Christopher J. Cramer

Date of birth: September 23, 1961

Curriculum Vitae

(as of November 20, 2016)

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EDUCATION

Doctor of Philosophy, Chemistry, University of Illinois, Urbana-Champaign, 1988.

Artium Baccalaurei, *summa cum laude*, Washington University, St. Louis, Missouri, Mathematics and Chemistry, 1983.

PROFESSIONAL EXPERIENCE

University of Minnesota, Minneapolis-St. Paul, College of Science and Engineering,	
Associate Dean for Academic Affairs	2013–present
Distinguished McKnight and University Teaching Professor	2000–present
Associate Professor of Chemistry, Chemical Physics, and Scientific Computation	1996–2000
Assistant Professor of Chemistry and Chemical Physics	1992–1996
Director, Center for Charge Transfer and Charge Transport in Photoactivated Systems (DOE SciDAC)	2012–2017
Fellow, Committee on Institutional Cooperation Academic Leadership Program	2013–2014
Faculty Liaison for eLearning Initiatives, Office of the Senior Vice President for Academic Affairs and Provost	2012–2013
Professeur Invité, University of Geneva, Switzerland	2007–2008
Visiting Professor, University of Barcelona, Catalonia, Spain	2000–2001
Hubert H. Humphrey Institute Policy Fellow	1996
Officer, United States Army, Chemical Corps	1988–1992

SELECTED AWARDS AND HONORS

Labex MiChem Professeur Invité, Sorbonne Universités, Paris	2015
George W. Taylor Distinguished Service Award	2013
University of Minnesota Morse-Alumni Undergraduate Teaching Award	2011
Fellow of the American Chemical Society	2010
Elmore H. Northey Chair, Chemistry	2009–2014
University of Minnesota Inventor Recognition Award	2005, 2008
University of Minnesota Postbaccalaureate, Graduate, and Professional Education Award	2005
Distinguished McKnight University Professor	2003
John Simon Guggenheim Fellowship	2000
George W. Taylor Distinguished Research Award	1999
Fellow of the Minnesota Supercomputer Institute	1996
Alfred P. Sloan Research Fellow	1996

University of Minnesota McKnight Land-Grant Assistant Professor 1994
8th Annual Army Materiel Command Outstanding Research Award 1992
Arthur S. Flemming Award 1991
Army Research and Development Achievement Award 1991
Army Special Act Award in Recognition of Research Excellence 1991
National Science Foundation Graduate Fellow 1984
Phi Beta Kappa 1983

RESEARCH INTERESTS

Modeling catalysis, including the exploitation of metal-organic frameworks, to advance sustainable chemistry and chemical processes
Molecular and material phenomena associated with solar energy devices
Theoretical characterization of small-molecule activation at transition-metal centers
Modeling remediation of environmental contaminants and chemical warfare agents
Development and application of condensed-phase quantum chemical models

RESEARCH SUPPORT

Current:

Vietnam Education Foundation, *Graduate Student Fellowship Program* (administrative PI), $28,000/student, May 13, 2005 – August 26, 2017

Department of Energy, *SCIDAC Charge Transfer and Charge Transport in Photoactivated Systems* (as PI, with co-investigators Gagliardi, Siepmann, Truhlar), $3,000,000, September 1, 2012 – August 31, 2017.

Department of Energy, *Nanoporous Materials Genome: Methods and Software to Optimize Gas Storage, Separations, and Catalysis*, (with PI Gagliardi and many co-PIs), $8,100,000, January 1, 2013 – December 31, 2017.

National Science Foundation, *Modeling Catalysis for Sustainable Processes*, July 1, 2014 – June 30, 2017, $420,000.

Department of Energy, *Energy Frontier Research Center for Inorganometallic Catalyst Design*, (with PI Gagliardi and many co-PIs), September 1, 2014 – August 31, 2018, $12,000,000.

National Science Foundation, *Center for Sustainable Polymers*, (with PI Hillmyer and many co-PIs), September 1, 2014 – August 31, 2019, $20,000,000.

