

Name: Lawrence Que, Jr.

Birthdate: April 23, 1949

Current Position: Regents Professor and 3M/Alumni Distinguished Professor of Chemistry

Education:

Ateneo de Manila University	B.S.	1969	Chemistry
University of Minnesota	Ph.D.	1973	Chemistry

Professional Experience:

Postdoctoral Study, Massachusetts Institute of Technology, 1973-74
Postdoctoral Study, Gray Freshwater Biological Institute, 1975-77
Assistant Professor of Chemistry, Cornell University, 1977-83
Associate Professor of Chemistry, University of Minnesota, 1983-1987
Professor of Chemistry, University of Minnesota, 1987-present.
3M/Alumni Distinguished Professor of Chemistry, University of Minnesota, 1999-present
Regents Professor, University of Minnesota, 2009-present

Visiting Professor, University of Florence, 1989; Université Paris-Sud, 1992; Ateneo de Manila University, 1993; Nankai University, 1993; University of Heidelberg, 2005.
Visiting Examiner, Chinese University of Hong Kong, 1997-2001
Advisory Committee, Institute of Chemistry, Academia Sinica, Taipei, Taiwan, 2004-2007

Awards and Honors:

Lubrizol Corporation Fellowship 1971-72; 3M Fellowship 1972-73
1982-86 Alfred P. Sloan Research Fellowship
1982-87 NIH Research Career Development Award
1996 NIOK Lectureship (Dutch National Graduate School in Catalysis)
1997 Distinguished Lectureship in Inorganic Chemistry at Northwestern University
2000 University of Minnesota Award for Outstanding Contributions in Post-Baccalaureate, Graduate, and Professional Education
2000-2010 National Institutes of Health MERIT Award
2000 Karcher Medal and Lectureship at University of Oklahoma
2001 Elected Fellow of the American Association for the Advancement of Science
2005 Cady Lectureship at University of Washington
2005 Frontiers in Biological Chemistry Award from the Max-Planck-Institut für Bioorganische Chemie
2006 Japan Society for the Promotion of Science Lecturer
2008 American Chemical Society Alfred Bader Award in Bioorganic or Bioinorganic Chemistry
2008 Designated Fellow of the Royal Society of Chemistry
2009 Habermann Distinguished Lectureship at Marquette University
2009 Appointed Regents Professor of the University of Minnesota
2010 Moses Gomberg Lecturer at the University of Michigan
2011 Royal Society of Chemistry Inorganic Reaction Mechanisms Award
2011 Elected American Chemical Society Fellow
2005-2011 Top 100 most cited living chemists (from [http://www.rsc.org/images/H-index%20ranking%20of%20living%20chemists\(March%202011\)_tcm18-85867.pdf](http://www.rsc.org/images/H-index%20ranking%20of%20living%20chemists(March%202011)_tcm18-85867.pdf))

Major Service at the University of Minnesota

Organizer, Metalloprotein Interest Group (MPIG) monthly meetings since 1986
 Co-Director, Center for Metals in Biocatalysis, University of Minnesota, 1994-present
 Director, Chemistry/Biology Interface Training Grant, 1999-2004, 2007-present
 Member, Molecular Biophysics Training Grant Steering Committee, 1988-96
 Member, Graduate School Fellowship Committee, 1993-96
 Chair, Chemistry NMR Committee, 1987-1999
 Chemistry Planning, Staffing, and Resources Committee, 1989-92
 Member, Graduate School Interdisciplinary Research, Scholarly and Creative Activity Review Committee 2001
 Chair, Kolthoff Hall Renovation Committee, 2005-2008
 Member, Chemistry Promotion and Tenure Committee, 2009-2011
 Member, College of Science and Engineering Promotion and Tenure Committee, 2010-2013

Major Service outside the University of Minnesota

Chief Editor, *Journal of Biological Inorganic Chemistry*, 2000-present
 Bioinorganic Chemistry Section Editor, *Chemtracts*, 1997-1999
 Editorial Advisory Boards: *Inorganic Chemistry* (1984-1987; 1999-2000), *Journal of Biological Inorganic Chemistry*, (1996-1999), *Current Opinion in Chemical Biology* (1997-present), *Accounts of Chemical Research* (2000-2002), *Inorganica Chimica Acta* (2004-present), and *Nature Communications* (2010-present).
 Chair-elect, 1992; Chair, 1993, ACS Division of Inorganic Chemistry, Bioinorganic Subdivision.
 Member, NIH Metallobiochemistry Study Section, 1984-1988.
 Ad hoc member, National Advisory General Medical Sciences Council, Sept. 1996
 Member, Site visit team for synchrotron research facilities funded by NIH, 1990, 1995, 1999
 Organizer, Symposium on "Metal Clusters in Proteins", Fall 1987 Meeting of the American Chemical Society (New Orleans)
 Member, National Committee for 4th Int'l Conference on Bioinorganic Chemistry, 1989.
 Chair, 1990 Gordon Conference on "Metals in Biology."
 Co-Organizer, Symposium on "Alkane Functionalization" held at Spring 1994 Meeting of the American Chemical Society (San Diego)
 Chair of the Organizing Committee for 1995 Midwest Bioinorganic Workshop (June 24-25, 1995, Minneapolis, Minnesota)
 Organizer, Kitajima Memorial Symposium on "Bioinorganic Chemistry" at Pacificchem95 (December, 1995, Honolulu, HI)
 Chair of the Organizing Committee for "1996 Conference on Oxygen Intermediates in Nonheme Metallobiochemistry" (June 23-27, 1996, Minneapolis, Minnesota)
 Chair of the Organizing Committee for 9th Int'l Conference on Bioinorganic Chemistry, 1999 (July 11-16, 1999, Minneapolis, Minnesota)
 Organizer, Symposium on Oxygen Activation in Biology at Pacificchem2000 (December 14-19, 2000, Honolulu, HI)
 Organizer, Symposium on Oxygen Activation in Biology at Pacificchem2005 (December 15-19, 2005, Honolulu, HI)
 Member, NSF Chemistry of Life Processes panel, April 2011.

