Gimarc, J.F. Liebman and M. Kohn, “The Shapes and Other Properties of Non‑Transition Element Complexes. I. AB6,” J. Am. Chem. Soc., 100, 2334‑2339 (1978).

J30. J.F. Liebman, D.L. Yeager and J. Simons, “A Simple Approach to Reson­ance Levels,” Chem. Phys. Lett., 48, 227‑232 (1977).

J29. J.F. Liebman, “Conceptual Problems in Noble Gas and Fluorine Chemistry, VI: The Anomalous Reactions of Cl2O and F2O with Lewis Acids,” J. Fluor. Chem., 9, 153‑159 (1977).

J28. J.F. Liebman, “Conceptual Problems in Noble Gas and Fluorine Chemistry, V: The Difference in the Reactions of the Isoelectronic XeOF4 and IF5 with KrF+,” J. Fluor. Chem., 9, 147‑151 (1977). (Article J26 is number IV in this series.)

J27. J.F. Liebman, P. Politzer and W.A. Sanders, “Trends in Molecular Properties by the Method of Structural Fragments,” J. Am. Chem. Soc., 95, 5115‑5119 (1976).

J26. J.F. Liebman, “On the Existence of the Trifluoroxenate (II) Ion, XeF3‑; Comments on `The `Base' Catalyzed Fluorination of SO2 by XeF2,'“ J. Fluor. Chem., 7, 531‑535 (1976).

J25. J.F. Liebman, “Conceptual Problems in Noble Gas and Fluorine Chemistry, III: The Equivalence of the Structural Chemistry of Dicarbon, C2 and Xenon,” Inorg. Nucl. Chem. Lett., 11, 687‑690 (1975).

J24. J.F. Liebman, “Conceptual Problems in Noble Gas and Fluorine Chemistry, II: The Nonexistence of Radon Tetrafluoride,” Inorg. Nucl. Chem. Lett., 11, 683‑685 (1975). (Paper R1 was renamed paper I in this series).

J23. J.F. Liebman and J.S. Vincent, “Systematics of the Molecular Geometry of Excited States and Free Radi­cals,” J. Am. Chem. Soc., 97, 1373-­1376 (1975).

J22. M. Pomerantz and J.F. Liebman, “Is 100% s Character Necessary?” Tetrahedron Lett., 2385‑2388 (1975).

J21. J.F. Liebman, “Nucleophilic Displacement Reactions on Fluorine, II: The Role of σ- and π‑bond Nucleophiles,” J. Fluor. Chem., 5, 55‑59 (1975).

J20. J.F. Liebman and B.B. Jarvis, “Nucleophilic Displace­ment Reactions on Fluorine, I: General Phenomenon and Lone Pair Nucleophiles,” J. Fluor. Chem., 5, 41‑54 (1975).

J19. A. Johannson, P.A. Kollman, J.F. Liebman and S. Rothenberg, “Substi­tuent Effects on Proton Affinities of Simple Molecules,” J. Am. Chem. Soc., 96, 3750‑­3754 (1974).

J18. J.F. Liebman, “Comment on `Polymerization of Nitrogen Dioxide,’” J. Chem. Phys., 60, 2944 (1974).

J17. J.F. Liebman, “Predictions of Molecular Geometry from Structural Fragments,” J. Am. Chem. Soc., 96, 3053‑3061 (1974).

J16. J.F. Liebman and A. Greenberg, “The Origin of Rota­tional Barriers in Amides and Esters,” Biophys. Chem., 1, 222‑226 (1974).

J15. J.F. Liebman and A. Greenberg, “Estimation by Bond Additivity Schemes of the Relative Thermodynamic Stabilities of Three‑Membered Ring Systems and Their Open Dipolar Forms,” J. Org. Chem., 39, 123‑130 (1974).

J14. J.F. Liebman and R.M. Pollack, “Aromatic Transition States and the α‑Effect,” J. Org. Chem., 38, 3444‑3445 (1973).

J13. J.F. Liebman, “Oxidant for Trapping Radiokrypton,” Nature, 244, 84‑85 (1973).

J12. Liebman, “On the Electron Affinity of Perfluoro­alkanes and Perfluorocycloalkanes,” J. Fluor. Chem., 3, 27‑33 (1973/4).

J11. J.F. Liebman, “Simple Regularities and Relations among Ionization Potentials of Non‑Transition Elements,” J. Chem. Ed., 50, 831‑834 (1973).

J10. J.F. Liebman and T.H. Vanderspurt, “Polarization of X‑F Bonds,” J. Fluor. Chem., 2, 413‑424 (1972/3).

J9. J.F. Liebman, “Comment on the Paper `Oxygen Monofluor­ide (OF, 2π): Hartree‑Fock Wavefunction, Binding Energy, Ionization Potential, Electron Affinity, Dipole and Quadrupole Moments and Spectroscopic Constants. A Comparison of Theoretical and Experi­mental Results,'“ by P.A.G. O'Hare and A.C. Wahl, J. Chem. Phys., 56, 4242‑4243 (1972).

J8. J.F. Liebman, “Why is the Oxygen in Water Negative?” J. Chem. Ed., 49, 415‑417 (1972).

J7. J.F. Liebman and L.C. Allen, “Noble Gas Boron Com­pounds,” Inorg. Chem., 11, 1143‑1145 (1972).

J6. J.F. Liebman, “The Relative Electric Dipole Moments of Singlets and Triplets,” Mol. Phys., 21, 563‑565 (1971).

J5. J.F. Liebman and L.C. Allen, “Bonding in Rare Gas Diatomic ions Containing Nitrogen or Oxygen,” Intl. J. Mass. Spectry. Ion Phys., 7, 27‑31 (1971).

J4. J.F. Liebman, “Comments and a Warning about Isoelec­tronic Systems,” J. Chem. Ed., 48, 188‑189 (1971).

J3. J.F. Liebman and L.C. Allen, “A Salt Chemistry of Light Noble Gas Compounds,” J. Am. Chem. Soc., 92, 3539‑3543 (1970).

J2. P.A. Kollman, J.F. Liebman and L.C. Allen, “The Lithium Bond,” J. Am. Chem. Soc., 92, 1142‑1150 (1970).

J1. J.F. Liebman and L.C. Allen, “Possible Argon Com­pounds,” Chem. Comm., 1355 (1969).

**Review Articles and Book Chapters**

R137. M. Ponikvar-Svet, D.N. Zeiger and J.F. Liebman, “Interplay of Thermochemistry and *Structural Chemistry*, the Journal (Volume 28, 2017, Issues 5 and 6) and the Discipline,” Struct. Chem., 29, (in press).

R136. M. Ponikvar-Svet, D.N. Zeiger and J.F. Liebman, “Interplay of Thermochemistry and *Structural Chemistry*, the Journal (Volume 28, 2017, Issues 3 and 4) and the Discipline,” Struct. Chem., 29, 1235-1245 (2018).

# R135. M. Ponikar-Svet and J.F. Liebman, “The Chemical Energetics of the Hypervalent Organohalogen Halosyl, Halyl And Perhalyl Species” in Patai’s Chemistry of Functional Groups: The Chemistry of Hypervalent Halogens (ed. B. Olofsson, Z. Rappoport and I. Marek), Wiley, Chichester (in press).

R134. M. Ponikvar-Svet, D.N. Zeiger and J.F. Liebman, “Interplay of Thermochemistry and *Structural Chemistry*, the Journal (Volume 28, 2017, Issues 1 and 2) and the Discipline,” Struct. Chem., 29, 942-955 (2018).

R133. M. Ponikvar-Svet and J.F. Liebman, “Contemporary Use of Azophenolates and Related Species in the Determination of Metal Cations” in Patai’s Chemistry of Functional Groups: The Chemistry of Metal Phenolates, Vol. 2 (ed. J. Zabicky), Wiley, Chichester 484 – 405 (2018).

R132. D.N. Zeiger, J. F. Liebman and M. Ponikvar-Svet. “Aspects Of The Energetics of Metal β-Diketonates and Their Derivatives,” in Patai’s Chemistry of Functional Groups: The Chemistry of Metal Enolates, Vol. 2 (ed. J. Zabicky), Wiley, Chichester, 1 – 24 (2018)..

R131. S.W. Slayden and J.F. Liebman, Aspects of the Chemical Energetics of Carbon-Aluminum Bonded Species, in Patai’s Chemistry of Functional Groups: The Chemistry of Organoaluminum Compounds, (ed. L. Micouin, I. Marek and Z. Rappoport) Wiley, Chichester, 33 – 70 (2017).

R130. K.F. Edwards and J.F. Liebman, “"Neil Bartlett: No Nobel for Noble Gases – Some Guesses Why" in The Posthumous Nobel Prize in Chemistry: Correcting the Errors and Oversights of the Nobel Prize Committee (Ed. E.T. Strom and V.V. Mainz) ACS Symposium Series, Vol. 1262, 261 – 281 (2017) Washington DC.

R129. M. Ponikvar-Svet, D.N. Zeiger and J.F. Liebman, “Interplay of Thermochemistry and *Structural Chemistry*, the Journal (Volume 27, 2016, Issues 5 and 6) and the Discipline,” Struct. Chem., 28, 1981-8 (2017).

R128. M. Ponikvar-Svet, D.N. Zeiger and J.F. Liebman, “Interplay of Thermochemistry and *Structural Chemistry*, the Journal (Volume 27, 2016, Issues 3 and 4) and the Discipline,” Struct. Chem., 28, 1265-1273 (2017).

R127. M. Ponikvar-Svet, D.N. Zeiger and J.F. Liebman, “Interplay of Thermochemistry and *Structural Chemistry*, the Journal (Volume 27, 2016, Issues 1 and 2) and the Discipline,” Struct. Chem., 28, 889-99 (2017).

R126. M. Ponikvar-Svet, D.N. Zeiger and J.F. Liebman, “Interplay of Thermochemistry and *Structural Chemistry*, the Journal (Volume 26, 2015, Issue 5) and the Discipline,” Struct. Chem., 28, 879-87 (2017).

(Issue 6 was subsumed in issue 5.)

R125. K.D. McDonald, E.O. Ojo and J.F. Liebman, “What are the Structures of the Octet Rule Obeying All-Carbon Species Cx (2 ≤ x ≤ 7 and Larger x): A Pedagogical, Mathematical and Pictorial Study” in Sustainable Nanosystems: Development, Properties, and Applications (ed. M.V. Putz and M. C.

Mirica) , IGI Global, Hershey, 1-45. (2017).

R124 M. Ponikvar-Svet and J.F. Liebman, “Interplay of Thermochemistry and *Structural Chemistry*, the Journal (Volume 26, 2015, Issues 3 and 4) and the Discipline,” Struct. Chem., 27, 1869-1678 (2016).

R123 M. Ponikvar-Svet, D.N. Zeiger and J.F. Liebman, “Interplay of Thermochemistry and *Structural Chemistry*, the Journal (Volume 26, 2015, Issues 1 and 2) and the Discipline,” Struct. Chem., 27, 1017-1026 (2016).

