## 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)

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Orcid #[0000-0002-6109-7753](https://orcid.org/0000-0002-6109-7753?lang=en)

### 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

Coeditor, 2022 -- present, Special Issue of Chemical Thermodynamics and Thermal Analysis, “Chemical Energetics: Rules, Regularities and Estimates”.(CTTA)

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/General/Series Co-Editor: 2009 – present, “Patai’s Chemistry of Functional Groups” (a series of research monographs published by Wiley, Chichester, UK). (I have coedited six volumes in this series, and I have contributed chapters to over 30 volumes, others are in preparation.) I am now also a general editor of “e-Patai: Patai’s Chemistry of Functional Groups,” published by Wiley, Chichester, UK and accordingly coauthor of the preface to individual volumes. 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 (with A. Greenberg): 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” or more recently, “Paradigms and Paradimgs” In 2007, a new column “Chemistry, Commentary and Community” was initiated but discontinued soon afterwards.

Coeditor and cofounder (with A. Greenberg): 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

Visiting Scholar/Adjunct Associate Professor, Sponsor, 2020 - a

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

Presidential Research Professor at UMBC, 2006-2009

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

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

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

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

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 – 1972l

Honorary Ramsay Fellow, 1970 – 1971*m*

NATO Postdoctoral Fellow, 1970 – 1971n

Recipient of Osgood Honorarium, 1968 – 1970o

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, 1964p

California State Regents Scholarship, 1963q

aSponsor of Prof. Maja Ponikvar (now, Ponikvar-Svet) (Jožef Stefan Institute, Slovenia).

bIt 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 for Excellence in Research, Scholarship and Creative Activity (v.i). and the ACS Chemist of the Year award (v.i.).

cBook 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.)

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 through 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).

lAt US National Bureau of Standards – Gaithersburg, for research with Dr. Thomas D. Coyle

nAt Cambridge University, for research with Prof. A. David Buckingham and Prof. John W. Linnett

*n*English Award.

oPrinceton Award.

pResearch with Prof. Norman Indictor.

qAt 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 Earth and Space Chemistry,ACS Omega, Acta Aeronautica, Acta Chemica Scandinavica, Acta Crystallograhica B, 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, Atoms, 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 Papers, Chemical Physics, Chemical Physics Letters, Chemical Reviews, Chemical Thermodynamics and Thermal Analysis, Chemistry: An Asian Journal, Chemistry: A European Journal, Chemistry Open, Chemistry Selects, Croatica Chemica Acta, Crystals, Energy and Fuels, Entropy, Environmental Science and Technology, Environmental Science – Atmosphere, European Journal of Inorganic Chemistry, European Journal of Organic Chemistry, Fluid Phase Equilibria, Graphene, Heteroatom Chemistry, Industrial and Engineering Chemistry-Research, Inorganic Chemistry, Inorganic and Nuclear Chemistry Letters, Inorganica Chimica Acta, Inter­national Journal of Chemical Kinetics, Inorganics, Inter­national Journal of Chemical Modeling, International Journal of Quantum Chemistry, Internet Journal of Molecular Sciences, Inorganic Chemistry, International Journal of Mass Spectrometry, International Journal of Thermophysics, Journal of Alloys and Compounds, Internet Electronic Journal of Molecular Design, Journal of the American Chemical Society, Journal of the American Society of Mass Spectrometry, Journal of the Brazilian Chemical Society, Journal of Chemical and Engineering Data, 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 Energetic 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 Graphics and Modelling, 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, Materials, 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, Photochemistry and Photobiology. Physical Chemistry Chemical Physics, Plasma, 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, Thermochimica Acta and Wiley Interdisciplinary Reviews: Computational Molecular Science. 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”)\*\*

Ethics in Chemistry/Biochemistry\*

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\*\*

Physical Organic Chemistry\*

Quantum Chemistry\*, \*\*

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\*

Arbitrary 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)

Hiring New Faculty\*

Honors and Awards\* (chair dept. committee), \*\* (including University System of Maryland Regents and Demorest mentoring awards)\*\*

Honors College Advisory Council\*\*

Honors College Governance Board\*\*

Honors Program\*\*

Honors University Task Force\*\*

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

Library Liaison\*,\*\*

Louis Stokes Alliuance for Minority Participation Scholar Mentor (LSAMP)\*\*

McNair Scholar Mentor\*\*

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

Presidential Professor Advisory Committee\*\*

*Promotion and Tenure*\*,\*\* (including Habilitation evaluator) at Baruch College (CUNY, USA) University of Rostock (Germany) and Ruswe Bošković Institute (Croatia), Jožef Stefan International Postgraduate School (Slovenia), Yarmuk University (Jordan) 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**

J392. M. Ponikvar-Svet, K.F. Edwards and J.F. Liebman. “Acetylacetone: Metal Complexes and Keto-Enol Tautomerism – Which Tautomer is More/Less Stable?" Special Issue of Acta Chim. Slovenica (invited, refereed, primary, research article dedicated to the memory of Prof. Boris Žemva (in press).