Current Grant Support

NSF CHE-1058248 " High Valent Nonheme Iron-Oxo Complexes: Synthesis and Reactivity "

NIH GM-38767 "Synthetic Approaches for Modeling Metal-Oxo Proteins"

DOE DE-FG02-03ER15455 "Bio-inspired Iron Catalysts for Hydrocarbon Oxidations"

Publications: 440**Patents:** 7**Invited lectures at major conferences:** 115 since 1984 (22 plenary or keynote lectures)**Invited lectures at universities and companies:** over 200 since 1984 (5 endowed lectureships)**Teaching, University of Minnesota**

3301	Elementary Organic Chemistry I	84
4701	Inorganic Chemistry	00,01,02,03,04,07,08, 09,10 (2x),11
5302/8302	Interpretation of Organic Spectra	86-99 (except for 88,92,97)
5361/8361	Interpretation of Organic Spectra	99,00,04,05
5526/5527	Biophysical Chemistry	85-99 (except for 88,91,97)
5751/8751	Physical Inorganic Chemistry	85,87,89,90,98
8993	Special Topics/Molecular Recognition	90
5765/8765	Bioinorganic Chemistry	85,87,89,90,93,95,96
4735/8735	Bioinorganic Chemistry	99,04,08,11,12

Students Trained**Doctoral students (40+7)**

Robert H. Heistand, 1982	Manager, AVX Corporation
Randall B. Lauffer, 1983	CSO, Epix Medical
Ruth J. Mayer, 1983	Smith Kline Beecham
A. Lawrence Roe, 1983	Intel Corporation
L. Steven White, 1985	W. R. Grace
Joseph W. Pyrz, 1986	(Doylestown, Pennsylvania)
Bruce P. Murch, 1987	Proctor & Gamble
David D. Cox, 1988	Director of Regulatory Affairs, Navigant Biotechnologies
John B. Lynch, 1989	Director of Innovation, Strategy, and Management, Millipore Corporation
Sheila S. David, 1989	Professor, U of California Davis
Theodore R. Holman, 1991	Professor, U of California, Santa Cruz
Bridget A. Brennan, 1991	(Wilmington, Delaware)
Clayton R. Randall, 1993	Tech. Support, Amersham Biosciences
Leah T. Schnaith, 1994	(Red Wing, Minnesota)
Zhigang Wang, 1994	Research Scientist, Pfizer
Yu-min Chiou, 1994	L'Oreal Corporation
Jinheung Kim, 1995	Professor, Ewha Womans University
Charlene J. McMahon, 1996	Associate Professor, Milwaukee Area Technical College
Lijin Shu, 1997	Minneapolis Community and Technical College
Teresa Lehmann, 1997	Asst. Professor, University of Wyoming
Xuedong Wang, 1998	(Boston, Massachusetts)
Elizabeth C. Wilkinson, 1998	Asst. Professor, Lyndon State College, VT
Mark E. Branum, 1999	Senior Scientist, Theraclone Sciences, WA

Feben T. Gobena, 2000	Boston Scientific
Amy M. Rocklin, 2000	Foley & Lardner Inc., Washington, D.C.
Hui Zheng, 2000	D. Pharm program, University of Minnesota
Kui Chen, 2000	Research Scientist, 3M Co.
Vicki MacMurdo, 2002	Asst. Prof., Anoka Ramsey Community College
Mark E. Mehn, 2003	Asst. Professor, U of Wyoming
Michael R. Bukowski, 2005	Asst. Professor, Penn State Altoona
Kevin D. Koehntop, 2005	Postdoctoral, Scripps Institute, La Jolla, CA
Paul Oldenburg, 2007	Exxon Mobil Corporation
Eric Klinker, 2007	Senior Chemist, Dow Chemical Corporation
Jonathan R. Frisch, 2010	Instrumentation Lab Manager, Mississippi State University
Erik R. Farquhar, 2010	Research Scientist, Brookhaven National Lab
Dong Wang, 2010	Postdoctoral associate, Princeton University
Anusree Mukherjee, 2011	Postdoctoral associate, Argonne National Lab
Partha Das, 2011	Postdoctoral associate, Pacific Northwest National Lab
Yan Feng, 2011	Postdoctoral associate, Georgia Tech
Feifei Li, 2011	Postdoctoral associate, Brookhaven National Lab
Van Vu, 2011	Postdoctoral associate, Scripps Research Institute
Andrew J. Fielding, 2012 (expected)	
Gregory T. Rohde, 2013 (expected)	
Jennifer Bigelow, 2014 (expected)	
Scott Kleespiess, 2015 (expected)	
Mayank Puri, 2015 (expected)	
Andrew Janiewski, 2016 (expected)	
Anna Komor, 2016 (expected)	

Postdoctoral associates (70 total)

Michael J. Maroney, 1983-85	Professor, U of Massachusetts Amherst
Fontaine C. Bradley, 1984-86	Instructor at a New England prep school
Robert C. Scarrow, 1985-88	Professor, Haverford College
Andrew S. Borovik, 1986-88	Professor, U of California Irvine
Richard E. Norman, 1988-90	Professor, Sam Houston State U
Randolph E. Leising, 1989-91	Wilson-Greatbach Company
Anne E. True, 1988-91	(Huntsville, TX)
Li-June Ming, 1988-91	Professor, U of South Florida
Richard C. Holz, 1989-92	Professor, Loyola University
Timothy E. Elgren, 1989-92	Professor, Hamilton College
Ho G. Jang, 1989-92	Professor, Korea University
Stéphane Ménage, 1989-91	Directeur de Recherche, CNRS, Grenoble, France
Yan Zang, 1990-98	Control Data Corporation
Yanhong Dong, 1991-97	Staff Scientist, University of Minnesota
Takahiko Kojima, 1991-93	Professor, Tsukuba University
Hiroshi Fujii, 1992-93	Assoc. Prof., Inst. for Molecular Science, Okazaki
Michael P. Hendrich, 1992-3	Professor, Carnegie-Mellon University
Isabelle Michaud-Soret, 1993-94	Directeur de Recherche, CNRS, Grenoble, France
Masami Ito, 1994-95	Assistant Professor, Oita Nat'l University (Japan)
Roger G. Harrison, 1993-95	Associate Professor, Brigham Young U
Abhik Ghosh, 1992-95	Professor, U of Tromsø (Norway)
Cheal Kim, 1994-97	Assistant Professor, Seoul National Polytechnic U
Sanjay Mandal, 1995-97	Senior Scientist, Clariant Corporation
Adam K. Whiting, 1993-98	Senior Associate, Howrey LLP
Eric L. Hegg, 1996-99	Associate Professor, Michigan State University
Steven J. Lange, 1997-2000	Staff Scientist, Ecolab
Ulrich Bierbach, 1998-99	Professor, Wake Forest University
Manabendra Ray, 1998-1999	Associate Professor, IIT Guwahati, India