National Science Foundation, *EAGER: From 0 to 2*, (with PI Neuhauser and co-PIs Fisher and Schroeder), May 15, 2016 – May 14, 2017, $97,966.

National Science Foundation, *Design Principles for the Growth of High-quality Binary and Ternary Tin Oxides*, (with co-PIs Gladfelter and Jalan), July 1, 2016 — June 30, 2019, $435,000.

Defense Threat Reduction Agency, *Highly Stable and Bifunctional Bio-inspired Catalytic MOFs for Destruction of Chemical Threats*, (with PI Farha and other co-PIs), March 1, 2016 – February 29, 2020, $493,541 (Cramer portion; contract in negotiation).

Historical: From 1992–2015 approx. $10M in individual and small-team grant support from, inter alia, the U.S. Army Research Office, the National Science Foundation, the Department of Energy, the U.S. Army Engineering Research & Development Center, the Office of Naval Research, the State of Minnesota, the U.S. Environmental Protection Agency, the National Institute of Standards and Technology, Silicon Graphics, Cray, and Kodak Inc.

TECHNOLOGY TRANSFER

Licensed Software, *MNSOL Database*, University of Minnesota Office for Technology Commercialization 2008

Licensed Software, *AMSOL*, University of Minnesota Office for Technology Commercialization 2005

CONSULTING RELATIONSHIPS

SEED Research and Development	2015–2016
Global OLED Technology, LLC	2013–2016
Novartis Institutes for Biomedical Research	2010–2015
Medtronic Inc.	2012
E. I. du Pont de Nemours and Company	2011–2012
Alcon Research Laboratories	2008–2012
ExxonMobil Research and Engineering Company	2010–2011
Segetis Inc.	2010
St. Onge Steward Johnston & Reens LLC	2008–2009
CT Associates	2006
Wyeth-Ayerst Research	1998
Le Research	1997
Pfizer Inc.	1997
Monsanto	1995

SELECTED ADMINISTRATIVE EXPERIENCE

Leadership: Served as Chair of a 5,000-member division of the American Chemical Society, working with a divisional executive board and national organizational staff to develop, fund, implement, and manage programmatic and membership activities. Served as Chair of faculty governance at the University of Minnesota, working with staff and other governance bodies to contribute to University shared governance. Served for 14 years as Editor-in-Chief of a scientific journal, charged with budgetary, content, and thematic decisions, managing relevant staff. Principal investigator for single- and multi-investigator research awards totaling in excess of $10M over 20 years including Directorship of a multi-institution Scientific Discovery through Advanced Computing (SciDAC) application project.

Program management: Serving as Associate Dean for Academic Affairs in the University of Minnesota's College of Science and Engineering (entails (i) responsibility for oversight of faculty hiring, promotion, and tenure within the College, awards, diversity programs, salary equity, sabbaticals and leaves, governance activities, and a variety of other miscellaneous management and liaison activities and (ii) responsibility for oversight and support of graduate education programs within the College serving ~2,500 graduate students and administration of $2.4M per year associated annual budget). Served as Faculty Liaison for eLearning Initiatives in the Office of the Senior Vice President for Academic Affairs and Provost with institution-wide responsibilities for development and enhancement of digital curricular strategies and materials, including online learning, Massive Open Online Courses (MOOCs), and management of a $500K initiative to enhance undergraduate programs using digital technology. Served as Director of Graduate Studies for the University of Minnesota's largest Ph.D. program, Chemistry, managing associated budget and staff. Served as Director of Undergraduate Studies for Chemistry, managing associated budget and staff. Continuous management of a Chemistry/Chemical Physics research group having a typical annual budget of six figures and multiple direct reports.

Diversity: Managing recurring lecture and networking events designed to support underrepresented groups in the College of Science and Engineering. Led faculty-governance component of University of Minnesota Gender-Related Faculty Salary Analysis Working Group. Regular attendee and organizer of events devoted to increasing diversity, in STEM disciplines in particular. Served as Chair of Chemistry's faculty search committee from 2010–2012 and implemented a strategy that led to approx. 50% of interviewed candidates being women or underrepresented minorities.