R122. M. Ponikvar-Svet, D.N. Zeiger and J.F. Liebman, “Interplay of Thermochemistry and *Structural Chemistry*, the Journal (Volume 25, 2014, Issues 5 and 6) and the Discipline,” Struct. Chem., 26, 1729-1739 (2015).

R121. M. Ponikvar-Svet, D.N. Zeiger and J.F. Liebman, “Interplay of Thermochemistry and *Structural Chemistry*, the Journal (Volume 25, 2014, Issues 3 and 4) and the Discipline,” Struct. Chem., 26, 887–898 (2015).

R120. M. Ponikvar-Svet, D.N. Zeiger and J.F. Liebman, “Interplay of Thermochemistry and *Structural Chemistry*, the Journal (Volume 25, 2014, Issues 1 and 2) and the Discipline,” Struct. Chem., 26, 623- 635 (2015).

R119. H.M. Perks and J.F. Liebman, “Aurocarbons: Binary Gold Carbides, Binary Carbon Aurides and

Their Derivatives” in Patai’s Chemistry of Functional Groups: The Chemistry of Organogold Compounds, Wiley, Chichester, (ed. Z. Rappoport, J.F. Liebman and I. Marek), 31-40 (2014).

R118. M. Ponikvar-Svet, D.N. Zeiger, L.R. Keating and J.F. Liebman, “Interplay of Thermochemistry and *Structural Chemistry*, the Journal (Volume 24, 2013, Issues 5 and 6) and the Discipline,” Struc. Chem., 25, 1881 – 1894 (2014).

R117. A. Greer, A.T. Balaban and J.F. Liebman, “Consequences of Spin and Strength in the Chemistry of Oxygen and its Compounds” in Patai’s Chemistry of Functional Groups: The Chemistry of Peroxides, Vol. 3, Wiley, Chichester, (ed. A. Greer and J.F. Liebman) 1-20 (2014).

R116. A.T. Balaban, A. Greer and J.F. Liebman, “Aromaticity and Conjugation in 1,2-Benzoquinone Valence Isomers and Congeners” in Advances in Heterocyclic Chemistry (ed. A.R. Katritzky, Elsevier) 113, 111-142 (2014).

R115. J.F. Liebman, “Isidor Fankuchen (1904–1964): More than Memories of a Master Measurer of Molecules and Materials,” Struct. Chem., 25, 1593-1595 (2014).

R114. J.F. Liebman and S.W. Slayden, “The Thermochemistry and Energetics of Organoiron Compounds in Patai’s Chemistry of Functional Groups: The Chemistry of Organoiron Compounds, Wiley, Chichester, (ed. Z. Rappoport and I. Marek), 45-64 (2014).

R113. M. Ponikvar-Svet, D.N. Zeiger, L.R. Keating and J.F. Liebman, “Interplay of Thermochemistry and *Structural Chemistry*, the Journal (Volume 24, 2013, Issues 3 and 4) and the Discipline,” Struc. Chem., 25, 1581 – 1592 (2014).

R112. S.W. Slayden and J.F. Liebman, “The Experimental Thermochemistry of Metal Phenolates,” in Patai’s Chemistry of Functional Groups: The Chemistry of Metal Phenolates” (ed. J. Zabicky), Wiley, Chichester, 91-130 (2014).

R111. J.A. Martinho Simões, J.F. Liebman and M.J.S. Monte, “The Life and Career of Manuel Ribeiro da Silva,” J. Chem. Thermodyn., 73, 1-2 (2014) (This iarticle is in memory of Manuel A.V. Ribeiro da Silva. This special issue was edited by R.D. Weir, J.A. Martinho Simões, J.F. Liebman and M.J.S. Monte..)

R110. J.E. Hack and J.F. Liebman, “A Summary of Functional Groups Containing Selenium and Tellurium: A Catalog of the Many Groups That are Known and Some That are Not,” in Patai’s Chemistry of Functional Groups: The Chemistry of Organic Selenium and Tellurium Compounds Vol. 4, Wiley, Chichester, (ed. Z. Rappoport). While the considerably abbreviated print version appears as pp. 1515-21 (2013), the full version of the chapter appears in the online version of Patai’s Chemistry of Functional Groups: Organic Selenium and Tellurium (2013) http://onlinelibrary. wileycom. book.10.1002.9780470682531.doc

R109. M. Ponikvar-Svet, D.N. Zeiger, L.R. Keating and J.F. Liebman, “Interplay of Thermochemistry and *Structural Chemistry*, the Journal (Volume 24, 2013, Issues 1 and 2) and the Discipline,” Struc. Chem., 24, 2101 – 2114 (2013).

R108. J.F. Liebman, J.S. Chickos and R. Notario, “Introduction: Maria Victoria Roux: Calorimetrist, Colleague, Friend,” Struct. Chem., 24, 1785 – 1787 (2013). (This is the introductory article for the special issue of *Structural Chemistry* in honor of Maria Victoria Roux on the occasion of her retirement. This special issue was edited by J.F. Liebman, J.S. Chickos and R. Notario.)

R107. M. Ponikvar-Svet, K.F. Edwards and J.F. Liebman, “An Overview of the Understanding of Ions Containing Solely Fluorine Atoms,” Acta Chim. Slovenica, 60, 471 – 483 (2013). (This primary research, invited, refereed article is in honor of Boris Žemva on the occasion of his receiving the Zois’ lifetime achievement award. This special issue was edited by M. Tramšek and B. Malič.)

R106. K.F. Edwards, E. Lewars and J.F. Liebman, “On the Existence and Energetics of o- and p-Benzoquinone and Their Derivatives: Additional Understanding from the Vantage Point of the Conceptual Trichotomy of Convenience, Anthropocentrism and Folksonomy,” Advances in Molecular Modeling, Vol. 5, 433 - 440 (2015) (ed. M. V. Putz, Nova Science Publishers, New York). This is an amended reprinting of K.F. Edwards, E. Lewars and J.F. Liebman, “On the Existence and Energetics of o- and p-Benzoquinone and Their Derivatives: Additional Understanding from the Vantage Point of the Conceptual Trichotomy of Convenience, Anthropocentrism and Folksonomy,” Intl. J. Chem. Model., 5, 327-334 (2013).

R105. K.F. Edwards, S. Perişanu and J.F. Liebman, “The Aromaticity of Benzene and the Lack of Aromaticity of Cyclooctatetraene: Is Our Calorimetric Perspective a Manifestation of Convenience, Anthropocentrism, or Folksonomy?,” Advances in Molecular Modeling, Vol. 5, 417 – 432 (2015) (ed. M. V. Putz, Nova Science Publishers, New York). This is an amended reprinting of K.F. Edwards, S. Perişanu and J.F. Liebman, “The Aromaticity of Benzene and the Lack of Aromaticity of Cyclooctatetraene: Is Our Calorimetric Perspective a Manifestation of Convenience, Anthropocentrism, or Folksonomy?,” Intl. J. Chem. Model., 5, 51– 65 (2013).

R104. M. Ponikvar-Svet, D.N. Zeiger, L.R. Keating and J.F. Liebman, “Interplay of Thermochemistry and *Structural Chemistry*, the Journal (Volume 23, 2012, Issues 4–6) and the Discipline,” Struc. Chem., 24, 1759-1779 (2013).

R103. K.F. Edwards, J.C. Williams and J.F. Liebman, “Organizing Principles and Gaps in the Periodic Table: Do We Find Manifestations of Convenience, Anthropocentrism, or Folksonomy?,” Advances in Molecular Modeling, Vol. 4, 525 – 537 (2013) (ed. M. V. Putz, Nova Science Publishers, New York). This is an amended reprinting of K.F. Edwards, J.C. Williams and J.F. Liebman, “Organizing Principles and Gaps in the Periodic Table: Do We Find Manifestations of Convenience, Anthropocentrism, or Folksonomy?,” Intl. J. Chem. Model., 4, 391 – 404 (2012) .

R102. M. Ponikvar-Svet, D.N. Zeiger, L.R. Keating and J.F. Liebman, “Interplay of Thermochemistry and *Structural Chemistry*, the Journal (Volume 23, 2012, Issues 1–3) and the Discipline,” Struct. Chem., 23, 2019 – 2037 (2012).

R101. M. Ponikvar-Svet and J.F. Liebman, “Aspects of the Chemistry of Species with Carbon-Polonium Bonds,” in Patai’s Chemistry of Functional Groups: The Chemistry of Organic Selenium and Organic Tellurium Compounds Vol. 3, (ed. Z. Rappoport), Wiley, Chichester, 1359-1369 (2012).

R100.J.F. Liebman and S.W. Slayden, “Thermochemistry of Organoselenium and Organotellurium Compounds,” in Patai’s Chemistry of Functional Groups: The Chemistry of Organic Selenium and Organic Tellurium Compounds Vol. 3, (ed. Z. Rappoport), Wiley, Chichester, 139 – 165 (2012).

R99. M. Ponikvar-Svet, D.N. Zeiger and J.F. Liebman, “Interplay of Thermochemistry and *Structural Chemistry*, the Journal (Volume 22, 2011, Issues 4–6) and the Discipline,” Struct. Chem., 23, 1267 – 1280 (2012).

R98. K.F. Edwards and J.F. Liebman, “Amphoteric, Amphihydric and Ambisaline: Are These Descriptive Concepts Manifestations of Convenience, Anthropocentrism, or Folksonomy?,” in Advances in Molecular Modeling, Vol. 3 (ed. M. V. Putz, Nova Science Publishers, New York, 2012). This is an amended reprinting of K.F. Edwards and J.F. Liebman, “Amphoteric, Amphihydric and Ambisaline: Are These Descriptive Concepts Manifestations of Convenience, Anthropocentrism, or Folksonomy?” Int. J. Chem. Model., 3, 213 – 223 (2011). (This primary, invited, research paper is in honor of Eduardo A. Castro on the occasion of his 65th birthday).

R97. M. Ponikvar-Svet and J.F. Liebman, “Interplay of Thermochemistry and *Structural Chemistry*, the Journal (Volume 22, 2011, Issues 1–3) and the Discipline,” Struct. Chem, 22, 1179 ‒ 1192 (2011).

R96. J.F. Liebman and S.W. Slayden, “Energetics of Organomanganese Compounds,” in Patai’s Chemistry of Functional Groups: The Chemistry of Organomanganese Compounds, (ed. Z. Rappoport and I. Marek), Wiley, Chichester, 171 – 221 (2011).

R95. M. Ponikvar-Svet and J.F. Liebman, “Interplay of Thermochemistry and *Structural Chemistry*, the Journal (Volume 21, 2010) and the Discipline,” Struct. Chem., 22, 717 – 740 (2011).

R94. S.W. Slayden, A. Greer and J.F. Liebman, “Peroxynitrogen: A Study of Nitrogen/Oxygen Heterocycles with N-O and O-O or N-O-O Bonding” in Patai’s Chemistry of Functional Groups,: The Chemistry of Hydroxylamines, Oximes and Hydroxamic Acids, Vol. 2, (ed. Z. Rappoport and J.F. Liebman), Wiley, Chichester, 549 – 576 (2011).