J391. A. Pavlovič, L. Janžič, L. Sršen, A.N. Kopitar, K.F. Edwards, J.F. Liebman and M. Ponikvar-Svet, “Mononuclear Aluminum-Fluoride Ions, AlFx (+/-) -- Study of Plausible Frameworks of Complexes with Biomolecules and Their *In Vitro* Toxicity”, Molecules (in press).

J390. L. Glasser and J.F. Liebman, “Thermochemistry of Monocharged Cation Substitutions in Ionic Solids”, Struct. Chem., 35, 407–412 (2024).

J389. Z. Salta, N. Tasinato, J.F. Liebman and O.N. Ventura, “Enthalpy of Formation of Carbocycles: A Precise Theoretical Determination of Experimentally Imprecise Measurements”, Chem. Thermodynam. Thermal Anal., 100121 (2023) (appearing in a VSI of CTTA, “Rules, Regularities and Estimates”, guest editors L. Glasser and J.F. Liebman.).

J388. M. Ponikvar-Svet, K.F. Edwards and J.F. Liebman, "Paradoxes and Paradigms: Elements and Compounds: Similar Names, Very Different Energetics. Part 5, Selected Examples of Exotic Species and Isotopes (H, He, C, F, U)", Struct. Chem., 34, 2365-2374 (2023).

J387. M. Ptaszek and J.F. Liebman, “Paradoxes and Paradigms: Are Maleimides Antiaromatic, Aromatic, or Neither?”, Struct. Chem., 34, 2015-2019 (2023).

J386. M. Ponikvar-Svet., K.F. Edwards and J.F. Liebman, "Paradoxes and Paradigms: Elements and Compounds: Similar Names, Very Different Energetics. Part 2, Potassium-to-Xenon (K -- Xe) Z = 19 - 54", Struct. Chem., 34, 1995-2004 (2023).

J385. M. Ponikvar-Svet, K.F. Edwards and J.F. Liebman, “Paradoxes and Paradigms: Elements and Compounds: Similar Names, Very Different Energetics. Part 4, Francium to Oganesson (Fr – Og) Z = 87-118”, Struct. Chem., 34, 1985-93 (2023).

J384. M. Ponikvar-Svet., K.F. Edwards and J.F. Liebman, "Paradoxes and Paradigms: Elements and Compounds: Similar Names, Very Different Energetics. Part 3, Cesium-to-Radon (Cs – Rn) Z = 37 - 86", Struct. Chem., 34, 1603-11 (2023).

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J383. A. Rágyanszki, B. Fiser, E. Lee-Ruff and J.F. Liebman, “Strained Small Nitrogen Heterocycles-Azabicyclobutanes and Azirines”, Chem. Select, 8, e202301405 (2023).

J382. M. Ponikvar-Svet., K.F. Edwards and J.F. Liebman, "Correction to: ‘Paradoxes and Paradigms: Elements and Compounds: Similar Names, Very Different Energetics. Part I, Hydrogen-to-Argon (H -- Ar) Z = 1 - 18", Struct. Chem. 34, 1219 (2023).

J381. M. Ponikvar-Svet., K.F. Edwards and J.F. Liebman, "Paradoxes and Paradigms: Elements and Compounds: Similar Names, Very Different Energetics. Part I, Hydrogen-to-Argon (H -- Ar) Z = 1 - 18", Struct. Chem., 34, 1205-17 (2023) (now corrected on line.)

J380. J.F. Liebman, “Paradigms and Paradoxes: Stabilization, Destabilization and Resonance Energy of α- Diketones, Dienes and Derived Radical Ions”, Struct. Chem., 34, 729-732 (2023).

J379. Z. Salta, N.Tasinato, O.N. Ventura, and J.F. Liebman, “Paradigms and Paradoxes: Systematics in the Study of the Simplest Sulfenic Acids and Sulfoxides, and a Comparison Between Sulfur–Oxygen and Nitrogen–Oxygen Bonds”, Struct. Chem., 34, 723-727 (2023).