Public Engagement: Testimony before the Minnesota State House and Senate Higher Education Committees. Author and quoted source for commentaries and articles in the *Minneapolis Star-Tribune*, *St. Paul Pioneer Press*, and other newspapers and higher education journals. Active in new media.

Military: Exercised staff and command responsibilities in administrative and tactical operations, including armed combat (Operations Desert Shield and Desert Storm).

SELECTED SERVICE

Service to University of Minnesota

Faculty Consultative Committee (and Senate Consultative Committee)
- past-chair (and University senator) 2012–2013
- chair (and University senator) 2011–2012
- vice-chair (and University senator) 2010–2011
- member (and University senator) 2009–2010

executive body of the Faculty Senate (and University Senate)

Senate Research Committee, member 2003–2006
University Senate body advising on all research-related issues

Senate Subcommittee on Research Openness, member 2006–2013
University Senate body handling all request for exceptions to policy in grants and contracts

Standing Comprehensive Review Committee for Deans, member 2011–2012
Advisory to senior vice president to whom a dean reports

Ad hoc Committee on Educational Materials Copyright/IP, member 2012–2013
Advisory body to the Provost

Research and Scholarship Advisory Panel, member 2012–2013
Advisory body to Office of the Vice President for Research

Public Engagement Council, member 2012–2013, 2015–present
Advisory body to Office of Public Engagement

Academy of Distinguished Teachers, Executive Committee, member 2012–2013
Steering committee working with Vice-Provost for Faculty Affairs

University Gender-Related Faculty Salary Analysis Working Group, member 2010–2012
Oversight of study to assess gender-related salary inequities

Search Committees
- University of Minnesota Alumni Association CEO, member 2013
- Northrup Director, member 2012
- Army High Performance Computing Research Center Director, member 1998

National Board of the University of Minnesota Alumni Association, member 2010–2011
Oversight of UMAA activities and strategic planning

University Working Group on Effort Issues, member 2010–2011
Examination of professorial appointments, effort certification, risk, and related issues

Regents Committee to Recommend Naming a Building for a Past President, member 2010

University Task Force on Research Infrastructure, member 2005–2006
Contributor to Strategic Positioning planning

Graduate School
- Quality Metrics Block Grant Allocation Committee, member 2013–present
- Council of Graduate Associate Deans 2013–present
- Ad Hoc Student Fellowship Committee, member 2001–2003
- Review Committee for David & Lucille Packard Award, member 2000–2003
- Physical Sciences Policy & Review Committee, member 1997–2000

Minnesota Supercomputing Institute
- Director's Advisory Board, member 2014–present
- Resources Peer Review Panel, member 1996–1997, 2002–2005
- IBM SP Advisory Committee, member 1998–2000
- Planning Committee, member 1996–2000
- Workstation Cluster Steering Committee, member 1996–1999
- Nominating Committee, member 1997–1998
- Symmetric Multiprocessing Initiative Committee, member 1996–1998

Center for Transportation Studies
- Executive Council, member (CSE representative) 2013–2016
- Strategic Management Subcommittee, member 2013–2016

Service to College of Science and Engineering

Strategic Planning ("Blue Ribbon") Committee, member 2009–2011

Merit Scholarship Review Committee, member 2007

Curriculum Committee, member 2004–2007

Promotion and Tenure Committee, member 2001–2004

Service to Chemistry Department

Director of Undergraduate Studies (and Honors Advisor) 2004–2007
Responsible for program graduating ~100 students per year

Director of Graduate Studies 1997–2000
Responsible for program of ~200 doctoral students total

Planning, Staffing and Resources Committee
- Chair 2004–2005
- Member 2002–2004

Executive advisory committee to the Departmental Chair

Faculty Search Committees
- Chair 2010, 2011
- Member 1993, 1995, 1997, 2002

Tenured and tenure-track faculty recruitment

Other Committees
- Mentor committee (Tonks) 2013–present

Awards Committee, member and chair 2009–2011
Graduate Student Symposium Committee, founding chair 2001–2002
Tenure Committee (York), member 1998–2001
Internal Search Committee (Chemistry Chair), member 1998–1999
Website Steering Committee, member 1996–1998
Seminar Committee 1996–1997
Graduate Admissions Committee, member 1993–1997
Named Lecture Series and Departmental Colloquia, member and chair 1992–1994