R93. M. Ponikvar-Svet and J.F. Liebman, “Interplay of Thermochemistry and *Structural Chemistry*, the Journal (Volume 20, 2009) and the Discipline,” Struct. Chem., 21, 1131 – 1149 (2010).

R92. M. Ponikvar-Svet, L.R. Keating, B.J. Dodson and J.F. Liebman, “Interplay of Thermochemistry and Structural Chemistry, the Journal (Volume 16, 2005) and the Discipline,” Struct. Chem., 21, 527 – 540 (2010).

R91. J.F. Liebman and S.W. Slayden, “Thermochemistry of Organocopper Compounds,” in The Chemistry of Organocopper Compounds (ed. Z. Rappoport and I. Marek), Wiley, Chichester, 145 - 162 (2009).

R90. M. Ponikvar-Svet and J.F. Liebman, “Interplay of Thermochemistry and Structural Chemistry, the Journal (Volume 17, 2006) and the Discipline,” Struct. Chem., 20, 1019 – 1037 (2009).

R89. M. Ponikvar-Svet, L.R. Keating, B.J. Dodson and J.F. Liebman, “Interplay of Thermochemistry and Structural Chemistry, the Journal (Volume 19, 2008) and the Discipline,” Struct. Chem., 20, 719 – 741 (2009).

R88. J.F. Liebman and S.W. Slayden, “Thermochemical Considerations of Metal Enolates,” in The Chemistry of Metal Enolates (ed. J. Zabicky), Wiley, Chichester, 185 – 221 (2009).

R87. M.A.R. Matos and J.F. Liebman, "Recent Advances in the Experimental Thermochemistry of Heterocycles and Their Aromaticity: A Study of Nitrogen, Oxygen and Sulfur Derivatives of Indane and Indene" in Topics in Heterocyclic Chemistry: Aromaticity in Heterocyclic Chemistry 19 (series ed., R.R. Gupta, vol. ed. T. M. Krygowski and M.K. Cyranski), Springer, Heidelberg, 1- 26 (2009).

R86. P.J. Smith, J.F. Liebman, H. Hopf, S. Ivo and B. Halton, “Distorted Aromatics” in Strained Hydrocarbons: Beyond the van’t Hoff and LeBel Hypothesis (ed. H. Dodziuk), Wiley-VCH, Weinheim, 147 - 203 (2009).

R85. D. Lenoir, P.J. Smith, J.F. Liebman, A. Nicolaides, R.P. Johnson, and K.M. Konrad, “Nonplanar Alkenes” in Strained Hydrocarbons: Beyond the van’t Hoff and LeBel Hypothesis (ed. H. Dodziuk), Wiley-VCH, Weinheim, 103 - 146 (2009).

R84. M. Ponikvar and J.F. Liebman, “Use of Oximes, Hydroxamic Acids and Related Species as Reagents in Inorganic Analytical Chemistry” in The Chemistry of Hydroxylamines, Oximes and Hydroxamic Acids, Vol. 1, (ed. Z. Rappoport and J.F. Liebman), Wiley, Chichester, 515 - 552 (2009).

R83. S.W. Slayden and J.F. Liebman, “The Organic Thermochemistry of Hydroxylamines, Oximes, Hydroxamic Acids and Their Derivatives” in The Chemistry of Hydroxylamines, Oximes and Hydroxamic Acids (ed. Z. Rappoport and J.F. Liebman), Wiley, Chichester, 53 ‒ 83 (2009).

R82. M. Ponikvar and J.F. Liebman, “Interplay of Thermochemistry and *Structural Chemistry*, the Journal (Volume 18, 2007) and the Discipline.” Struct. Chem., 19, 849 – 872 (2008).

R81. J.F. Liebman, T. Holm and S.W. Slayden, “The Thermochemistry of Organomagnesium Compounds” in The Chemistry of Organomagnesium Compounds (ed. Z. Rappoport and I. Marek), Wiley, Chichester, 101–129 (2008).

R80. S.W. Slayden and J.F. Liebman, “Thermochemistry of Anilines,” in The Chemistry of Anilines (ed. Z. Rappoport), Wiley, Chichester, 259-292 (2007).

R79. J.F. Liebman and S.W. Slayden, “Thermochemistry of Organozinc Compounds,” in The Chemistry of Organozinc Compounds, (eds. Z. Rappoport and I. Marek), Wiley, Chichester, 135-145 (2006).

R78. M.R. Stem and J.F. Liebman, “Interplay of Thermochemistry and *Structural Chemistry*, the Journal (Volume 15, 2004) and the Discipline,” Struct. Chem., 17, 367-373 (2006).

R77. S.W. Slayden and J.F. Liebman, “Thermochemistry of Peroxides,” in The Chemistry of Peroxides, Vol. 2, (ed. Z. Rappoport), Wiley, Chichester, 145-169 (2006).

R76. M.R. Stem and J.F. Liebman, “Interplay of Thermochemistry and *Structural Chemistry*, the Journal (Volume 14, 2003) and the Discipline,” Struct. Chem., 16, 593-603 (2005).

R75. M.V. Roux, P. Jiménez, R. Notario, M. Temprado, G.Martín-Valcarcel and J.F. Liebman, “Thermochemical Study of Arene Carboxylic Acids,” Arkivoc, 364-374 (2005). (This invited research/review article is in honor of José Elguero on the occasion of his 70th birthday.)

R74. M.R. Stem-Berenand J.F. Liebman, “Interplay of Thermochemistry and *Structural Chemistry*, the Journal (Volume 13, 2002) and the Discipline,” Struct. Chem., 16, 159-168 (2005).

R73. H. Hopf, J.F. Liebman and H.M. Perks, “Cubanes, Fenestranes, Ladderanes, Prismanes, Staffanes and other Oligocyclobutanoids,” in The Chemistry of Cyclobutanes, (ed. Z. Rappoport and J.F. Liebman), Wiley, Chichester, 1061-1109 (2005).

R72. J.F. Liebman and S.W. Slayden, “Thermochemistry of Cyclobutane and its Derivatives,” in The Chemistry of Cyclobutanes, (ed. Z. Rappoport and J.F. Liebman), Wiley, Chichester, 133-175 (2005).

R71. S.W. Slayden and J.F. Liebman, “Thermochemistry of Organolithium Compounds,” in The Chemistry of Organic Lithium Compounds (eds. Z. Rappoport and I. Marek), Wiley, Chichester, 121-136 (2004).

R70. S.W. Slayden and J.F. Liebman, “Thermochemistry of Phenols and Related Arenols,” in The Chemistry of Phenols (ed. Z. Rappoport), Wiley, Chichester, 223-257 (2003).

R69. J.F. Liebman,“Interplay of Thermochemistry and *Structural Chemistry*, the Journal and the Discipline, Volume 12, 2001,” Struct. Chem., 14, 403-415 (2003).

R68. J.F. Liebman, “Interplay of Thermochemistry and *Structural Chemistry*, the Journal and the Discipline (Volume 11, 2000),” Struct. Chem., 14, 299-313 (2003).

R67. J.F. Liebman and C.A. Deakyne, “Noble Gas Compounds and Chemistry: A Brief Review of Interrelations and Interactions with Fluorine-containing Species,” J. Fluor. Chem., 121, 1-8 (2003). (This research/review article is in honor of Neil Bartlett on the occasion of his 70th birthday. A poem of mine, “Ode to Neil Bartlett” also appears as part of this paper.)

R66. J.F. Liebman, K. Severin and T.M. Klapötke, “Inorganic Exotic Molecules,” in The Encyclopedia of Physical Science and Technology, 3rd edn. (genl. ed., R.A. Meyers), Academic Press, San Diego, Vol.7, 817-838 (2002).

R65. S.W. Slayden and J.F. Liebman, “The Energetics of Aromatic Hydrocarbons: An Experimental Thermochemical Perspective,” Chem. Rev., 101, 1541-1566 (2001). This invited, review article is part of the special thematic issue entitled “Aromaticity” edited by P.v.R. Schleyer.

R64. J.F. Liebman and S.W. Slayden, “Some Relationships between Molecular Structure and Thermochemistry: Part 4,” in Advances in Molecular Structure Research, Volume 6, (eds. M. Hargittai and I. Hargittai), JAI Press, Greenwich, CT, 2000, 443-459.

R63. J.F. Liebman, H.Y. Afeefy and S.W. Slayden, “The Thermochemistry of Amides,” in The Amide Linkage: Structural Significance in Chemistry, Biochemistry and Materials Science, (ed. A. Greenberg, C.M. Breneman and J.F. Liebman), Wiley, New York, 2000, 115-136. (Also see amended paperback version of this book, Wiley, New York, 2003, 115-136.)

R62. J.S. Chickos, W.E. Acree, Jr. and J.F. Liebman, “Estimating Solid-Liquid Phase Change Enthalpies and Entropies,” J. Phys. Chem. Ref. Data, 28, 1535-1673 (1999).

R61. J.F. Liebman and S.W. Slayden, “Some Relationships between Molecular Structure and Thermochemistry: Part 3,” in Advances in Molecular Structure Research, Volume 5, (eds. M. Hargittai and I. Hargittai), JAI Press, Greenwich, CT, 1999, 359-382.

R60. S.W. Slayden and J.F. Liebman, “Bond Energies, Enthalpies of Formation and Homologies: The Energetics of Aliphatic and Alicyclic Hydrocarbons and Some of their Derivatives,” in Pauling's Legacy: Modern Modelling of the Chemical Bond, (eds. Z.B. Maksić and W.J. Orville-Thomas), Elsevier, Amsterdam, 1999, 303-320.

R59. J.F. Liebman, J.A. Martinho Simões and S.W. Slayden, “Thermochemistry of the Organometallic Compounds of Silver and Gold,” in The Chemistry of Organic Silver and Gold Compounds, (eds. S. Patai and Z. Rappoport), Wiley, Chichester, 1999, 52-66.

R58. I. Černušák, C.A. Deakyne, H. Lischka, J.F. Liebman, A. Pappová and A. Skancke, “Ionic and Neutral Complexes of Borane (1),” in Fundamentals and Applications of Gas Phase Ion Chemistry, (ed. K.R. Jennings), NATO ASI, Series C, Vol. 521, Kluwer Academic Publishers, Dordrecht, 1999, 459-460.

R57. J.F. Liebman, P.P. Gaspar and D.J. Berger, “The Proton Affinities of Pyridine, Phosphabenzene and Arsabenzene,” in Fundamentals and Applications of Gas Phase Ion Chemistry, (ed. K.R. Jennings), NATO ASI, Series C, Vol. 521, Kluwer Academic Publishers, Dordrecht, 1999, 432-434.

R56. K.K. Irikura, M. Meot-Ner (Mautner), L.W. Sieck, A.D. Fant and J.F. Liebman, “Protonated para-Benzoquinone,” in Fundamentals and Applications of Gas Phase Ion Chemistry, (ed. K.R. Jennings), NATO ASI, Series C, Vol. 521, Kluwer Academic Publishers, Dordrecht, 1999, 410-411.