John R. Hagadorn, 1998-2000	Research Scientist, Exxon/Mobil
Huafen Hsu Konopka, 1997-2000	Assistant Professor, National Cheng Kung U
Shuorong Zhu, 1998-2000	Associate Professor, Nankai University
Alex Tipton, 2000-01	Research Scientist, Clorox Services Co.
Adrienne Tipton, 2000-01	Research Scientist, Clorox Services Co.
Jingyan Zhang, 2000-2001	Assistant Professor, East China University of Science and Technology.
Du-Hwan Jo, 1998-2001	Staff Scientist, POSCO, Korea
Raymond Y. N. Ho, 1995-2001	Research Scientist, Ecolab
Stéphane Torelli, 2000-2001	Maitre de Recerche, CNRS, Grenoble, France
Mark F. Reynolds, 1999-2002	Associate Professor, St. Joseph's University
Ferman A. Chavez, 1999-2002	Associate Professor, Oakland University
Aimin Liu, 1999-2002	Associate Professor, Georgia State U
Miquel Costas, 1999-2002	Associate Professor, Universitat de Girona
Luca Quaroni, 1999-2002	Staff Scientist, Canadian Light Source
Joszeif Kaizer, 2001-2003	Associate Professor, University of Pannonia, Hungary
Antoni Mairata, 2002-2004	ICREA Researcher at Bayer Polimeros, Tarragona, Spain
Megumi Fujita, 2001-2004	Assistant Professor, Southwest Georgia State U
Michael P. Jensen, 2000-2005	Assistant Professor, Ohio U
Jan-Uwe Rohde, 2000-2005	Assistant Professor, University of Iowa
Tapan K. Paine, 2003-2005	Assistant Professor, Indian Association for the Cultivation of Science
Alexander Pocutsa, 2004-2005	Ukranian Academy of Sciences
Yoshimitsu Tachi, 2004-2005	Assistant Professor, Osaka City University
Chun-Yen Ke, 2004-2006	(Corvalis, Oregon)
David P. Klein, 2004-2006	Internet Sales, Discount Steel, Inc.
Timothy A. Jackson, 2005-2007	Assistant Professor, University of Kansas
Seth J. Friese, 2005-2007	Assistant Professor, Salisbury College
Joseph P. Emerson, 2003-2007	Assistant Professor, Mississippi State University
Ruben Más, 2004-2007	Research Associate, Univ Autonoma Madrid, Spain
Xiaopeng Shan, 2003-2008	Research Chemist, Eastman Chemical
Xi Zhang, 2007-2008	(Beijing, China)
Paul Vecchi, 2007-2008	(St. Paul, MN)
Kallol Ray, 2006-2008	Assistant Professor, Humboldt University Berlin
Adam T. Fiedler, 2006-2009	Assistant Professor, Marquette University
Jason England, 2006-2010	Staff Scientist, MPI Muelheim
Yuming Zhou, 2004-2008, 2009-2010	(St. Paul, MN)
V. K. K. Praneeth, 2008-2011	Research Associate, U of Basel
Gen-Qiang Xue, 2006-2011	Dow Corning
Matthew A. Cranswick, 2008-2012	Assistant Professor, Colorado State U at Pueblo
Kathy van Heuvelen, 2009-2012	Assistant Professor, Harvey Mudd College
Aidan R. McDonald, 2008-2012	Assistant Professor, Trinity College Dublin
Williamson Oloo, 2011-present	
Lisa Engstrom, 2012-present	

Publications:

1. L. Que, Jr. and L. H. Pignolet, "Proton Magnetic Resonance Study of Stereochemistry of Four Coordinate Nickel (II) Complexes. Dihalobis(tertiary phosphine)nickel(II) Complexes" *Inorg. Chem.* **1973**, *12*, 156.
2. L. H. Pignolet, D. J. Duffy, and L. Que, Jr., "Stereochemically Nonrigid Ruthenium(III) and Cobalt(III) Tris-Chelate Complexes" *J. Am. Chem. Soc.* **1973**, *95*, 295.
3. M. C. Palazzotto, D. J. Duffy, L. Que, Jr. and L. H. Pignolet, "Dynamic Stereochemistry of Tris-Chelate Complexes I. Tris(dithiocarbamate) Complexes of Iron, Cobalt, and Rhodium" *J. Am. Chem. Soc.* **1973**, *95*, 4537.
4. L. Que, Jr., G. R. Willie, M. Cashel, J. W. Bodley, and G. R. Gray, "Guanosine 5'-Diphosphate, 3'-Diphosphate: Assignment of Structure by ^{13}C Nuclear Magnetic Resonance Spectroscopy" *Proc. Nat. Acad. Sci., U.S.A.* **1973**, *70*, 2563.
5. L. Que, Jr., R. H. Holm, and L. E. Mortenson, "Extrusion of Fe_2S_2 and Fe_4S_4 Cores from the Active Sites of Ferredoxin Proteins" *J. Am. Chem. Soc.* **1973**, *97*, 463.
6. L. Que, Jr. and G. R. Gray, " ^{13}C Nuclear Magnetic Resonance Spectra and the Tautomeric Equilibria of Keto-hexoses in Solution" *Biochemistry* **1974**, *13*, 146.
7. M. A. Bobrik, L. Que, Jr., and R. H. Holm, "Synthetic Analogs of the Active Sites of Iron-Sulfur Proteins IV. Ligand Substitution Reactions of the Tetranuclear Clusters $[\text{Fe}_4\text{S}_4(\text{SR})_4]^{2-}$ " *J. Am. Chem. Soc.* **1974**, *96*, 285.
8. L. Que, Jr. and L. H. Pignolet, "Dynamic Stereochemistry of Tri-Chelate Complexes II. Tri(dithiocarbamate) Complexes of Manganese(III), Vanadium(III), Chromium(III), Gallium(III), and Indium(III)" *Inorg. Chem.* **1974**, *13*, 351.
9. B. V. DePamphilis, B. A. Averill, T. Heroskovitz, L. Que, Jr., and R. H. Holm, "Synthetic Analogs of the Active Sites of Iron-Sulfur Proteins. VI. Spectral and Redox Characteristics of the Tetranuclear Clusters $[\text{Fe}_4\text{S}_4(\text{SR})_4]^{2-}$ " *J. Am. Chem. Soc.* **1974**, *96*, 4199.
10. L. Que, Jr., M. A. Bobrik, J. A. Ibers, and R. H. Holm, "Synthetic Analogs of the Active Sites of Iron-Sulfur Proteins. VII. Ligand Substitution Reactions of the Tetranuclear Clusters $[\text{Fe}_4\text{S}_4(\text{SR})_4]^{2-}$ and the Structure of $[\text{CH}_3)_4\text{N}]_2.[\text{Fe}_4\text{S}_4(\text{SC}_6\text{H}_5)_4]$ " *J. Am. Chem. Soc.* **1974**, *96*, 4168.
11. L. Que, Jr., J. R. Anglin, M. A. Bobrik, A. Davison, and R. H. Holm, "Synthetic Analogs of the Active Sites of Iron-Sulfur Proteins. IX. Formation and Some Electronic Reactivity Properties of Fe_4S_4 Glycyl-L-Cysteiny-Glycyl Oligopeptide Complexes Obtained by Ligand Substitution Reactions" *J. Am. Chem. Soc.* **1974**, *96*, 6042.
12. G. V. Rao, L. Que, Jr., L. D. Hall, and T. P. Fondy, "Deoxyfluoroketohexoses: -4-Deoxy-4-fluoro-D-sorbose and -tagatose and 5-deoxy-5-L-sorbose" *Carbohydr. Res.* **1975**, *40*, 311.
13. J. B. Howard, T. Lorsbach, and L. Que, Jr., "Iron-Sulfur Clusters and Cysteine Distribution in a Ferredoxin from *Azotobacter Vinelandii*" *Biochem. Biophys. Res. Comm.* **1976**, *70*, 582.
14. R. A. Haberkorn, L. Que, Jr., W. O. Gillum, R. H. Holm, C. S. Liu, and R. C. Lord, "Cadmium-113-Fourier Transform NMR and Raman Spectroscopic Studies of Cadmium(II)-Sulfur Complexes, Including $[\text{Cd}_{10}(\text{SCH}_2\text{CH}_2\text{OH})_{16}]^{4+}$ " *Inorg. Chem.* **1976**, *16*, 2408.