Service to Profession

Theoretical Chemistry Accounts
Editor-in-chief 2000–2014
Associate editor 1997–2000
Professional journal receiving ~500 submissions per year

Journal of Physical Organic Chemistry
Associate editor for North America 1997–present
Professional journal receiving ~300 submissions per year

Selection committee, Award of the American Chemical Society
Chair 2008–2009
Member 2006–2008
National award of professional organization of 161,000 members

Governing Board, Reaction Mechanisms Conference, member 2002–2008
Oversight of biennial international conference

Editorial Advisory Board
Journal of Organic Chemistry, member 2003–2006
Progress in Physical Organic Chemistry, member 1997–2000

International Society of Quantum Biology and Pharmacology, Councilor 2001–2003
Oversight of professional organization and international conference

Ad Hoc Task Force to Monitor the *Journal of Chemical Information and Computer Sciences*, member 1996

American Chemical Society, Division of Computers in Chemistry
Chair 1995–1996
Chair-elect 1994–1995
Leadership and oversight of professional Division of 5,000 members

Organization of Symposia at National and International Conferences
ESPA 2016, Scientific Committee, member 2016
Midwest Undergraduate Computational Chemistry Conference 2005, 2011
Pacifichem 2010, 2015
Meetings of the American Chemical Society 1994, 1997, 2000, 2002, 2008
Midwest Theoretical Chemistry Conference 2001
Computational Chemical Dynamics 2000
Computers in Chemical Research and Education 1997

Editor, symposium volume
Perspectives on Theoretical Chemistry: Five Decades of Theoretical Chemistry Accounts and Theoretica Chimica Acta 2012
Structure, Energetics, and Reactivity in Aqueous Solution 1994

Editor, *Highlights in Theoretical Chemistry*, book series, volumes 1-11 2012–2016

Service to Broader Scientific and Technical Organizations and Community Engagement

Complete set of lecture videos and printed materials for *Chemistry 4021/8021, Computational Chemistry* made available freely online at http://pollux.chem.umn.edu/4021 and on YouTube 2013–present

Massive Open Online Course *Statistical Molecular Thermodynamics* taught through Coursera and all videos (including all additional lectures/exercises comprising UMN Chem 4501) made available on YouTube 2013–present

Non-routine Reviewing/Workshop Commitments (with agency reports)

Department of Homeland Security 2008–2013
Ad hoc technical reviewer, Chemical Security Analysis Center

American Association for the Advancement of Science 2009, 2012
Strategic Technologies Programs for the Kingdom of Saudi Arabia

National Institutes of Health 2004, 2005
Computational Biophysics and National Research Service Award Study sections

National Science Foundation 1999, 2004
CAREER evaluation and Workshop on Cyberinfrastructure

National Academy of Sciences 1999
Roundtable on Graduate Education in the Chemical Sciences

Department of Energy 1998
Workshop on Research Needs and Opportunities in Radiation Chemistry

Judge

North Star STEM Alliance Research Symposium 2010

St. Louis Park public schools' science fairs 2001, 2002, 2004, 2006

National Finals of Siemens-Westinghouse Science Competition 2002
evaluation of student research posters/presentations

RESEARCH MENTORSHIP

University of Minnesota, 1992-2015

Postdoctoral Associates: 33 (9 current)

Graduate Students: 29 doctoral students (3 current); 7 masters students

Undergraduate Students: 66 (a large majority of whom went on to pursue post-graduate studies in doctoral or professional programs; 2 current)

High-school students: 3 (who went on to attend Stanford, MIT, and the University of Illinois, respectively)

Visiting scientists/faculty: 26

RECENT INVITED SEMINARS

Cambridge University, May 16, 2012.