R55. C.A. Deakyne and J.F. Liebman, “Isoelectronic Isogyric Reactions,” in The Encyclopedia of Computational Chemistry, (eds. P.v.R. Schleyer, N.L. Allinger, T. Clark, J. Gasteiger, P.A. Kollman, H.F. Schaefer III and P.R. Schreiner), Wiley, Chichester, Vol. 2, 1439-1449 (1998).

R54. J.F. Liebman and S.W. Slayden, “Some Relationships between Molecular Structure and Thermochemistry, Part 2,” in Advances in Molecular Structure Research, Volume 4, (eds. M. Hargittai and I. Hargittai), JAI Press, Greenwich, CT, 343-371 (1998).

R53. J.F. Liebman and H. Afeefy, “Thermochemical Mimicry,” in Thermodynamical Modeling and Materials Data Engineering, (eds. J.-P. Caliste, E. Truyol and J. Westbrook) Springer Verlag, Berlin, 71-78 (1998).

R52. J.S. Chickos, W.E. Acree, Jr. and J.F. Liebman, “Estimating Phase Change Enthalpies and Entropies,” in Computational Thermochemistry: Prediction and Estimation of Molecular Thermodynamics, 63-91 (eds. D.J. Frurip and K.K. Irikura), (ACS Symposium Series 677), Washington, DC (1998).

R51. H.Y. Afeefy and J.F. Liebman, “Estimation of the Enthalpies of Formation of Organic Compounds in the Solid Phase: The Study of 2-Acetoxybenzoic Acid (Aspirin) and its Isomers,” in Computational Thermochemistry: Prediction and Estimation of Molecular Thermodynamics, 94-104 (eds. D.J. Frurip and K.K. Irikura), (ACS Symposium Series 677), Washington, DC (1998).

R50. J.F. Liebman, “Hydride,” in McGraw-Hill Encyclopedia of Science and Technology, Vol. 8, pp. 642-643 (8th ed., S.P. Parker, editor-in-chief, McGraw-Hill, New York, 1997).

R49. J.F. Liebman, H.Y. Afeefy and S.W. Slayden, “Thermochemistry of Azo, Hydrazo, Azoxy and Related Species,” in The Chemistry of Hydrazo, Azo and Azoxy Groups, Vol. 2 (ed. S. Patai), Wiley, Chichester, 79-104 (1997).

R48. J.F. Liebman and S.W. Slayden, “Some Relationships between Molecular Structure and Thermochemistry,” in Advances in Molecular Structure Research, Volume 3, (eds. M. Hargittai and I. Hargittai), JAI Press, Greenwich, CT 313-337 (1997).

R47. S.W. Slayden and J.F. Liebman, “Thermochemistry of Olefins, Carbonyl Compounds and Imines,” in The Chemistry of Functional Groups Supplement A3: The Chemistry of Doubly-Bonded Functional Groups, (ed. S. Patai), Wiley, Chichester, 537-609 (1997).

R46. J.F. Liebman, “Thermochemistry of Dienes and Polyenes,” in The Chemistry of Functional Groups Supplement A2: The Chemistry of Dienes and Polyenes, Vol. 1 (ed. Z. Rappoport), Wiley, Chichester, 67-110 (1997).

R45. J.F. Liebman, M.S. Campbell and S.W. Slayden, “Thermochemistry of Amines, Nitroso Compounds, Nitro Compounds and Related Species,” in The Chemistry of Functional Groups Supplement F2: The Chemistry of Amino, Nitroso, Nitro and Related Groups, (ed. S. Patai), Wiley, Chichester, 337-378 (1996).

R44. A. Greenberg and J.F. Liebman, “Resonance and 1,2-Rearrangement Enthalpies in Radicals: From Alkyl Radicals to Alkylcobalamins,” on Energetics of Organic Free Radicals, (ed. J.A. Martinho Simões, A. Greenberg and J.F. Liebman), (Blackie Academic & Professional, an imprint of Chapman & Hall, London), 196-223 (1996).

R43. J.F. Liebman, “Interrelations in the Thermochemistry of Cyclopropanes,” in The Chemistry of the Cyclopropyl Group, Vol. 2, (ed. Z. Rappoport), Wiley, Chichester, 223-260 (1995).

R42. R.Y.N. Ho, J.F. Liebman and J.S. Valentine, “Biological Reactions of Dioxygen,” in Active Oxygen in Biochemistry, (ed. J.S. Valentine, C.S. Foote, A. Greenberg and J.F. Liebman), (Blackie Academic & Professional, an imprint of Chapman & Hall, London), 1-36 (1995).

R41. J.F. Liebman, J.A. Martinho Simões and S.W. Slayden, “Thermochemistry of Organometallic Compounds of Germanium, Tin and Lead,” in The Chemistry of Organic Germanium, Tin and Lead Compounds, (ed. S. Patai), Wiley, Chichester, 245-266 (1995).

R40. R.Y.N. Ho, J.F. Liebman and J.S. Valentine, “Overview of the Energetics and Reactivity of Oxygen,” in Active Oxygen in Chemistry, (ed. C.S. Foote, J.S. Valentine, A. Greenberg and J.F. Liebman), (Blackie Academic & Professional, an imprint of Chapman & Hall, London), 1-23 (1995).

R39. S.W. Slayden, J.F. Liebman and W.G. Mallard, “Thermochemistry of Halogenated Organic Compounds,” in The Chemistry of Functional Groups Supplement D2: The Chemistry of Organic Halides, Pseudohalides and Azides, (ed. S. Patai and Z. Rappoport), Wiley, Chichester, 361-402 (1995).

R38. J.F. Liebman, J.A. Martinho Simões and S.W. Slayden, “Aspects of the Thermochemistry of Lithium Compounds,” in Lithium Chemistry: A Theoretical and Experimental Overview, (ed. A.-M. Sapse and P.v.R. Schleyer), Wiley, New York, 173-193 (1995).

R37. J.F. Liebman and H.M. Perks, “Thermochemistry of Enamines,” in The Chemistry of Enamines, (ed. Z. Rappoport), Wiley, Chichester, 255-277 (1994).

R36. J.F. Liebman, J.A. Martinho Simões and S.W. Slayden, “Thermochemistry of Organo-Arsenic, Antimony and Bismuth Compounds,” in The Chemistry of Organic Arsenic, Antimony and Bismuth Compounds, (ed. S. Patai), Wiley, Chichester, 153-168 (1994).

R35. J.F. Liebman, K.S.K. Crawford and S.W. Slayden, “Thermochemistry of Organosulphur Compounds,” in The Chemistry of Functional Groups Supplement S: The Chemistry of Sulphur-containing Functional Groups, (ed. S. Patai and Z. Rappoport), Wiley, Chichester, 197-243 (1993).

R34. S.W. Slayden and J.F. Liebman, “Thermochemistry of Ethers, Alcohols, Arenols, Enols and Peroxides,” in The Chemistry of Functional Groups Supplement E2: Chemistry of Hydroxyl, Ether and Peroxide Groups, (ed. S. Patai), Wiley, Chichester, 103-200 (1993).

R33. J.S. Chickos, D.G. Hesse and J.F. Liebman, “Estimating Enthalpies of Sublimation of Hydrocarbons,” in Energetics of Organometallic Species (ed. J.A. Martinho Simes), NATO ASI, Series C, Vol. 367, Kluwer Academic Publishers, Dordrecht, 1992, 159-169.

R32. J.F. Liebman, S.O. Yee and C.A. Deakyne, “Normalizing/Formalizing the Ion/Neutral Thermochemistry of Fluorinated Species,” in Fundamentals of Gas Phase Ion Chemistry (ed. K.R. Jennings), NATO ASI, Series C, Vol. 347, Kluwer Academic Publishers, Dordrecht, 1991, 284.

R31. J.F. Liebman, M.J. Romm, M. Meot-Ner, S.M. Cybulski and S. Scheiner, “Isotropy of Ion Interactions: NH4+ vs K+, in Fundamentals of Gas Phase Ion Chemistry (ed. K.R. Jennings), NATO ASI, Series C, Vol. 347, Kluwer Academic Publishers, Dordrecht, 1991, 148.

R30. J.F. Liebman, S.O. Yee and C.A. Deakyne, “Systematics and Surprises in Bond Energies of Fluorinated Reactive Intermediates,” in Effect of Selective Fluorination on Reactivity in Organic and Bioorganic Chemistry (ed. J.T. Welch), American Chemical Society, Washington, DC, ACS Symposium Series, 456, 36-54 (1991).

R29. J.F. Liebman, “Thermochemistry of Sulphonic Acids and their Deriva­tives,” in The Chemistry of the Sulphonic Acids, Esters and their Derivatives, (ed. S. Patai and Z. Rappoport), Wiley, Chichester, 283-321 (1991).

R28. J.F. Liebman and C.D. Hoff, “The Thermochemistry of Hydrocarbon Activation Reactions. A View from the Organic and Metal Perspectives,” in Selective Hydrocarbon Activation:  Principles and Progress, (ed. J.A. Davies, P.L. Watson, J.F. Liebman and A. Greenberg), VCH Publishers, Inc., NewYork,149-206 (1990).

R27. J.F. Liebman and A. Greenberg, “Survey of the Heats of Formation of Three‑Membered Ring Species,” Chem. Rev., 89, 1225‑1246 (1989).

R26. G. Frenking, W. Koch and J.F. Liebman, “A Comparison of Isoelectronic Hydrogen and Helium(+) Compounds” in From Atoms to Polymers: Isoelec­tronic Reasoning, (ed. J.F. Liebman and A. Greenberg), VCH Publish­ers, Inc., New York, 169‑213 (1989).

R25. J.F. Liebman and R.M. Pollack “Thermochemistry of Enones and Related Species” in The Chemistry of the Enone Functional Group (ed. S. Patai and Z. Rappoport), Wiley, Chichester, 107‑128 (1989).

R24. J.F. Liebman, “Fluorine Chemistry Without Fluorine: Substituent Effects and Empirical Mimicry, in Fluorine‑containing Molecules: Structure, Reactivity, Synthesis and Applications (ed. J.F. Liebman, A. Greenberg and W.R. Dolbier, Jr.), VCH Publishers, Inc., New York, 309‑329 (1988).

R23. J.A. Berson, D.M. Birney, W.P. Dailey III and J.F. Liebman, “Ethyl­enedione, Its Ions and Analogues” in Modern Models of Bonding and Delocalization (ed. J.F. Liebman and A. Greenberg), VCH Publishers, Inc., New York, 391‑441 (1988).

R22. A. Greenberg and J.F. Liebman, “Structure/Energy Studies on Substituted Strained Molecules,” in Molecular Structure: Chemical Reactivity and Biological Activity (ed. J.J. Stezowski, J.‑L. Huang and M.‑C. Shao), Oxford University Press, Oxford, 313‑318 (1988).