15. E. Münck, R. Zimmermann, J. D. Lipscomb, L. Que, Jr., and W. H. Orme-Johnson, "Characterization of an Oxygenated Intermediate in a Dioxygenase Reaction by EPR and Mössbauer Spectroscopy" *J. de Physique* **1976**, *37*, C6-203.
16. L. Que, Jr., J. D. Lipscomb, R. Zimmermann, E. Münck, N. R. Orme-Johnson, and W. H. Orme-Johnson, "EPR and Mössbauer Studies of Protocatechuate-3,4-Dioxygenase from *Pseudomonas Aeruginosa*" *Biochim. Biophys. Acta* **1976**, *452*, 320.
17. P. G. Debrunner, E. Münck, L. Que, Jr., and C. E. Schulz, "Recent Mössbauer Results of Some Iron-Sulfur Proteins and Model Complexes" in "Iron-Sulfur Proteins," (W. Lovenberg, ed.) Academic Press, New York, **1977**, pp. 381.
18. J. M. Wood, J. D. Lipscomb, L. Que, Jr., R. S. Stephens, W. H. Orme-Johnson, E. Münck, W. P. Ridley, L. Dizikes, A. Cheh, M. Francia, T. Frick, R. Zimmermann, and J. Howard, "Some Bioinorganic Chemical Reactions of Environmental Significance" "Biological Aspects of Inorganic Chemistry" (Proceedings of the International Symposium) D. Dolphin, ed. Wiley-Interscience **1977**.
19. L. Que, Jr., J. D. Lipscomb, E. Münck, and J. M. Wood, "Protocatechuate 3,4-Dioxygenase: Inhibitor Studies and Mechanistic Implications" *Biochim. Biophys. Acta* **1977**, *485*, 60.
20. M. H. Emptage, R. Zimmermann, L. Que, Jr., E. Münck, W. Hamilton, and W. H. Orme-Johnson, "Mössbauer and EPR Studies of Cytochrome c' from *Rhodospirillum Rubrum*" *Biochim. Biophys. Acta* **1977**, *495*, 12.
21. J. M. Wood, R. L. Crawford, E. Münck, R. Zimmermann, J. D. Lipscomb, R. S. Stephens, J. W. Bromley, L. Que, Jr., J. B. Howard, and W. H. Orme-Johnson, "Structure and Function of Dioxygenases. One Approach to Lignin Degradation" *J. Agric. Food. Chem.* **1977**, *25*, 698.
22. L. Que, Jr., "Extradial Cleavage of o-Aminophenol of Pyrocatechase" *Biochem. Biophys. Res. Comm.* **1978**, *84*, 60.
23. L. Que, Jr., R. H. Heistand II, "Resonance Raman Studies of Pyrocatechase" *J. Am. Chem. Soc.* **1979**, *101*, 2219.
24. L. Que, Jr., "Non-Heme Iron Dioxygenases: Structure and Mechanism" *Struct. Bonding* **1980**, *40*, 39.
25. L. Que, Jr., R. H. Heistand II, R. Mayer, and A. L. Roe, "Resonance Raman Studies of Pyrocatechase-Inhibitor Complexes" *Biochemistry* **1980** *19*, 2588.
26. L. Que, Jr. and R. M. Epstein, "Resonance Raman Studies of Protocatechuate 3,4-Dioxygenase-Inhibitor Complexes" *Biochemistry* **1981**, *20*, 2545.
27. R. B. Lauffer, R. H. Heistand II, and L. Que, Jr., "Dioxygenase Model Studies: The Reaction of Oxygen with Iron Catecholates" *J. Am. Chem. Soc.* **1981**, *103*, 3947.
28. L. Que, Jr., J. Widom, and R. L. Crawford, "3,4-Dihydroxyphenylacetate 2,3-Dioxygenase. A Manganese Dioxygenase from *Bacillus brevis*" *J. Biol. Chem.* **1981**, *256*, 10941.
29. R. H. Heistand II, A. L. Roe, and L. Que, Jr., "Dioxygenase Models. The Crystal Structures of Fe(saloph)catH and [Fe(salen)]₂hq" *Inorg. Chem.* **1982**, *21*, 676.
30. L. Que, Jr. and R. Mayer, "Intermediates in the Reaction of Catechol 1,2-Dioxygenase with Pyrogallol and Oxygen" *J. Am. Chem. Soc.* **1982**, *104*, 875.