Ripon College, November 30, 2012.

Washington University, February 7, 2013.

University of Alberta, February 14, 2013.

University of Calgary, February 15, 2013.

North Carolina State University, September 13, 2013.

EcoLab, October 9, 2013.

Centro de Investigacion y de Estudios Avanzados, Mérida, September 20, 2014.

Université de Nancy, June 9, 2015.

Institut de Recherche Chimie Paris (6 lectures), June 12-14, 2015

L'École Nationale Supérieure de Chimie de Paris, April 1, 2016.

Université d'Evry, Paris, April 5, 2016.

Università degli Studi di Torino, May 25, 2016.

Università di Milano Biccoca, May 26, 2016.

University of Kansas, November 4, 2016.

University of Wisconsin, Eau Claire, December 2, 2016.

RECENT INVITED CONFERENCE CONTRIBUTIONS

243rd National ACS Meeting (COMP), *Charge Model 5 for the Accurate Description of Molecular Interactions in the Gas Phase and Solution*, Truhlar, D. G.; Marenich, A.; Cramer, C. J., San Diego, CA, March 26, 2012 (co-senior author, not presenter).

Targeting and Triggering Basic Research Workshop, *Modeling Intermolecular Interactions Relevant to Targeting and Triggering*, Cramer, C. J.; Gagliardi, L.; Isley, W., III; Semrouni, D. Cambridge, England, May 15, 2012.

Electronic Structure Theory for Strongly Correlated Systems, *Modeling the Activation of Small Molecules at Supported Transition-Metal Centers*, Cramer, C. J., Palermo, Italy, June 1, 2012.

Xth Girona Seminar, *Scope and Limitations of Continuum Solvation Models*, Cramer, C. J., Girona, Catalonia, July 2, 2012.

International Symposium on Reactive Intermediates and Unusual Molecules 2012, *Reactive Intermediates in Supported Transition-Metal Mediated Catalytic Cycles*, Cramer, C. J.; Ascona, Switzerland, July 9, 2012.

245th National ACS Meeting (PHYS), *Modeling Host-Guest Interactions in Metal-Templated Self-Assembled Molecular Cages*, Isley III, W. C.; Semrouni, D.; League, A. B.; Nitschke, J. R.; Gagliardi, L.; Cramer, C. J., New Orleans, LA, April 8, 2013.

245th National ACS Meeting (COMP), *Universal Solvation Models: Theory and Application*, Marenich, A. V.; Cramer, C. J.; Truhlar, D. G., New Orleans, LA, April 9, 2013.

223rd Electrochemical Society Meeting, *Continuum Solvation Models for Computational Electrochemistry: Recent Advances*, Marenich, A.; Cramer, C. J.; Truhlar, D. G., Calgary, Canada, May 13, 2013 (co-senior author, not presenter).

Challenges in Computational Homogeneous Catalysis - 2013, *Modeling Catalysis Relevant to Energy Sustainability*, Cramer, C. J., Stockholm, Sweden, June 13, 2013.

The Scott E. Denmark Symposium, *Mechanistic analysis of water-splitting catalysis*, Cramer, C. J., Urbana, IL, August 3, 2013.

246th National ACS Meeting (ENVR), *Modeling remediation pathways available to environmental contaminants*, Cramer, C. J., Indianapolis, IN, September 9, 2013.

Southeast Regional ACS Meeting 2013, *Modeling condensed-phase effects on electronic structure and spectroscopy*, Cramer, C. J., Atlanta, GA, November 15, 2013.

2014 Annual Meeting of the Center for Sustainable Polymers, *Structure, Reactivity, Mechanistic Insight: Theory in Your Toolbox*, Minneapolis, MN, April 22, 2014.

Electronic Structure Principles and Applications 2014 (ESPA2014), *Modeling condensed-phase effects on electronic structure and spectroscopy*, Cramer, C. J., Badajoz, Spain, July 2, 2014.

248th National ACS Meeting (PHYS), *Mechanistic analysis of water-splitting catalysis*, Cramer, C. J., San Francisco, CA, August 11, 2014.