R21. A. Greenberg, P.‑C. Lyu, J.F. Liebman and C.J. Cheer, “Structural Studies of Substituted Prismanes and Nitrocyclopropenes: Comparisons of Ab‑Initio Calculations, Experimental X‑Ray Data and Analysis of Structural Trends,” Report 6th Annual Working Group on Synthesis of High Energy Density Materials, US Army Armament Research, Development and Engineering Center, (AARDEC, May, 1987), 40‑62 (1988).

R20. J.F. Liebman, J.S. Chickos and J. Simons, “Aspects of the Estimation of Physical Properties of Boron Compounds by the Use of Isoelectronic and Plemeioelectronic Analogies” in Advances in Boron and the Boranes: A volume in honor of Anton B. Burg (ed. J.F. Liebman, A. Greenberg and R.E. Williams), VCH Publishers, Inc., New York, 491‑516 (1988).

R19. A. Greenberg, W.J. Simonsick, Jr. and J.F. Liebman, “Experimental and Calculated Reactivity Parameters of Potential Environmental Signifi­cance for Nitro‑Polycyclic Aromatic Hydrocarbons” in Proceedings of the 1987 EPA/APCA Symposium on the Measurement of Toxic Air Pollutants (ed. R.K.M. Jayanty and S. Hochheiser), APCA, Pittsburgh, 329‑340 (1987).

R18. J.F. Liebman and A. Greenberg, “Cyclopropanes with Additional Strain,” in The Chemistry of the Cyclopropyl Functional Group (ed. Z. Rappoport), Wiley, Chichester, 1083‑1119 (1987).

R17. J.F. Liebman, “Estimation and Mimicry in Cage and Substituted Cage Energetics.” Report Working Group on Synthesis of High Energy Density Materials, US Army Armament Munitions and Chemical Command (ARDEC, May, 1986), 53‑71 (1987).

R16. J.F. Liebman, “Are the Numerical Magnitudes of Proton Affinities Intuitively `Plausible'?” in Molecular Structure and Energetics: Biophysical Aspects, Vol. 4, (ed. J.F. Liebman and A. Greenberg), VCH Publishers, Inc., Deerfield Beach, FL and New York, NY, 49‑70 (1987).

R15. J.F. Liebman, “The Limiting Values of Ionization Potentials of 1‑Substituted Alkanes,” in Structure/Reactivity and Thermochemistry of Ions (ed. P. Ausloos and S.G. Lias), NATO ASI, Series C, Vol. 193, D. Reidel Publishing Co., Dordrecht, 371‑373 (1987).

R14. J.F. Liebman, “Estimation of Phase Change Enthalpies for Deriving Thermo­chemical Properties of Organic Compounds,” in Structure/Reacti­vity and Thermochemistry of Ions (ed. P. Ausloos and S.G. Lias), NATO ASI, Series C, Vol. 193, D. Reidel Publishing Co., Dordrecht, 404‑406 (1987).

R13. J.F. Liebman and D. Van Vechten, “Universality: Interre­lationships among Heats of Formation, Resonance Energies and Strain Energies,” in Molecular Structure and Energetics: Physical Measurements, Vol. 2, (ed. J.F. Liebman and A. Greenberg), VCH Publishers, Inc., Deerfield Beach, FL and New York, NY, 315‑374 (1987).

R12. J.F. Liebman, “Macroincrementation: A ‘Holistic' Estimation Approach,” in Molecular Structure and Energetics: Studies of Organic Molecules, Vol. 3, (ed. J.F. Liebman and A. Greenberg), VCH Publishers, Inc., Deerfield Beach, FL and New York, NY, 267‑328 (1986).

R11. J.F. Liebman and J. Simons, “Carbenes: A Study in Quantita­tive and Qualitative Theory,” in Molecular Structure and Energetics: Chemical Bonding Models, Vol. 1, (ed. J.F. Liebman and A. Greenberg), VCH Publishers, Inc., Deerfield Beach, FL and New York, NY, 51‑99 (1986).

R10. L.A. Nottingham, J.S. Plotkin and J.F. Liebman, “Improved Calculation of Strain Energies for Cage Mole­cules.” Report Working Group on Synthesis High Energy Density Materials, US Armament Munitions and Chemical Command, (ARDC, June 1985), 31‑47 (1986).

R9. J.F. Liebman, “Estimation Methods and Regularities in the Chemical Energetics of Organic Compounds: Sublimation Energies of Hydrocarbons, Resonance Energies of Nitroanil­ines and Entropies of Formation and Reaction,” Proc. Working Group Meeting on the Synthesis of High Density Energetic Materials, US Army and Armaments Research and Development Command (ARDC, May, 1984), 23‑44 (1985).

R8. S.G. Lias, J.F. Liebman and R.D. Levin, “Evaluated Gas Phase Basicities and Proton Affinities of Molecules; Heat of Formation of Protonated Molecules,” J. Phys. Chem. Ref. Data, 13, 695‑808 (1984).

R7. M.W. Victor and J.F. Liebman, “Macroincrementation of Densities and Molar Volumes,” Proc. Seminar High Density Energetic Materials, US Army Armaments Research and Develop­ment Command (ARRDCOM, May, 1982), 35‑65 (1984).

R6. J.F. Liebman, “The Conceptual Chemistry of the Cyclophanes,” in The Cyclophanes, (ed. P.M. Keehn and S.M. Rosenfeld), Academic Press, New York, NY, 23‑68 (1983).

R5. J.S. Chickos, A. Greenberg, L.H. Ladon, C.M. Lee, H.M. Ro­senstock, P.J. Rybcyznski, C.C. Van Vechten, Jr. and J.F. Liebman, “Macroincrementation: Simple Methods for Estimating Molecular Properties,” Proc. High Energy Hydro­carbon Fuels Workshop, Naval Air Systems Command (NAVAC, Nov. 1981), 161‑191 (1982).

R4. H.M. Rosenstock, J. Dannacher and J.F. Liebman, “The Role of Excited Electronic States in Ionic Fragmentation, C6H6+,” Radiat. Phys. Chem., 20, 7‑27 (1982).

R3. J.F. Liebman, P. Politzer and D.C. Rosen, “The π‑Fluoro Effect; An `Empirical' Application of Atomic Electrostatic Potentials,” in Applications of Electrostatic Potentials in Chemistry, (ed. P. Politzer and D.G. Truhlar), Plenum, New York, NY, 295‑308 (1981).

R2. J.F. Liebman and A. Greenberg, “A Survey of Strained Organic Molecules,” Chem. Rev., 76, 311‑365 (1976).

R1. J.F. Liebman, “An Attempt to Reconcile Conflicting Measure­ments of the Bond Strengths in the Xenon Fluorides,” in Inorganic and Nuclear Chemistry: Herbert H. Hyman Memorial Volume (ed. J.J. Katz and I. Sheft), Pergamon Press, New York, NY, 155‑157 (1976). This paper is also considered article I in the series “Conceptual Problems in Noble Gas and Fluorine Chemistry.”

## Coauthored or Coedited Books, and other works

B28. C.A. Deakyne and J.F. Liebman (coeditors), Special Issue of International Journal of Chemical Modeling”, in dedication and memory of Henry A. Bent, Intl. J. Chem. Model, 8 , issues 3 + 4, 253-434 (2016).

B27. C.A. Deakyne and J.F. Liebman (coeditors), Special Issue of International Journal of Chemical Modeling”, in dedication and memory of Leland C. Allen, Intl. J. Chem. Model, 8 , issues 1 + 2 (2016), 1 – 250 (2016).

B26. Z. Rappoport, J.F. Liebman and I. Marek (coeditors) “Patai’s Chemistry of Functional Groups: The Chemistry of Organogold Compounds” part 1, pp. 1 – 525 + xix and part 2, 527 – 1017 + xix (Wiley, Chichester, 2014).

B25, R.D. Weir, J.A. Martinho Simões, J.F. Liebman and M.J.S. Monte*),* A Special Issue of *The Journal of Chemical Thermodynamics* J. Chem. Thermodyn., in memory of Manuel A.V. Ribeiro da Silva, J. Chem. Thermodyn,., 73 (2014)..

B24. A. Greer and J.F. Liebman (coeditors), “Patai’s Chemistry of Functional Groups: The Chemistry of Peroxides, Vol. 3” part 1, 1 – 435 + xxiv and part 2, pp. 437 – 906 + xxiv (Wiley, Chichester, 2014).

B23. J.F. Liebman, J.S. Chickos and R. Notario (special editors), “Maria Victoria Roux: Calorimetrist, Colleague, Friend” (A special issue of *Structural Chemistry* in honor of Maria Victoria Roux on the occasion of her retirement.) Struct. Chem., 24, issue 6 (2013).

B22. Z. Rappoport and J.F. Liebman (coeditors), “Patai’s Chemistry of Functional Groups: The Chemistry of Hydroxylamines, Oximes and Hydroxamic Acids, Vol. 2” part 1, pp. 1 – 547 + xix and part 2, pp. 549 – 1078 + xix (Wiley, Chichester, 2011).

B21. Z. Rappoport and J.F. Liebman (coeditors), “The Chemistry of Hydroxylamines, Oximes and Hydroxamic Acids, Vol. 1” part 1, pp. 1 – 514 + xix and part 2, pp. 515 – 1038 + xix (Wiley, Chichester, 2009).

B20. Z. Rappoport and J.F. Liebman (coeditors), “The Chemistry of Cyclobutanes,” part 1, pp. 1-616 + xix; part 2, pp. 617-1226 + xix (Wiley, Chichester, 2005).

B19. A. Greenberg, C.M. Breneman and J.F. Liebman (coeditors), “The Amide Linkage: Structural Significance in Chemistry, Biochemistry and Materials Science,” pp. 653 + xii, (Wiley, New York, hardcover, 2000; amended paperback, 2003).

B18. J.A. Martinho Simões, A. Greenberg and J.F. Liebman (coeditors), “Energetics of Organic Free Radicals,” pp. 301 + xii, (Blackie Academic & Professional, an imprint of Chapman & Hall, London, 1996).

B17. J.S. Valentine, C.S. Foote, A. Greenberg and J.F. Liebman (coeditors), “Active Oxygen in Biochemistry,” pp. 463 + xvii, (Blackie Academic & Professional, an imprint of Chapman & Hall, London, hardcover, 1995; paperback, 1995).

B16. C.S. Foote, J.S. Valentine, A. Greenberg and J.F. Liebman (coeditors), “Active Oxygen in Chemistry,” pp. 342 + x, (Blackie Academic & Professional, an imprint of Chapman & Hall, London, hardcover, 1995; paperback, 1995).

B15. G.D. Mendenhall, A. Greenberg and J.F. Liebman (coeditors), “Mesomolecules: From Molecules to Materials,” pp. 199 + xi (Chapman & Hall, New York, 1995).

B14. J.A. Davies, P.L. Watson, J.F. Liebman and A. Greenberg (coeditors), “Selective Hydrocarbon Activation: Principles and Progress,” pp. 568 + xiv (VCH Publishers, Inc., New York, 1990).

B13. J.F. Liebman and A. Greenberg (coeditors), “From Atoms to Polymers: Isoelectronic Analogies,” pp. 473 + xv (VCH Publishers, Inc., New York, 1989).