31. R. H. Heistand II, R. B. Lauffer, E. Fikrig, and L. Que, Jr., "Catecholate and Phenolate Iron Complexes as Models for the Dioxygenases" *J. Am. Chem. Soc.* **1982**, *104*, 2789.
32. L. Que, Jr., "Spectroscopic Studies on Catechol 1,2-Dioxygenase," in "Oxygenases and Oxygen Metabolism" (M. Nozaki, T. Ishimura, A. Yamamoto, M. J. Coon, R. W. Estabrook, L. Ernster, eds.) Academic Press, New York, **1982**, pp. 39-50.
33. L. S. White, E. J. Hellman, and L. Que, Jr., "On the Oxidative Cleavage of 3,5-Di-tert-butyl-o-benzoquinone" *J. Org. Chem.* **1982**, *47*, 3766.
34. R. B. Lauffer and L. Que, Jr., "¹H NMR and ²H NMR Studies of the Catechol Dioxygenases" *J. Am. Chem. Soc.* **1982**, *104*, 7324.
35. R. B. Lauffer, R. H. Heistand II, and L. Que, Jr., "The Crystal Structures of Fe(salen)acac, Fe(salen)PSQ, and K⁺[Fe(salen)cat]⁻" *Inorg. Chem.* **1983**, *22*, 50.
36. L. Que, Jr., R. B. Lauffer, and R. H. Heistand II, "The Enzyme-Substrate Interaction in the Catechol Dioxygenases," in "Coordination Chemistry of Metalloenzymes in Hydrolytic and Oxidative Processes" (I. Bertini, R. S. Drago, C. Luchinat, eds.) D. Reidel Publishing Company, Dordrecht, **1983**, pp. 265-271.
37. L. Que, Jr., R. B. Lauffer, B. C. Antanaitis, and P. Aisen, "NMR Studies of Porcine Uteroferrin: Evidence for a Spin-Coupled Binuclear Cluster" *Inorg. Chim. Acta* **1983**, *79*, 137.
38. L. Que, Jr., "Metalloproteins with Phenolate Coordination" *Coord. Chem. Rev.* **1983**, *50*, 73.
39. L. Que, Jr., "The Catechol Dioxygenases," in "Iron Binding Proteins Without Cofactors or Sulfur Clusters," Advances in Inorganic Biochemistry, Vol. 5 (E. C. Theil, G. L. Eichhorn, L. G. Marzilli, eds.) Elsevier, New York, **1983**, pp. 167-199.
40. R. B. Lauffer, L. Que, Jr., B. C. Antanaitis, and P. Aisen, "NMR Studies of Porcine Uteroferrin" *J. Biol. Chem.* **1983**, *258*, 14212-14218.
41. T. Walsh, D. P. Ballou, R. Mayer, and L. Que, Jr., "Rapid Kinetic Studies on the Oxygenation Reactions of Catechol of Dioxygenase" *J. Biol. Chem.* **1983**, *258*, 14422-14427.
42. A. L. Roe, D. J. Schneider, R. Mayer, J. W. Pyrz, J. Widom, and L. Que, Jr., "X-ray Absorption Studies of the Iron-Tyrosinate Proteins" *J. Am. Chem. Soc.* **1984**, *106*, 1676-1681.
43. D. J. Schneider, A. L. Roe, R. J. Mayer, and L. Que, Jr., "Evidence for Synergistic Anion Binding to Iron in Ovotransferrin Complexes from Resonance Raman and EXAFS Analysis" *J. Biol. Chem.* **1984**, *259*, 9699-9703.
44. R. J. Mayer and L. Que, Jr., "¹⁸O Studies of Pyrogallol Cleavage by Catechol 1,2-Dioxygenase" *J. Biol. Chem.* **1984**, *259*, 13056-13060.
45. M. J. Maroney, R. B. Lauffer, L. Que, Jr., and D. M. Kurtz, Jr., "Paramagnetic ¹H-NMR Spectra of Hemerythrin from *Phascolopsis gouldii*" *J. Am. Chem. Soc.* **1984**, *106*, 6445-6446.
46. L. S. White, P. V. Nilsson, L. H. Pignolet, and L. Que, Jr., "Iron(III)-Catalyzed Oxygenation of Catechols. Structure of [Fe(NTA)DBC]⁻" *J. Am. Chem. Soc.* **1984**, *106*, 8312-8313.

47. J. W. Pyrz, K. D. Karlin, T. N. Sorrell, G. C. Vogel, and L. Que, Jr., "Resonance Raman Studies of Phenolate Bridged Binuclear Copper Complexes. Relevance to Hemocyanin and Tyrosinase" *Inorg. Chem.* **1984**, *23*, 4581-4584.
48. J. W. Pyrz, A. L. Roe, L. J. Stern, and L. Que, Jr., "Model Studies of Iron-Tyrosinate Proteins" *J. Am. Chem. Soc.* **1985**, *107*, 614-620.
49. J. M. Nocek, D. M. Kurtz, Jr., J. T. Sage, P. G. Debrunner, M. J. Maroney, and L. Que, Jr., "A Nitric Oxide Adduct of the Binuclear Iron Center in Deoxyhemerythrin from *Phascolopsis gouldii*. Analogue of a Putative Intermediate in the Oxygenation Reaction" *J. Am. Chem. Soc.* **1985**, *107*, 3382-3384.
50. J. B. Howard, T. L. Deits, G. L. Anderson, M. Maroney, L. Que, Jr. and R. P. Hausinger, "Mechanism and Structure of Nitrogenase Fe-Protein," in "Nitrogen Fixation and CO₂ Metabolism" (P. W. Ludden and J. E. Burris, eds.) Elsevier, **1985**, pp. 153-162.
51. L. S. White and L. Que, Jr., "Cobalt-Catalyzed Oxidative Cleavage of Semi-quinones" *J. Mol. Catal.* **1985**, *33*, 139-149.
52. B. P. Murch, P. D. Boyle, and L. Que, Jr., "Structures of Binuclear and Tetranuclear Iron(III) Complexes as Models for Ferritin Core Formation" *J. Am. Chem. Soc.* **1985**, *107*, 6728-6729.
53. L. Que, Jr., "Spectroscopic Studies of the Catechol Dioxygenases, *J. Chem. Ed.* **1985**, *62*, 938-943.
54. L. Que, Jr., L. S. White, and J. W. Pyrz, "Iron(III)-Catalyzed Cleavage of Catechols" in *Frontiers in Bioinorganic Chemistry* (A.V. Xavier, ed.) VCH, Weinheim **1986**, pp. 225-232.
55. J. W. Pyrz, J. T. Sage, P. G. Debrunner, and L. Que, Jr., "The Interaction of Phosphate with Uteroferrin. Characterization of a Reduced Phosphate Complex" *J. Biol. Chem.* **1986**, *261*, 11015-11020.
56. B. P. Murch, F. C. Bradley, and L. Que, Jr., "A Binuclear Iron Peroxide Complex Capable of Olefin Epoxidation" *J. Am. Chem. Soc.* **1986**, *108*, 5027-5028.
57. F. C. Bradley, S. Lindstedt, J. D. Lipscomb, L. Que, Jr., A. L. Roe, and M. Rundgren, "4-Hydroxyphenylpyruvate Dioxygenase Is an Iron-Tyrosinate Protein" *J. Biol. Chem.* **1986**, *261*, 11693-11696.
58. R. C. Scarrow, M. J. Maroney, S. M. Palmer, L. Que, Jr., S. P. Salowe, and J. Stubbe, "EXAFS Studies of the B₂ Subunit of the Ribonucleotide Reductase from *E. coli*" *J. Am. Chem. Soc.* **1986**, *108*, 6832-6834.
59. M. J. Maroney, D. M. Kurtz, Jr., J. N. Nocek, L. L. Pearce, and L. Que, Jr., "¹H NMR Probes of the Binuclear Iron Cluster in Hemerythrin" *J. Am. Chem. Soc.* **1986**, *108*, 6871-6879.
60. I. M. Arafa, H. M. Goff, S. S. David, B. P. Murch, and L. Que, Jr., "Hydrogen and Deuterium NMR Studies of Carboxylate Coordination to Iron(III) Complexes: Diverse Chemical Shift Values for Coordinated Carboxyl Residues" *Inorg. Chem.* **1987**, *26*, 2779-2784.
61. L. Que, Jr. and M. J. Maroney, "NMR Studies of Magnetically Coupled Metalloproteins" *Metal Ions in Biological Systems* **1987**, *21*, 87-120.
62. T. A. Kent, E. Münck, J. W. Pyrz, J. Widom, and L. Que, Jr., "Mössbauer and EPR Spectroscopy of Catechol 1,2-Dioxygenase" *Inorg. Chem.* **1987**, *26*, 1402-1408.