National Mexican Chemical Society Meeting, Plenary Lecture, *Mechanistic Characterization of Homogeneous Catalytic Processes for Water Splitting*, Mérida, Mexico, September 18, 2014.

Meeting of Committee on Institutional Cooperation (CIC) Academic Leadership Program (ALP) Fellows, *Flipped Classrooms, MOOCs, and Other eLearning Initiatives at the University of Minnesota*, Minneapolis, MN, October 25, 2014.

249th National ACS Meeting (COMP), *Concertedness and synchronicity—from arynes to electrochemistry*, Cramer, C. J., Denver, CO, March 24, 2015.

249th National ACS Meeting (PHYS), *25 years of SMx models: Quantum and classical continuum solvation*, Cramer, C. J., Truhlar, D. G., Denver, CO, March 25, 2015.

Labex MiChem International Symposium, *How Can Theory Contribute to Catalyst Design for Solar Fuels?*, Paris, France, June 26, 2015.

250th National ACS Meeting (COMP), *Pushing around protons and electrons: What could possibly go wrong?* Cramer, C. J., Boston, MA, August 17, 2015.

250th National ACS Meeting (INOR), *Computational models applied to homogeneous water oxidation catalysis: What's the value proposition?* Cramer, C. J., Boston, MA, August 18, 2015.

3rd Challenges in Computational Homogeneous Catalysis Meeting, *Exploiting the Metal-Organic Frameworks NU-1000 and UiO-6*n *for Catalysis at the Homogeneous/Heterogeneous Interface*, Cramer, C. J., Stockholm, Sweden, September 4, 2015.

Pacifichem 2015, *Role of computational models in the design cycle of catalysts*, Cramer, C. J., Honolulu, HI, December 16, 2015.

Electronic Structure Principles and Applications 2016 (ESPA2016), *Catalysis on Metal-Organic Framework Nodes*, Cramer, C. J., Valencia, Spain, June 30, 2016.

MERCURY 2016, *Spiral Feedback for Catalyst Design: Experiment and Theory*, Cramer, C. J., Lewisburg, PA, July 22, 2016.

253rd National ACS Meeting (INOR), *Factors controlling the activity of Fe-based catalysts for the polymerization of lactide and epoxides*, Cramer, C. J., San Francisco, CA, April 2, 2017.

253rd National ACS Meeting (INOR), *Factors controlling the activity of Al-based catalysts for the ring-opening transesterification polymerization of caprolactone*, Cramer, C. J., San Francisco, CA, April 3, 2017.

PUBLICATIONS (~34,000+ citations, *h* index = 83, Google Scholar)

Books, Authored

1. Cramer, C. J. *Essentials of Computational Chemistry: Theories and Models*, Wiley: Chichester, 2002.
2. Cramer, C. J. *Essentials of Computational Chemistry: Theories and Models, 2nd Edition*, Wiley: Chichester, 2004.

Journal Articles/Refereed Book Chapters, Authored

1. Denmark, S. E.; Dappen, M. S.; Cramer, C. J. "Intramolecular [4+2]-Cycloadditions of Nitroalkenes with Olefins." *J. Am. Chem. Soc.* **1986**, *108*, 1306.
2. Denmark, S. E.; Cramer, C. J.; Sternberg, J. A. "The Stereostructures of [1,1´-Bicyclohexyl]-2,2´-diones: A Reassignment" *Tetrahedron Lett.* **1986**, *27*, 3693.
3. Denmark, S. E.; Cramer, C. J.; Sternberg, J. A. "Intermolecular [4+2]-Cycloadditions of Nitroalkenes with Cyclic Olefins. Transformations of Cyclic Nitronates" *Helv. Chim. Acta* **1986**, *69*, 1971.
4. Denmark, S. E.; Cramer, C. J.; Dappen, M. S. "Intramolecular [4+2]-Cycloadditions of Vinylnitrosonium Cations with Olefins" *J. Org. Chem.* **1987**, *52*, 877.
5. Cramer, C. J.; Dykstra, C. E.; Denmark, S. E. "An Ab Initio Study of the [1,2] Proton Transfer from Phosphine Oxide to Phosphinous Acid" *Chem. Phys. Lett.* **1987**, *136*, 17.
6. Denmark, S. E.; Cramer, C. J. "The Theoretical Structures of Neutral, Anionic and Lithiated *P*-Allylphosphonic Diamide" *J. Org. Chem.* **1990**, *55*, 1806.