B12. J.F. Liebman and A. Greenberg (coeditors), “Environmental Influences and Recognition in Enzyme Chemistry,” pp. 349 + xv (VCH Publishers, Inc., New York, 1989).

B11. J.F. Liebman and A. Greenberg (coeditors), “Mechanistic Principles of Enzyme Activity,” pp. 404 + xii (VCH Publish­ers, Inc., New York, 1988).

B10. J.F. Liebman, A. Greenberg and W.R. Dolbier, Jr. (coeditors), “Fluor­ine‑Containing Molecules: Structure, Reactivity, Synthesis and Applica­tions,” pp. 346 + xvii (VCH Publishers, Inc., New York, 1988).

B9. J.F. Liebman and A. Greenberg (coeditors), “Structure and Reactivity,” pp. 385 + xiii (VCH Publishers, Inc., New York, 1988).

B8. J.F. Liebman and A. Greenberg (coeditors), “Modern Models of Bonding and Delocaliza­tion,” pp. 461 + xiv (VCH Publishers, Inc., New York, 1988).

B7. S.G. Lias, J.E. Bartmess, J.F. Liebman, J.L. Holmes, R.D. Levin and W.G. Mallard, “Gas‑Phase Ion and Neutral Thermochemistry,” pp. 861 + iii (J. Phys. Chem. Ref. Data, 17, supplement 1, 1988).

B6. J.F. Liebman, A. Greenberg and R.E. Williams (coeditors), “Advances in Boron and the Boranes: A volume in honor of Anton B. Burg,” pp. 547 + xiv (VCH Publishers, Inc., New York, 1988).

B5. J.F. Liebman and A. Greenberg (coeditors), “Molecular Structure and Energetics: Biophysical Aspects,” (Vol. 4), pp. 405 + xvi (VCH Publish­ers Inc., Deerfield Beach, 1987).

B4. J.F. Liebman and A. Greenberg (coeditors), “Molecular Structure and Energetics: Physical Measurements,” (Vol. 2), pp. 388 + xiii (VCH Publishers Inc., Deerfield Beach, 1987).

B3. J.F. Liebman and A. Greenberg (coeditors), “Molecular Structure and Energetics: Studies of Organic Molecules,” (Vol. 3), pp. 385 + xiv (VCH Publishers, Inc., Deerfield Beach, 1986).

B2. J.F. Liebman and A. Greenberg (coeditors), “Molecular Structure and Energetics: Chemical Bonding Models,” (Vol. 1), pp. 360 + xiv (VCH Publishers, Inc., Deerfield Beach, 1986).

B1. A. Greenberg and J.F. Liebman (invited authors), “Strained Organic Molecules,” pp. 406 + xi, (Academic Press, New York, 1978).

### Electronic Data Bases and Other Documents

ED46. S.G. Lias, H.M. Rosenstock, K. Draxl, B.W. Steiner, J.R. Herron, J.L. Holmes, R.D. Levin, J.F. Liebman and S.A. Kafafi, “Ion Energetics (IE, AE) Data,” in “NIST Chemistry WebBook,” NIST Stand. Ref. Data Base, (Ed. P.J. Linstrom, 2015).

ED45. J.S. Chickos, W.E. Acree, Jr., J.F. Liebman and Students of CHEM 202, University of Missouri-St. Louis, “Heat of Fusion,” in “NIST Chemistry WebBook,” NIST Stand. Ref. Data Base, (Ed. P.J. Linstrom, 2015).

.

ED45. H.Y. Afeefy, J.F. Liebman and S.E. Stein, “Neutral Thermochemical Data,” in “NIST Chemistry WebBook,” NIST Stand. Ref. Data Base, (Ed. P.J. Linstrom, 2015).

ED44. S.G. Lias, H.M. Rosenstock, K. Draxl, B.W. Steiner, J.R. Herron, J.L. Holmes, R.D. Levin, J.F. Liebman and S.A. Kafafi, “Ion Energetics (IE, AE) Data,” in “NIST Chemistry WebBook,” NIST Stand. Ref. Data Base, (Eds. P.J. Linstrom and W.G. Mallard, 2014).

ED43. J.S. Chickos, W.E. Acree, Jr., J.F. Liebman and Students of CHEM 202, University of Missouri-St. Louis, “Heat of Fusion,” in “NIST Chemistry WebBook,” NIST Stand. Ref. Data Base, (Eds. P.J. Linstrom and W.G. Mallard, 2014).

ED42. H.Y. Afeefy, J.F. Liebman and S.E. Stein, “Neutral Thermochemical Data,” in “NIST Chemistry WebBook,” NIST Stand. Ref. Data Base, (Eds. P.J. Linstrom and W.G. Mallard, 2014).

ED41. S.G. Lias, H.M. Rosenstock, K. Draxl, B.W. Steiner, J.R. Herron, J.L. Holmes, R.D. Levin, J.F. Liebman and S.A. Kafafi, “Ion Energetics (IE, AE) Data,” in “NIST Chemistry WebBook,” NIST Stand. Ref. Data Base, (Eds. P.J. Linstrom and W.G. Mallard, 2013).

ED40. J.S. Chickos, W.E. Acree, Jr., J.F. Liebman and Students of CHEM 202, University of Missouri-St. Louis, “Heat of Fusion,” in “NIST Chemistry WebBook,” NIST Stand. Ref. Data Base, (Eds. P.J. Linstrom and W.G. Mallard, 2013).

ED39. H.Y. Afeefy, J.F. Liebman and S.E. Stein, “Neutral Thermochemical Data,” in “NIST Chemistry WebBook,” NIST Stand. Ref. Data Base, (Eds. P.J. Linstrom and W.G. Mallard, 2013).

ED41. S.G. Lias, H.M. Rosenstock, K. Draxl, B.W. Steiner, J.R. Herron, J.L. Holmes, R.D. Levin, J.F. Liebman and S.A. Kafafi, “Ion Energetics (IE, AE) Data,” in “NIST Chemistry WebBook,” NIST Stand. Ref. Data Base, (Eds. P.J. Linstrom and W.G. Mallard, 2012).

ED40. J.S. Chickos, W.E. Acree, Jr., J.F. Liebman and Students of CHEM 202, University of Missouri-St. Louis, “Heat of Fusion,” in “NIST Chemistry WebBook,” NIST Stand. Ref. Data Base, (Eds. P.J. Linstrom and W.G. Mallard, 2012).

ED39. H.Y. Afeefy, J.F. Liebman and S.E. Stein, “Neutral Thermochemical Data,” in “NIST Chemistry WebBook,” NIST Stand. Ref. Data Base, (Eds. P.J. Linstrom and W.G. Mallard, 2012).

ED38. S.G. Lias, H.M. Rosenstock, K. Draxl, B.W. Steiner, J.R. Herron, J.L. Holmes, R.D. Levin, J.F. Liebman and S.A. Kafafi, “Ion Energetics (IE, AE) Data,” in “NIST Chemistry WebBook,” NIST Stand. Ref. Data Base, (Eds. P.J. Linstrom and W.G. Mallard, 2011).

ED37. J.S. Chickos, W.E. Acree, Jr., J.F. Liebman and Students of CHEM 202, University of Missouri-St. Louis, “Heat of Fusion,” in “NIST Chemistry WebBook,” NIST Stand. Ref. Data Base, (Eds. P.J. Linstrom and W.G. Mallard, 2011).

ED36. H.Y. Afeefy, J.F. Liebman and S.E. Stein, “Neutral Thermochemical Data,” in “NIST Chemistry WebBook,” NIST Stand. Ref. Data Base, (Eds. P.J. Linstrom and W.G. Mallard, 2011).

ED35. M. Rothlisberger, L. Portsmouth, Z. Rappoport, J.F. Liebman and I. Marek, “Instructions to Contributors: Patai’s Chemistry of Functional Groups” (Wiley, Chichester, 2010).

ED34. S.G. Lias, H.M. Rosenstock, K. Draxl, B.W. Steiner, J.R. Herron, J.L. Holmes, R.D. Levin, J.F. Liebman and S.A. Kafafi, “Ion Energetics (IE, AE) Data,” in “NIST Chemistry WebBook,” NIST Stand. Ref. Data Base, (Eds. P.J. Linstrom and W.G. Mallard, 2010).

ED33. J.S. Chickos, W.E. Acree, Jr., J.F. Liebman and Students of CHEM 202, University of Missouri-St. Louis, “Heat of Fusion,” in “NIST Chemistry WebBook,” NIST Stand. Ref. Data Base, (Eds. P.J. Linstrom and W.G. Mallard, 2010).

ED32 H.Y. Afeefy, J.F. Liebman and S.E. Stein, “Neutral Thermochemical Data,” in “NIST Chemistry WebBook,” NIST Stand. Ref. Data Base, (Eds. P.J. Linstrom and W.G. Mallard, 2010).

ED31. S.G. Lias, H.M. Rosenstock, K. Draxl, B.W. Steiner, J.R. Herron, J.L. Holmes, R.D. Levin, J.F. Liebman and S.A. Kafafi, “Ion Energetics (IE, AE) Data,” in “NIST Chemistry WebBook,” NIST Stand. Ref. Data Base, (Eds. P.J. Linstrom and W.G. Mallard, 2009).

ED30. J.S. Chickos, W.E. Acree, Jr., J.F. Liebman and Students of CHEM 202, University of Missouri-St. Louis, “Heat of Fusion,” in “NIST Chemistry WebBook,” NIST Stand. Ref. Data Base, (Eds. P.J. Linstrom and W.G. Mallard, 2009).

ED29 H.Y. Afeefy, J.F. Liebman and S.E. Stein, “Neutral Thermochemical Data,” in “NIST Chemistry WebBook,” NIST Stand. Ref. Data Base, (Eds. P.J. Linstrom and W.G. Mallard, 2009).

ED28. S.G. Lias, H.M. Rosenstock, K. Draxl, B.W. Steiner, J.R. Herron, J.L. Holmes, R.D. Levin, J.F. Liebman and S.A. Kafafi, “Ion Energetics (IE, AE) Data,” in “NIST Chemistry WebBook,” NIST Stand. Ref. Data Base, (Eds. P.J. Linstrom and W.G. Mallard, 2008).

ED27. J.S. Chickos, W.E. Acree, Jr., J.F. Liebman and Students of CHEM 202, University of Missouri-St. Louis, “Heat of Fusion,” in “NIST Chemistry WebBook,” NIST Stand. Ref. Data Base, (Eds. P.J. Linstrom and W.G. Mallard, 2008).

ED26. H.Y. Afeefy, J.F. Liebman and S.E. Stein, “Neutral Thermochemical Data,” in “NIST Chemistry WebBook,” NIST Stand. Ref. Data Base, (Eds. P.J. Linstrom and W.G. Mallard, 2008).

