#### 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%3A1F23774FX86F350AFX7B36BE62591BF578F5/2.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%3A1F23774FX86F350AFX7B36BE62591BF578F5/6.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).)

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## J351. Y, Ortiz, D. J. Klein and J. F. Liebman, [Tetrahedral Units: for Dodecahedral Super-​Structures](https://scifinder.cas.org/scifinder/references/answers/87808E58X86F3514BX44B25B45436F677081%3A8780E69DX86F3514BX71C72C3C4494ED6717/1.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%3A6F121B73X86F3514CX5B566BFD25AC068F2B/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).

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