63. L. Que, Jr., R. C. Kolanczyk, and L. S. White, "Functional Models for Catechol 1,2-Dioxygenase. Structure, Reactivity, and Mechanism" *J. Am. Chem. Soc.* **1987**, *109*, 5373-5380.
64. L. Que, Jr., R. B. Lauffer, J. B. Lynch, B. P. Murch, and J. W. Pyrz, "Elucidation of the Coordination Chemistry of the Enzyme-Substrate Complex of Catechol 1,2-Dioxygenase by NMR Spectroscopy" *J. Am. Chem. Soc.* **1987**, *109*, 5381-5385.
65. R. C. Scarrow, M. J. Maroney, S. M. Palmer, L. Que, Jr., A. L. Roe, S. P. Salowe, and J. Stubbe, "EXAFS Studies of Binuclear Iron Proteins: Hemerythrin and Ribonucleotide Reductase" *J. Am. Chem. Soc.* **1987**, *109*, 7857-7864.
66. B. P. Murch, F. C. Bradley, P. D. Boyle, V. Papaefthymiou, and L. Que, Jr., "Iron-Oxo Aggregates. Crystal Structures and Solution Characterization of 2-Hydroxy-1,3-xylylenediaminetetraacetic Acid Complexes" *J. Am. Chem. Soc.* **1987**, *109*, 7993-8003.
67. A. S. Borovik, B. P. Murch, L. Que, Jr., V. Papaefthymiou, and E. Münck, "Models for Iron-Oxo Proteins. A Mixed Valence Fe(II)-Fe(III) Complex" *J. Am. Chem. Soc.* **1987**, *109*, 7190-7191.
68. L. Que, Jr., "Metal-Tyrosinate Proteins" in "Biological Applications of Raman Spectroscopy" (T.G. Spiro, ed.) Wiley, New York **1988**, pp. 491-521.
69. A. S. Borovik, L. Que, Jr., V. Papaefthymiou, E. Münck, L. F. Taylor and O. P. Anderson, "Heterobimetallic Complexes with (μ -Phenoxo)bis(μ -carboxylato) Cores" *J. Am. Chem. Soc.* **1988**, *110*, 1986-1988.
70. A. S. Borovik and L. Que, Jr., "Models for the Fe(II) Fe(III) Forms of Iron-Oxo Proteins" *J. Am. Chem. Soc.* **1988**, *110*, 2345-2347.
71. D. D. Cox, S. J. Benkovic, L. M. Bloom, F. C. Bradley, M. J. Nelson, L. Que, Jr., and D. E. Wallick, "Catecholate LMCT Bands as Probes for the Active Sites of Nonheme Iron Oxygenases" *J. Am. Chem. Soc.* **1988**, *110*, 2026-2032.
72. S. Yan, L. Que, Jr., L. F. Taylor, and O. P. Anderson, "A Model for the Chromophoric Site of Purple Acid Phosphatases" *J. Am. Chem. Soc.* **1988**, *110*, 5222-5224.
73. L. Que, Jr., D. D. Cox, and R. C. Kolanczyk, "Functional Models for Catechol 1,2-Dioxygenase" in *The Role of Oxygen in Chemistry and Biochemistry* (W. Ando and Y. Moro-Oka, eds.) Elsevier, Amsterdam, **1988**, pp. 399-405.
74. Q. Chen, J. B. Lynch, P. Gomez-Romero, A. Ben-Hussein, G. B. Jameson, C. J. O'Connor, and L. Que, Jr., "Iron-Oxo Aggregates. Binuclear and Tetranuclear Complexes of N,N,N',N'-Tetrakis(2-benzimidazolylmethyl)-2-hydroxy-1,3-diaminopropane" *Inorg. Chem.* **1988**, *27*, 2673-2681.
75. L. Que, Jr. and R. C. Scarrow, "Active Sites of Binuclear Iron-Oxo Proteins," in "Metal Cluster in Proteins" (Que, L., Jr., ed.) *ACS Symp Ser.* **1988**, *372*, 152-177.
76. D. D. Cox and L. Que, Jr., "Functional Models for Catechol 1,2-Dioxygenase. The Role of the Iron(III) Center" *J. Am. Chem. Soc.* **1988**, *110*, 8085-8092.
77. E. P. Day, S. S. David, J. Peterson, N. R. Dunham, J. J. Bonviosin, R. H. Sands, and L. Que, Jr., "Magnetization and Electron Paramagnetic Resonance Studies of Reduced Uteroferrin and Its 'EPR-Silent' Phosphate Complex" *J. Biol. Chem.* **1988**, *263*, 15561-15567.