ED25. M. Ponikvar, H.D.B. Jenkins and J.F. Liebman, “Patterns and Estimation of the Entropies of Formation of Fluorine Containing Aqueous Anions,” “Papers Dedicated to Prof. Neil Bartlett on the occasion of his 75th Birthday from His Friends and Colleagues” (234th ACS National Meeting, Boston, August 2007) (a cd edited by Alain Tressaud, CNRS).

ED24. M. Ponikvar and J.F. Liebman, “Stability of PnF6 (Pn = P, As, Sb, Bi) Species in Aqueous Media,” “Slovenski Kemijski Dnevi, 11th, Maribor, Slovenia, Sept. 22-23, 2005, A9/1-A9/4.: Univerza v Mariboru, Fakulteta za Kemijo in Kemijsko Tehnologijo, Maribor, Slovenia) (a cd in Slovenian).

ED23. S.G. Lias, H.M. Rosenstock, K. Draxl, B.W. Steiner, J.R. Herron, J.L. Holmes, R.D. Levin, J.F. Liebman and S.A. Kafafi, “Ion Energetics (IE, AE) Data,” in “NIST Chemistry WebBook,” NIST Stand. Ref. Data Base, June 2005 Release (W.G. Mallard and P.J. Linstrom, general editors, 2005). Translations into Spanish, Portuguese, French and Czech, provided courtesy of European Union project "Eurospec - Access to Research Spectroscopic Data and Associated Chemical Knowledge - GTC1-2001-43000.”

ED22. J.S. Chickos, W.E. Acree, Jr., J.F. Liebman and Students of CHEM 202, University of Missouri-St. Louis, “Heat of Fusion,” in “NIST Chemistry WebBook,” NIST Stand. Ref. Data Base, June 2005 Release (W.G. Mallard and P.J. Linstrom, general editors, 2005). Translations into Spanish, Portuguese, French and Czech, provided courtesy of European Union project "Eurospec - Access to Research Spectroscopic Data and Associated Chemical Knowledge - GTC1-2001-43000.”

ED21. H.Y. Afeefy, J.F. Liebman and S.E. Stein, “Neutral Thermochemical Data,” in “NIST Chemistry WebBook,” NIST Stand. Ref. Data Base, June 2005 Release (W.G. Mallard and P.J. Linstrom, general editors, 2005). Translations into Spanish, Portuguese, French and Czech, provided courtesy of European Union project "Eurospec - Access to Research Spectroscopic Data and Associated Chemical Knowledge - GTC1-2001-43000.”

ED20. S.G. Lias, H.M. Rosenstock, K. Draxl, B.W. Steiner, J.R. Herron, J.L. Holmes, R.D. Levin, J.F. Liebman and S.A. Kafafi, “Ion Energetics (IE, AE) Data,” in “NIST Chemistry WebBook,” NIST Stand. Ref. Data Base, Eighth Release (W.G. Mallard and P.J. Linstrom, general editors, 2003).

ED19. J.S. Chickos, W.E. Acree, Jr., J.F. Liebman and Students of CHEM 202, University of Missouri-St. Louis, “Heat of Fusion,” in “NIST Chemistry WebBook,” NIST Stand. Ref. Data Base, Eighth Release (W.G. Mallard and P.J. Linstrom, general editors, 2003).

ED18. H.Y. Afeefy, J.F. Liebman and S.E. Stein, “Neutral Thermochemical Data,” in “NIST Chemistry WebBook,” NIST Stand. Ref. Data Base, Eighth Release (W.G. Mallard and P.J. Linstrom, general editors, 2003).

ED17. S.G. Lias, H.M. Rosenstock, K. Draxl, B.W. Steiner, J.R. Herron, J.L. Holmes, R.D. Levin, J.F. Liebman and S.A. Kafafi, “Ion Energetics (IE, AE) Data,” in “NIST Chemistry WebBook,” NIST Stand. Ref. Data Base, Seventh Release (W.G. Mallard and P.J. Linstrom, general editors, 2001).

ED16. J.S. Chickos, W.E. Acree, Jr., J.F. Liebman and Students of CHEM 202, University of Missouri-St. Louis, “Heat of Fusion,” in “NIST Chemistry WebBook,” NIST Stand. Ref. Data Base, Seventh Release (W.G. Mallard and P.J. Linstrom, general editors, 2001).

ED15. H.Y. Afeefy, J.F. Liebman and S.E. Stein, “Neutral Thermochemical Data,” in “NIST Chemistry WebBook,” NIST Stand. Ref. Data Base, Seventh Release (W.G. Mallard and P.J. Linstrom, general editors, 2001).

ED14. S.G. Lias, H.M. Rosenstock, K. Draxl, B.W. Steiner, J.T. Herron, J.L. Holmes, R.D. Levin, J.F. Liebman and S.A. Kafafi, “Ion Energetics (IE, AE) Data,” in “NIST Chemistry WebBook” , NIST Stand. Ref. Data Base, Sixth Release (W.G. Mallard and P.J. Linstrom, general editors, 2000).

ED13. H.Y. Afeefy, J.F. Liebman and S.E. Stein, “Neutral Thermochemical Data,” in “NIST Chemistry WebBook,” NIST Stand. Ref. Data Base, Sixth Rlease (W.G. Mallard and P.J. Linstrom, general editors, 2000).

ED12. S.G. Lias, H.M. Rosenstock, K. Draxl, B.W. Steiner, J.T. Herron, J.L. Holmes, R.D. Levin, J.F. Liebman and S.A. Kafafi, “Ion Energetics (IE, AE) Data,” in “NIST Chemistry WebBook,” NIST Stand. Ref. Data Base, Fifth Release, (W.G. Mallard and P.J. Linstrom, general editors, 1998).

ED11. H.Y. Afeefy, J.F. Liebman and S.E. Stein, “Neutral Thermochemical Data,” in “NIST Chemistry WebBook,” NIST Stand. Ref. Data Base, Fifth Release, (W.G. Mallard and P.J. Linstrom, general editors, 1998).

ED10. S.G. Lias, H.M. Rosenstock, K. Draxl, B.W. Steiner, J.T. Herron, J.L. Holmes, R.D. Levin, J.F. Liebman and S.A. Kafafi, “Ion Energetics (IE, AE) Data,” in “NIST Chemistry WebBook,” NIST Stand. Ref. Data Base, Fourth Release (W.G. Mallard and P.J. Linstrom, general editors, 1997).

ED9. H.Y. Afeefy, J.F. Liebman and S.E. Stein, “Neutral Thermochemical Data,” in “NIST Chemistry WebBook,” NIST Stand. Ref. Data Base, Fourth Release, (W.G. Mallard and P.J. Linstrom, general editors, 1997).

ED8. H.Y. Afeefy, J.F. Liebman and S.E. Stein, “Neutral Thermochemical Data,” in “NIST Chemistry WebBook,” NIST Stand. Ref. Data Base, Third Release, (W.G. Mallard and P.J. Linstrom, general editors, 1997).

ED7. S.G. Lias, H.M. Rosenstock, K. Draxl, B.W. Steiner, J.T. Herron, J.L. Holmes, R.D. Levin, J.F. Liebman and S.A. Kafafi, “Ion Energetics (IE, AE) Data,” in “NIST Chemistry WebBook,” NIST Stand. Ref. Data Base, Third Release, (W.G. Mallard and P.J. Linstrom, general editors, 1997).

ED6. S.G. Lias, H.M. Rosenstock, K. Draxl, B.W. Steiner, J.T. Herron, J.L. Holmes, R.D. Levin, J.F. Liebman and S.A. Kafafi, “Ion Energetics (IE, AE) Data,” in “NIST Chemistry WebBook,” NIST Stand. Ref. Data Base, Second Release, (W.G. Mallard and P.J. Linstrom, general editors, 1997).

ED5. H.Y. Afeefy, J.F. Liebman and S.E. Stein, “Neutral Thermochemical Data,” in “NIST Chemistry WebBook,” NIST Stand. Ref. Data Base, Second Release, (W.G. Mallard and P.J. Linstrom, general editors, 1997).

ED4. S.G. Lias, H.M. Rosenstock, K. Draxl, B.W. Steiner, J.T. Herron, J.L. Holmes, R.D. Levin, J.F. Liebman and S.A. Kafafi, “Ion Energetics (IE, AE) Data,” in “NIST Chemistry WebBook,” NIST Stand. Ref. Data Base, First Release, (W.G. Mallard and P.J. Linstrom, general editors, 1996).

ED3. H.Y. Afeefy, J.F. Liebman and S.E. Stein, “Neutral Thermochemical Data,” in “NIST Chemistry WebBook,” NIST Stand. Ref. Data Base, First Release, (W.G. Mallard and P.J. Linstrom, general editors, 1996).

ED2. S.G. Lias, J.F. Liebman, R.D. Levin and S.A. Kafafi, “Positive Ion Energetics Version 2.0,” NIST Stand. Ref. Data Base 19A (1993).

ED1. S.G. Lias, J.F. Liebman, J.L. Holmes, R.D. Levin and W. G. Mallard, “Positive Ion Energetics Version 1.0,” NIST Stand. Ref. Data Base 19A (1989).

### Book Reviews

BR38. “Computational Organic Chemistry” (2nd Edition) by S.M.Bachrach, Mol. Crysr, Liq. Cryst., 616, 257–258 (2015).

.

BR37. “Time-Dependent Density-Functional Theory: Concepts and Applications” by C.A. Ullrich, Mol. Cryst. Liq. Cryst., 569, 165-166 (2012).

BR36. “Neither Physics nor Chemistry: A History of Quantum Chemistry” by K. Gavroglu and A. Simões, Mol. Cryst. Liq. Cryst., 569, 163-164 (2012).

BR35. “Density Functional Theory: A Practical Introduction” by D.S. Sholl and J.A. Steckel, Mol. Cryst. Liq. Cryst., 515, 249-250 (2009).

BR34. “Molecular Modeling for Beginner” (2nd Ed.) by A. Hinchliffe, Mol. Cryst. Liq. Cryst., 515, 247-248 (2009).

BR33. “Number Theory and the Periodicity of Matter” by J.C.A. Boeyens and D.C. Levendis, Mol. Cryst. Liq. Cryst., 503, 164-165 (2009).

BR32. “The Basics of Theoretical and Computational Chemistry” by B.M. Rode, T.S. Hofer and M.D. Kugler, Mol. Cryst. Liq. Cryst., 473, 105-106 (2007).

BR31. “Molecular Physics: Theoretical Principles and Experimental Methods” by W. Demtröder, Mol. Cryst. Liq. Cryst., 460, 151-152 (2006).

BR30. “Molecular Modelling for Beginners,” by A. Hinchliffe, Mol. Cryst. Liq. Cryst., 442, 203-205 (2005) (reviewed with S.K. Gregurick).

BR29. “New Theories for Chemistry” by J.C.A. Boeyens, J. Am. Chem. Soc., 127, 14526-14527 (2005).

BR28. “An Introduction to Theoretical Chemistry” by J. Simons, Mol. Cryst. Liq. Cryst., 420, 97-98 (2004).

BR27. “The Theories of Chemistry,” by J.C.A. Boeyens, J. Am. Chem. Soc., 126, 8350 (2004).