## J378. J.F. Liebman, “Paradigms and Paradoxes: Can the Energy of a π-orbital, εi, Equal e or π, or Some rational multiple of either number?” (this invited, primary, research article), for a special issue of *Structural Chemistry,* ed. Y. V. Novakavaskaya and I. Hargittai, “Structure and Bonding”. Struct. Chem., 34. 55-58 (2023).

J377. M. Ponikvar-Svet and J.F. Liebman, "Paradoxes and Paradigms: The Stabilization/Resonance Energy of Some –C(O)– Species: Acetyl Derivatives, Metal Carbonyls and Amides Alike", Struct. Chem. (this invited, primary, research article appears in a special issue of *Structural Chemistry,* ed. Y. V. Novakavaskaya and I. Hargittai, “Structure and Bonding”) Struct. Chem., 34, 51-54 (2023) (Our paper was dedicated to László Markó (1928-2022).)

J376. K.F. Edwards and J.F. Liebman, "Paradigms and Paradoxes: Fractional and Other Non-Integer Charges in Chemistry: An Understanding of Aromaticity", Struct. Chem., 33, 551-554 (2022).

## J375. A. Rágyanszki, B. Fiser, E. Lee-Ruff and J.F. Liebman,  "Photochemical Valence Isomerization to High Energy Products – Bicyclobutanes and Oxabicyclobutanes,” Photochem. Photobiol., 97, 1353-1364  (2021) (this invited, primary, research article, ed. A. Greer, for the special issue of *Photochemistry and Photobiology* “Retirement Issue of E. L. Clennan”).

J374. M. Ponikvar-Svet, D.N. Zeiger and J.F. Liebman, “Alkaloids and Selected Topics in their Thermochemistry” Molecules, 26, 6715 (2021) (13 pages) (this invited, primary, research article, ed. V.L.S. Freitas and M.D.M.C. Ribeiro da Silva for a special issue of *Molecules* “Synergies on the Trio Energy-Structure-Reactivity: Nitrogen-containing Heteropolycyclic Compounds”,

J373. M. Ponikvar-Svet, K.F. Edwards and J.F. Liebman, “Paradigms and Paradoxes: “The Ionization Potential of Atomic Astatine (Z = 85), Polonium (Z =84) and Some other Elements: What Does This Value Tell Us About the Energetics of Atomic and Diatomic Halogens,” Struct. Chem., 32, 973-976 (2021).

J372. M. Ponikvar-Svet, K.F. Edwards and J.F. Liebman, “Paradoxes and Paradigms: On Ambisaline Ions of Nitrogen,” Struct. Chem., 32, 529-37 (2021).

J371. M. Ponikvar-Svet, K.F. Edwards and J.F. Liebman, "Paradoxes and Paradigms: On Ambisaline Ions of Oxygen, Fluorine, and Related Oxyfluorides,” Struct. Chem., 32, 11-17 (2021).

J370. R. Fournier, A.R. Green, A. Greenberg, E. Lee-Ruff, J.F. Liebman and A. Rágyanszki, “Predicted Reversal in N-Methylazepine/N-Methyl-7-azanorcaradiene, Equilibrium Upon Formation of Their N-Oxides,” Molecules, 25, 4767 (2020). (this invited, primary, research article, ed. E. Lee-Ruff., for a special issue of *Molecules*, “Reactive Intermediates in Organic Chemistry,”)

J369. S. Jabeen, A. Greer, K.F. Edwards and J.F. Liebman, “Why are the Elemental Nonmetals (F2, Cl2, Br2, I2, S8, P4) of so Many Hues or of Any Hues and Where is the Chromophore? Insight into Intera‐X–X Bonds,” Photochem. Photobiol., 96, 1140-3 (2020). (This paper was a “Featured article” at the Journal Website.)

J368. A. Greenberg, A.R. Green and J.F. Liebman, “Computational Study of Selected Amine and Lactam N-oxides: Including Comparisons of N-O Bond Dissociation Enthalpies with Those of Pyridine  
N-oxides,” (this invited, primary, research article, ed. E. Lee-Ruff, appeared in a special issue on “Reactive Intermediates in Organic Chemistry,” Molecules, 25, 3703 (2020).

J367. J.A.M. Lucker and J.F. Liebman, “​Hückel Theory and Distinguishing between Isospectral Molecules: 1,4-Divinylbenzene and 2-Phenylbutadiene, and Tetramethylenemethane and Cyclobutadiene + Carbon,” Struct. Chem., 31, 1119-24 (2020).