7. Denmark, S. E.; Moon, Y.-C.; Cramer, C. J.; Dappen, M. S.; Senanayake, C. B. "Intramolecular [4+2]-Cycloadditions of Nitroalkenes with Olefins. 2" *Tetrahedron* **1990**, *46*, 7373.
8. Cramer, C. J.; Famini, G. R. "Computational Studies of Open-Shell Phosphorus Oxyacids 1. P-H Bond Homolysis in H_2PO_2" *J. Am. Chem. Soc.* **1990**, *112*, 5460.
9. Cramer, C. J.; Famini, G. R. "Computational Studies of Open-Shell Phosphorus Oxyacids. Cheletropic Reaction of PO_2 with H_2" *Chem. Phys. Lett.* **1990**, *169*, 405.
10. Cramer, C. J. "Theoretical Rotation, Pseudorotation and Pseudoinversion Barriers for the Hydroxyphosphoranyl Radical" *J. Am. Chem. Soc.* **1990**, *112*, 7965.
11. Cramer, C. J. "The Fluorophosphoranyl Series: Computational Insights into Relative Stabilities and Localization of Spin" *J. Am. Chem. Soc.* **1991**, *113*, 2439.
12. Cramer, C. J. "Calculation of the Electronic Structures and Spectra of Several Organic and Inorganic Radicals Containing Aluminum" *J. Mol. Struct. (Theochem)* **1991**, *235*, 243.
13. Cramer, C. J. "Dependence of Isotropic Hyperfine Coupling in the Fluoromethyl Radical Series on Inversion Angle" *J. Org. Chem.* **1991**, *56*, 5229.
14. Cramer, C. J.; Truhlar, D. G. "General Parameterized SCF Model for Free Energies of Solvation in Aqueous Solution" *J. Am. Chem. Soc.* **1991**, *113*, 8305.
15. Cramer, C. J.; Truhlar, D. G. "Molecular Orbital Theory Calculations of Aqueous Solvation Effects on Chemical Equilibria" *J. Am. Chem. Soc.* **1991**, *113*, 8552.
16. Falvey, D. E.; Cramer, C. J. "Aryl- and Alkylnitrenium Ions: Singlet-Triplet Gaps via Ab Initio and Semi-Empirical Methods" *Tetrahedron Lett.* **1992**, *33*, 1705.
17. Urban, J. J.; Cramer, C. J.; Famini, G. R. "A Computational Study of Solvent Effects on the Conformation of Dopamine" *J. Am. Chem. Soc.* **1992**, *114*, 8226.
18. Cramer, C. J.; Truhlar, D. G. "An SCF Solvation Model for the Hydrophobic Effect and Absolute Free Energies of Aqueous Solvation Including Specific Water Interactions" *Science* **1992**, *256*, 213.
19. Cramer, C. J.; Truhlar, D. G. "PM3-SM3: A General Parameterization for Including Aqueous Solvation Effects in the PM3 Molecular Orbital Model" *J. Comput. Chem.* **1992**, *13*, 1089.
20. Cramer, C. J.; Truhlar, D. G. "Polarization of the Nucleic Acid Bases in Aqueous Solution" *Chem. Phys. Lett.* **1992**, *198*, 74.
21. Cramer, C. J.; Truhlar, D. G. "What Causes Aqueous Acceleration of the Claisen Rearrangement?" *J. Am. Chem. Soc.* **1992**, *114*, 8794.
22. Cramer, C. J.; Truhlar, D. G. "Comparative Analysis of the AM1-SM2 and PM3-SM3 Parametrized SCF Solvation Models for Free Energies in Aqueous Solution" *J. Comput.-Aid. Mol. Des.* **1992**, *6*, 629.
23. Cramer, C. J. "Anomeric and Reverse Anomeric Effects in the Gas Phase and Aqueous Solution" *J. Org. Chem.* **1992**, *57*, 7034.
24. Cramer, C. J. "Where is the Unpaired Electron in the Phosphoranyl Radicals H_3PS^- and H_3PSH?" *Chem. Phys. Lett.* **1993**, *202*, 297.
25. Cramer, C. J.; Truhlar, D. G. "Quantum Chemical Conformational Analysis of Glucose in Aqueous Solution" *J. Am. Chem. Soc.* **1993**, *115*, 5745.
26. Cramer, C. J.; Truhlar, D. G. "Correlation and Solvation Effects on Heterocyclic Equilibria in Aqueous Solution" *J. Am. Chem. Soc.* **1993**, *115*, 8810.
27. Cramer, C. J.; Gustafson, S. M. "Hyperconjugation vs. Apicophilicity in Trigonal Bipyramidal Phosphorus Species" *J. Am. Chem. Soc.* **1993**, *115*, 9315.
28. Cramer, C. J.; Famini, G. R.; Lowrey, A. "Use of Quantum Chemical Properties as Analogs for Solvatochromic Parameters in Structure-Activity Relationships" *Acc. Chem. Res.* **1993**, *26*, 599.
29. Ruggiero, C. E.; Carrier, S. M.; Antholine, W. E.; Whittaker, J. W.; Cramer, C. J.; Tolman, W. B. "Synthesis and Structural and Spectroscopic Characterization of Mononuclear Copper