78. K. K. Andersson, D. D. Cox, L. Que, Jr., T. Flatmark, and J. Haavik, "Resonance Raman Studies on the Blue-Green Colored Bovine Adrenal Tyrosine 3-Monooxygenase" *J. Biol. Chem.* **1988**, *263*, 18621-18626.
79. M. J. Maroney, R. C. Scarrow, L. Que, Jr., A. L. Roe, G. S. Lukat, and D. M. Kurtz, Jr., "X-ray Absorption Spectroscopic Studies of the Sulfide Complexes of Hemerythrin" *Inorg. Chem.* **1989**, *28*, 1342-1348.
80. J. B. Lynch, C. Juarez-Garcia, E. Münck, and L. Que, Jr., "Mössbauer and EPR Studies of the Binuclear Iron Center in Ribonucleotide Reductase for *Escherichia coli*. A New Iron-To-Protein Stoichiometry" *J. Biol. Chem.* **1989**, *264*, 8091-8096.
81. L. Que, Jr., "The Catechol Dioxygenases" in "Iron Carriers and Iron Proteins" (T. M. Loehr, ed.) VCH, New York, **1989**, pp. 467-523.
82. S. Yan, D. D. Cox, L. L. Pearce, C. Juarez-Garcia, L. Que, Jr., J. H. Zhang, and C. J. O'Connor, "A (μ -Oxo)(μ -carboxylato)diiron(III) Complex with Distinct Iron Sites" *Inorg. Chem.* **1989**, *28*, 2507-2509.
83. A. S. Borovik, V. Papaefthymiou, L. F. Taylor, O. P. Anderson, and L. Que, Jr., "Models for Iron-Oxo Proteins. Structures and Properties of $\text{Fe}^{\text{II}}\text{Fe}^{\text{III}}$, $\text{Zn}^{\text{II}}\text{Fe}^{\text{III}}$, and $\text{Fe}^{\text{II}}\text{Ga}^{\text{III}}$ Complexes with (μ -Phenoxo)bis(μ -carboxylato)dimetal Cores" *J. Am. Chem. Soc.* **1989**, *111*, 6183-6193.
84. R. E. Norman, S. Yan, L. Que, Jr., G. Backes, J. Ling, J. Sanders-Loehr, J. H. Zhang, and C. J. O'Connor, "(μ -Oxo)(μ -carboxylato)diiron(III) Complexes with Distinct Iron Sites. Consequences of the Inequivalence and Its Relevance to Dinuclear Iron-Oxo Proteins" *J. Am. Chem. Soc.* **1990**, *112*, 1554-1562.
85. L. Ming, L. Que, Jr., A. Kriauciunas, C. A. Frolik, and V. J. Chen, "Coordination Chemistry of the Metal Binding Site of Isopenicillin N Synthase" *J. Am. Chem. Soc.* **1990**, *29*, 1111-1112.
86. R. C. Scarrow, J. W. Pyrz, and L. Que, Jr., "NMR Studies of the Dinuclear Iron Site in Reduced Uteroferrin and Its Oxoanion Complexes" *J. Am. Chem. Soc.* **1990**, *112*, 657-665.
87. R. A. Leising, R. E. Norman, and L. Que, Jr., "Alkane Functionalization by Non-Porphyrin Iron Complexes: Mechanistic Insights" *Inorg. Chem.* **1990**, *29*, 2554-2555.
88. A. S. Borovik, M. P. Hendrich, T. R. Holman, L. Que, Jr., V. Papaefthymiou, and E. Münck, "Models for Diferrous Forms of Iron-Oxo Proteins. Structure and Properties of $[\text{Fe}_2\text{BPMP}(\text{O}_2\text{CR})_2]\text{BPh}_4$ Complexes" *J. Am. Chem. Soc.* **1990**, *112*, 6031-6038.
89. L. Ming, R. B. Lauffer, and L. Que, Jr., "Proton Nuclear Magnetic Resonance Studies of Iron(II/III)-Amide Complexes. Spectroscopic Models for Non-Heme Iron Proteins" *Inorg. Chem.* **1990**, *29*, 3060-3064.
90. S. Ménage, B. A. Brennan, C. Juarez-Garcia, E. Münck, and L. Que, Jr., "Models for Iron-Oxo Proteins: Dioxygen Binding to a Diferrous Complex" *J. Am. Chem. Soc.* **1990**, *112*, 6423-6425.
91. S. S. David and L. Que, Jr., "Anion Binding to Uteroferrin. Evidence for Phosphate Coordination to the Fe(III) Ion of the Dinuclear Active Site and Interaction with the Hydroxo Bridge" *J. Am. Chem. Soc.* **1990**, *112*, 6455-6463.

92. T. R. Holman, C. Juarez-Garcia, M. P. Hendrich, L. Que, Jr., and E. Münck, "Models for Iron-Oxo Proteins. Mössbauer and EPR Study of an Antiferromagnetically Coupled Fe^{III}Ni^{II} Complex" *J. Am. Chem. Soc.* **1990**, *112*, 7611-7618.
93. T. R. Holman, K. A. Anderson, O. P. Anderson, M. P. Hendrich, C. Juarez-Garcia, E. Münck, and L. Que, Jr., "Correlations Between Magnetism and Structure in Dinuclear Cu(II)Fe(III) Complexes with Integer Spin EPR Signals" *Angew. Chem. Int. Ed. Engl.* **1990**, *29*, 921-923.
94. S. Ménage and L. Que, Jr., "A Bis(μ -alkoxo)diiron Complex with Novel Terminally Ligated Carboxylates. Implications for Diiron-Oxo Proteins" *Inorg. Chem.* **1990**, *29*, 4293-4297.
95. L. Que, Jr. and A. E. True, "Dinuclear Iron- and Manganese-Oxo Centers in Biology" *Prog. Inorg. Chem.* **1990**, *38*, 97-200.
96. A. E. True, A. M. Orville, L. L. Pearce, J. D. Lipscomb, and L. Que, Jr., "An EXAFS Study of the Interaction of Substrate with the Ferric Active Site of Protocatechuate 3,4-Dioxygenase" *Biochemistry* **1990**, *29*, 10847-10854.
97. R. E. Norman, R. C. Holz, S. Ménage, C. J. O'Connor, J. Zhang, and L. Que, Jr., "Structures and Properties of Dibriged (μ -oxo)diiron(III) Complexes. Effects of the Fe-O-Fe Angle" *Inorg. Chem.* **1990**, *29*, 4629-4637.
98. C. Juarez-Garcia, M. P. Hendrich, T. R. Holman, L. Que, Jr., and E. Münck, "Combined Mössbauer and EPR Studies of the S = 3 State of an Exchange-Coupled Fe^{III}Cu^{II} Complex: Test for Quantitative EPR Analysis of Integer Spin Systems" *J. Am. Chem. Soc.* **1991**, *113*, 518-525.
99. M. P. Hendrich, L. L. Pearce, L. Que, Jr., N. D. Chasteen, and E. P. Day, "Multifield Saturation Magnetization and Multifrequency EPR Measurements of Deoxyhemerythrin Azide. A Unified Picture," *J. Am. Chem. Soc.* **1991**, *113*, 3039-3044.
100. B. A. Brennan, Q. Chen, C. Juarez-Garcia, A. E. True, C. J. O'Connor, and L. Que, Jr., "Models for Diiron-Oxo Proteins. The Peroxide Adduct of Fe₂(HPTB)(OH)(NO₃)₄," *Inorg. Chem.* **1991**, *30*, 1937-1943.
101. R. A. Leising, B. A. Brennan, L. Que, Jr., B. G. Fox, and E. Münck, "Models for Non-Heme Iron Oxygenases: A High Valent Iron-Oxo Intermediate," *J. Am. Chem. Soc.* **1991**, *113*, 3988-3990.
102. L. Que, Jr., "Oxygen Activation at the Diiron Center of Ribonucleotide Reductase" *Science* **1991**, *253*, 273-274.
103. M. P. Hendrich, T. E. Elgren, and L. Que, Jr., "A Mixed Valence Form of the Iron Cluster in the B2 Protein of Ribonucleotide Reductase from *Escherichia Coli*," *Biochem. Biophys. Res. Commun.* **1991**, *176*, 705-710.
104. D. L. Wang, R. C. Holz, S. S. David, L. Que, Jr., and M. T. Stankovich, "Electrochemical Properties of the Diiron Core of Uteroferrin and Its Anion Complexes," *Biochemistry* **1991**, *30*, 8187-8194.
105. M. J. Nelson, H. Jin, I. M. Turner, Jr., G. Grove, R. C. Scarrow, B. A. Brennan, and L. Que, Jr., "A Novel Iron-Sulfur Center in Nitrile Hydratase from *Brevibacterium sp.*," *J. Am. Chem. Soc.* **1991**, *113*, 7072-7073.
106. S. Ménage and L. Que, Jr., "(μ -Oxo)(μ -Carboxylato)diiron(III) Complexes. Effects of the Terminal Ligands," *New J. Chem.* **1991**, *15*, 431-438.