BR26. “The Road to Stockholm: Nobel Prizes, Science and Scientists,” by I. Hargittai, Chem. Intl., 25, 24 (2003).

BR25. “Deciphering the Chemical Code: Bonding Across the Periodic Table,” by N. Epiotis, Struct. Chem., 8, 233-234 (1997) (reviewed with A. Greenberg).

BR24. “Molecular Structure and Statistical Thermodynamics: Selected Papers of Kenneth S. Pitzer (ed. K.S. Pitzer), Chem. Intelligencer, 2, 52-53 (1995).

BR23. “Bonding Energetics in Organometallic Compounds,” ed. by T.J. Marks, Struct. Chem., 2, 607 (1991).

BR22. “Fluorine in Bioorganic Chemistry,” by J.T. Welch and S. Eswarakrishnan, J. Am. Chem. Soc., 113, 8195 (1991) (reviewed with M. Hulce).

BR21. “Handbook of the Thermodynamics of Organic Compounds,” by R.M. Stephenson and S. Malanowski, J. Am. Chem. Soc., 111, 2366 (1989).

BR20. “Annual Reviews in Physical Chemistry,” Vol. 38, ed. H.L. Strauss, G.T. Bobcock and C.B. Moore, J. Am. Chem. Soc., 111, 796 (1989).

BR19. “Partition Coefficient: Determination and Estimation,” by W.J. Dunn, III, J.H. Block and R.S. Pearlman, J. Am. Chem. Soc., 110, 3339 (1988).

BR18. “Molecular Volumes in Chemistry and Biology: Applications Including Partitioning and Toxicity,” J.C. McGowan and A. Mellors, J. Am. Chem. Soc., 110, 3339 (1988).

BR17. “CODATA Thermodynamic Tables. Selections for Some Compounds of Calcium and Related Mixtures,” ed. D. Garvin, V.B. Parker and H.J. White, Jr., J. Am. Chem. Soc., 110, 3340 (1988).

BR16. “Calculated Molecular Properties of Polynuclear Aromatic Com­pounds,” by R.A. Hites and W.J. Simonsick, Jr., J. Am. Chem. Soc., 110, 3340 (1988).

BR15. “JANAF Thermochemical Tables,” by M.W. Chase, Jr., C.A. Davies, J.R. Downey, Jr., D.J. Frurip, R.A. McDonald and A.N. Syverud, J. Am. Chem. Soc., 110, 2997 (1988).

BR14. “Magnetic Atoms and Molecules,” by W. Weltner, Jr., J. Am. Chem. Soc., 106, 6120 (1984).

BR13. “The Physics and Chemistry of Color: The Fifteen Causes of Color,” by K. Nassau, J. Am. Chem. Soc., 106, 6123 (1984).

BR12. “Ionization Potential and Appearance Potential Measure­ments 1971 ‑ 1981. NSRDS ‑ NBS 71,” by R.D. Levin and S.G. Lias, J. Am. Chem. Soc., 106, 829 (1984) (reviewed with C.C. Fenselau).

BR11. “Progress in Physical Organic Chemistry,” Vol. 13, ed. R.W. Taft, J. Am. Chem. Soc., 105, 7006 (1983) (reviewed with A. Greenberg).

BR10. “The Force Concept in Chemistry,” ed. B.M. Deb, J. Am. Chem. Soc., 105, 6773 (1983).

BR9. “Pattern Recognition in Chemistry. Lecture Notes in Chem­istry,” Vol. 21, by K. Varmuza, J. Am. Chem. Soc., 105, 6197 (1983).

BR8. “Quantum Theory of Chemical Reactions. Vol. II. Solvent Effects, Reaction Mechanisms, Photochemical Processes,” ed. R. Daudel, A. Pullman, L. Salem and A. Veillard, J. Am. Chem. Soc., 105, 5963 (1983).

BR7. “Annual Review of Physical Chemistry,” Vol. 33, (ed. B.S. Rabinovitch), J.M. Schurr and H.L.

Strauss, J. Am. Chem. Soc., 105, 5526 (1983).

BR6. “Current Applications of Quantum Chemistry 1981. Studies in Physical and Theoretical Chemistry,” Vol. 21, (ed. R. Carbo), J. Am. Chem. Soc., 105, 5526 (1983).

BR5. “Introduction to Applied Solid State Physics: Topics in the Applica­tions to Semiconductors, Superconductors and the Nonlinear Optical Properties of Solids,” by R. Dalven, J. Am. Chem. Soc., 104, 1456 (1982) (reviewed with E.D. Yorke).

BR4. “The Lewis Acid‑Base Concepts,” by W.B. Jensen, J. Am. Chem. Soc., 103, 3616 (1981).

BR3. “Rearrangements in Ground and Excited States,” (ed. P. de Mayo), J. Am. Chem. Soc., 103, 3615 (1981) (review­ed with A. Greenberg).

BR2. “Fitting Equations to Data: Computer Analysis of Multifactor Data,” (2nd Ed). by C. Daniel and F.S. Wood, J. Am. Chem. Soc., 102, 7822 (1980).

BR1. “Factor Analysis in Chemistry,” by E.A. Malinowski and D.G. Howery, J. Am. Chem. Soc., 102, 782(1980).

**Other Creative Activites Including Poems Appearing in Scientific Media**

OCA16, The poem “Ode to Gennady Kabo” as part of the t special issue of the Journal of Chemical Thermodynamics, 126, 544 (2018) in honor of Gennady Y. Kabo on the occasion of his 80th birthday.

OCA15. The poem “Let Us Recall Some Science, Much We Know Well”, part of the preface for an ACS book “The Posthumous Nobel Prize in Chemistry: Correcting the Errors and Oversights of the Nobel Prize Committee” (Ed. E.T. Strom and V. V. Mainz) ACS Symposium Series, Vol. 1262, 261 – 281 (2017) (American Chemical Society. Washington DC).

OCA14. The essay “Dedication to Professor Henry Bent”, part of the introductory material for a special issue of the International Journal of Chemical Modeling appearing in C.A. Deakyne and J.F. Liebman (eds.), “Special Issue Dedicated to and in Honor and Memory of Professsor Henry A. Bent, 8(3-4), 255-6 (2016).

OCA13. The poem “Ode to Henry A. Bent” part of the introductory material for a special issue of the International Journal of Chemical Modeling “Festschrift in Honor and Memory of Henry A. Bent on the occasion of his 90th Birthday” edited by C.A. Deakyne and J.F. Liebman (special editors) Intl. J. Chem. Model., 8(3-4). 253 (2016).

OCA12. The essay “Dedication and Memento to Professor Leland C, Allen”, part of the introductory material for a special issue of the International Journal of Chemical Modeling appearing in C.A. Deakyne and J.F. Liebman (eds.), “Special Issue Dedicated to and in Honor and Memory of Professsor Leland C. Allen, 8(1-2), 5-6 (2016).

OCA11. The poem “Ode to Lee Allen” part of the introductory material for a special issue of the International Journal of Chemical Modeling appearing in C.A. Deakyne and J.F. Liebman (eds.), “Special Issue Dedicated to and in Honor and Memory of Professor Leland C. Allen, Intl. J. Chem. Model., 8(1-2), 3 (2016).

OCA10. The poem “Ode to R.S. Brown” part of the introductory material for a special issue of the Canadian Journal of Chemistry in honor of R. Stanley Brown, (This primary research, refereed article is in honor of R. Stan Brown. Guest Editors, W. Leigh and V. Snieckus, Canad. J. Chem., 93(4), i – vii (2015). This issue contains our primary, invited, research article M.S. Miranda, P.J.O. Ferreira, J.C.G. Esteves da Silva and J.F. Liebman, “Three-Membered Ring Amides: A Calculational and Conceptual Study of the Structure and Energetics of 1,2-Oxaziridine-3-one and Aziridine-2,3-dione,” Canad. J. Chem., 93, 406-413 (2015).

OCA9. Authored foreword to “Quantum Molecule and Reactivity, Volume III,” of the five volune set “Quantum Nanochemistry” by M. V. Putz, Apple Academic Press (2016).

OCA8. The poem “Ode to Bob Moss” part of the introductory material for a special issue of the Journal of Physical Organic Chemistry on the occasion of ISRIUM at Pacifichem 2010 – Reactive Intermediates, Guest editors: D.C. Merrer and M.S. Platz, in honor of Robert A. Moss, J. Phys. Org. Chem., 24, 865 (2011).

OCA7. The poem “Ode to Neil Bartlett” appears in J.F. Liebman and C.A. Deakyne, “Noble Gas Compounds and Chemistry: A Brief Review of Interrelations and Interactions with Fluorine-containing Species,” J. Fluor. Chem., 121, 1-8 (2003). (This research/review article is in honor of Neil Bartlett on the occasion of his 70th birthday.)

OCA6. Miscellaneous untitled poems appearing in J.F. Liebman, K. Severin and T.M. Klapötke, “Inorganic Exotic Molecules,” in The Encyclopedia of Physical Science and Technology, 3rd edn. (genl. ed., R.A. Meyers), Academic Press, San Diego, Vol. 7, 817-838 (2002).

OCA5. The poem “Ode to Pat O’Hare” as part of the the frontsmatter of a special issue of the Journal of Chemical Thermodynamics, 34 (2002) in honor of Patrick A.G. O’Hare on the occasion of his 65th birthday. This issue contains our primary, invited, research article C.A. Deakyne, L. Li, W. Zheng, D. Xu and J.F. Liebman, “Regularities in the Bond Dissociation Enthalpies of Molecules of Type AB and BAB Energetics of Compounds of Groups 14 and 16,” J. Chem. Thermodyn., 34, 185-192 (2002).

OCA4. The poem “Ode to Van’t Hoff and LeBel,” as part of the frontsmatter of a special issue of Journal of Molecular Structure (1995) commemorating the 120th anniversary of the tetrahedral carbon atom edited by Z. Maksić and W.J. Orville-Thomas.) This issue contains our primary, invited, research article D.J. Berger, P.P. Gaspar and J.F. Liebman, “π-Overlap, Pyramidalization and Protonation of Group 15 Heterocycles: The Basicity of the ‘Higher Pyridines’,” J. Mol. Struct. (Theochem), 338, 51-70 (1995).

OCA3 Miscellaneous untitled poems in J.F. Liebman, “The Conceptual Chemistry of the Cyclophanes,” in The Cyclophanes, (ed. P.M. Keehn and S.M. Rosenfeld), Academic Press, New York, NY, 23‑68 (1983).

OCA2. Untitled poem appearing in J.F. Liebman, “An Attempt to Reconcile Conflicting Measure­ments of the Bond Strengths in the Xenon Fluorides,” in Inorganic and Nuclear Chemistry: Herbert H. Hyman Memorial Volume (ed. J.J. Katz and I. Sheft), Pergamon Press, New York, NY, 155‑157 (1976).

OCA1. Dedication in Ph.D. thesis, J.F. Liebman, “Bonding in Rare Gas and Fluorine Compounds and Other Quantum Chemical Considerations” (1970).