Nitrosyl Complexes: Models for Nitric Oxide Adducts of Copper Proteins and Copper-Exchanged Zeolites" *J. Am. Chem. Soc.* **1993**, *115*, 11285.

30. Cramer, C. J.; Truhlar, D. G. "Development and Biological Applications of Quantum Mechanical Continuum Solvation Models" in *Theoretical and Computational Chemistry: Solute/Solvent Interactions*, Vol. 2, Politzer, P., Murray, J. S., Eds.; Elsevier: Amsterdam, 1994; p. 9.
31. Cramer, C. J.; Gustafson, S. M. "Ab Initio Conformational and Stereopermutational Analysis of Dihydroxyphosphoranyl, $H_2P(OH)_2$" *J. Am. Chem. Soc.* **1994**, *116*, 723.
32. Cramer, C. J.; Denmark, S. E.; Miller, P. C.; Dorow, R. L.; Swiss, K. A.; Wilson, S. R. "Structure and Dynamics of Phosphorus(V)-Stabilized Carbanions: A Comparison of Theoretical, Crystallographic, and Solution Structures" *J. Am. Chem. Soc.* **1994**, *116*, 2437.
33. Cramer, C. J.; Truhlar, D. G. "Quantum Chemical Conformational Analysis of 1,2-Ethanediol: Correlation and Solvation Effects on the Tendency to Form Internal Hydrogen Bonds in the Gas Phase and Aqueous Solution" *J. Am. Chem. Soc.* **1994**, *116*, 3892.
34. Cramer, C. J.; Dulles, F. J.; Storer, J. W.; Worthington, S. E. "Full Valence Complete Active Space SCF, Multireference CI, and Density Functional Calculations of $^1A_1$–$^3B_1$ Singlet-Triplet Gaps for the Valence-Isoelectronic Series BH_2^-, CH_2, NH_2^+, AlH_2^-, SiH_2, PH_2^+, GaH_2^-, GeH_2, and AsH_2^+" *Chem. Phys. Lett.* **1994**, *218*, 387.
35. Giesen, D. J.; Cramer, C. J.; Truhlar, D. G. "Entropic Contributions to Free Energies of Solvation" *J. Phys. Chem.* **1994**, *98*, 4141.
36. Cramer, C. J. "Problems and Questions in the Molecular Modeling of Biomolecules" *Biochem. Ed.* **1994**, *22*, 140.
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