J366. J.M. Hudzik, L.R. Stoler, J.W. Bozzelli and J.F. Liebman, “Thermochemistry of Fluorinated Dimethyl and Ethyl Methyl Ethers and Corresponding Radical Species,” J. Chem. Eng. Data,  65, 1594-1616 (2020) (+ 168 supplemental pages).

J365. D.Z. Spera and J.F. Liebman, "Paradigms and Paradoxes: Additive Trends in the Absolute Entropy of Monoxides and Homonuclear Diatomic Molecules,” Struct. Chem., 31, 81-4 (2020).

J364. J.F. Liebman and A. Greenberg, “The Resonance Energy of Amides and their Radical Cations,” Struct. Chem., 30, 1631-4 (2019).

J363. A. Greenberg and J.F. Liebman, “Paradigms and Paradoxes: Revisiting the Relation of Oxidation State and Acidity of Polyhydride Cations,” Struct. Chem., 30, 1629-30 (2019).

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 in-print article is in honor of Gennady Kabo on the occasion of his 80th birthday. This paper was written for a special virtual issue of J. Chem. Thermodyn. edited by A. Bazyleva, E. Paulechka and R. Weir. This virtual issue was reprinted as J. Chem. Thermodyn., 134F (2019) using the original pagination of the individual papers.)

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, 1247-1254 (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).

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OCA23 An untitled poem appearing in M. Ponikvar-Svet, K.F. Edwards and J.F. Liebmanm Acetylacetone: Metal Complexes and Keto-Enol Tautomerism – Which tautomer is more/less stable?" Special Issue of Acta Chim. Slovenica (invited, refereed, primary, research article dedicated to the memory of Prof. Boris Žemva (in press).

OCA22. A poem “Structural Chemistry, some memories”, Struct. Chem., 35, 1035 (2024).

OCA21. An untitled poem appearing in the book chapter by M. Ponikvar-Svet and J.F. Liebman, “Some Aspects of the Energetics of Species Containing Cobalt–Carbon Bonds” in Patai’s Chemistry of Functional Groups: The Chemistry of Organocobalt Compounds” (ed. C. Gosmini and I. Marek), Wiley, Chichester, 65-81 (2023).

OCA20. The poem ”Ed Clennan on the Occasion of His ‘Official’ Retirement” (coauthored with K. F. Edwards) was written in honor of Edward L Clennan on the occasion of his retirement, appearing as part of the preface in a dedicated volume of Photochemistry and Photobiology, “[Retirement Issue Dedicated to Edward L. Clennan](https://scifinder-n-cas-org.proxy-bc.researchport.umd.edu/navigate/?appId=5d7e2512-2851-473a-a99f-511250caf0f3&backKey=61ca88f48b6a1b0c212ea4bd&backToPage=1&contentUri=document%2Fpt%2Fdocument%2F61010561&key=61ca88f48b6a1b0c212ea4bd&metricsOrdinal=5&metricsResultType=reference&ordinal=4&resultType=reference&resultView=DETAIL&sortBy=publication_date&sortOrder=descending&state=searchDetail.reference&uiContext=364&uiSubContext=551&uriForDetails=document%2Fpt%2Fdocument%2F61010561). edited by A. Greer,” Photochem. Photobiol., 97, 1166-7 (2021).

OCA19. The poem”Ode to Josef Michl” (coauthored with K.F. Edwards) was written in honor of Josef Michl on the occasion of his 80th birthday appearing in “Tribute to Josef Michl,” Chemistry, 3, 440-443 (2021) in a dedicated volume to JM edited by I. Alagubin and P. Klan.

OCA18. The poem in honor of Thomas M. Klapötke (coauthored with M. Ponikvar-Svet and K. Edwards) appearing as part of a Laudatio (written by K. Karaghisoff, B. Krumm and J. Stierstofer, Z. Anorg. Allg. Chem., 147, 135-6 (2021) (special issue in honor of Thomas M. Klapötke in Celebration of his 60th birthday, edited by T.F. Fãssler, C. Limberg and G. Qian).

OCA17. The invited poem “Onward with Hydrogen,” Chesapeake Chemist, 77(3), 10-11 (2020).

OCA16. The poem “Ode to Gennady Kabo” J. Chem.Thermodyn., 133, 54 (2019) was written in honor of Gennady Kabo on the occasion of his 80th birthday as part of a special virtual issue of J. Chem. Thermodyn., and appeared in print as was edited by A. Bazyleva, E. Paulechka and R. Weir. This virtual issue was reprinted as J. Chem. Thermodyn., 134F, (2019) with the original pagination of the individual papers.

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”, Intl. J. Chem. Model. 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).

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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 articles 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) and 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). .

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