107. J. W. Pyrz, X. Pan, D. Britton, and L. Que, Jr., "Models for Catechol Dioxygenases. Structure of Bromobis[2-(2'-hydroxyphenyl)benzothiazolato]iron(III) Derived from the Bromoiron(III) complex of 2,2'-Bis((salicylideneamino)phenyl) Disulfide," *Inorg. Chem.* **1991**, *30*, 4362-3464.
108. R. A. Leising, Y. Zang, and L. Que, Jr., "Oxidative Ligand Transfer to Alkanes: A Model for Iron-Mediated C–X Bond Formation in β -Lactam Antibiotic Biosynthesis," *J. Am. Chem. Soc.* **1991**, *113*, 8555-8557.
109. T. E. Elgren, J. B. Lynch, C. Juarez-Garcia, E. Münck, B-M. Sjöberg, and L. Que, Jr., "Electron Transfer Associated with Oxygen Activation in the B2 Protein of Ribonucleotide Reductase from *Escherichia coli*," *J. Biol. Chem.* **1991**, *266*, 19265-19268.
110. H. G. Jang, D. D. Cox, L. Que, Jr., "A Highly Reactive Functional Model for the Catechol Dioxygenases. Structure and Properties of [Fe(TPA)DBC]BPh₄," *J. Am. Chem. Soc.* **1991**, *113*, 9201-9204.
111. F. Jiang, J. Peisach, L.-J. Ming, and L. Que, Jr., V. J. Chen, "Electron Spin Echo Envelope Modulation Studies of the Cu(II)-Substituted Derivative of Isopenicillin N Synthase: A Structural and Spectroscopic Model," *Biochemistry* **1991**, *30*, 11437-11445.
112. L.-J. Ming, L. Que, Jr., A. Kriauciunas, C. A. Frolik, and V. J. Chen, "NMR Studies of the Active Site of Isopenicillin N Synthase, a Non-Heme Iron(II) Enzyme," *Biochemistry* **1991**, *30*, 11653-11659.
113. D. Britton, R. E. Norman, and L. Que, Jr., "Tris[(2-pyridinium)methyl]amine Perchlorate," *Acta Cryst.* **1991**, *C47*, 2415-2417.
114. L.-J. Ming, H. G. Jang, and L. Que, Jr., "2D NMR Studies of Paramagnetic Diiron Complexes," *Inorg. Chem.* **1992**, *31*, 359-364.
115. T. R. Holman, M. P. Hendrich, and L. Que, Jr., "EPR Studies of a Dinickel Complex in Its II,II and II,III Oxidation States," *Inorg. Chem.* **1992**, *31*, 937-939.
116. R. C. Holz, L.-J. Ming, and L. Que, Jr., "NOESY Studies on the Fe^{III}Co^{II} Active Site of the Purple Acid Phosphatase Uteroferrin," *J. Am. Chem. Soc.* **1992**, *114*, 4434-4436.
117. K. K. Andersson, C. Vassort, B. A. Brennan, L. Que, Jr., J. Haavik, T. Flatmark, F. Gros, and J. Thibault, "Purification and Characterization of the Blue-Green Rat Phaeochromocytoma (PC12) Tyrosine Hydroxylase with a Dopamine-Fe(III) Complex," *Biochem. J.* **1992**, *284*, 687-695.
118. Z. Wang, L.-J. Ming, L. Que, Jr., J. B. Vincent, M. W. Crowder, and B. A. Averill, "¹H NMR and NOE Studies of the Purple Acid Phosphatases from Porcine Uterus and Bovine Spleen," *Biochemistry* **1992**, *31*, 5263-5268.
119. D. J. Hirsh, W. F. Beck, J. B. Lynch, L. Que, Jr. and G. W. Brudvig, "Using Saturation-Recovery EPR to Measure Exchange Couplings in Proteins: Application to Ribonucleotide Reductase," **1992**, *114*, 7475-7481.
120. Y.-M. Chiou and L. Que, Jr., "Model Complexes for α -Keto Acid-Dependent Enzymes. Structure and Reactivity of {Fe^{II}[tris[(6-methyl-2-pyridyl)methyl]amine](benzoyl-formate)}(ClO₄)," *J. Am. Chem. Soc.* **1992**, *114*, 7567-7568.
121. P. E. Olson, B. Qi, L. Que, Jr., and L. P. Wackett, "Immunological Demonstration of a Unique 3,4-Dihydroxyphenylacetate 2,3-Dioxygenase in Soil *Arthrobacter* Strains," *Appl. and Environ. Microbiol.* **1992**, *58*, 2820-2826.

122. S. Ménage, Y. Zang, M. P. Hendrich and L. Que, Jr., "Structure and Reactivity of a Bis(μ -acetato-*O,O'*)diiron(II) Complex, $[\text{Fe}_2(\text{O}_2\text{CCH}_3)_2(\text{TPA})_2](\text{BPh}_4)_2$. A Model for the Diferrous Core of Ribonucleotide Reductase," *J. Am. Chem. Soc.* **1992**, *114*, 7786-7792.
123. D. C.-T. Siu, A. M. Orville, J. D. Lipscomb, D. H. Ohlendorf, and L. Que, Jr., "Resonance Raman Studies of the Protocatechuate 3,4-Dioxygenase from *Brevibacterium fuscum*," *Biochemistry* **1992**, *31*, 10443-10448.
124. K. K. Andersson, T. E. Elgren, L. Que, Jr., and J. D. Lipscomb, "Accessibility to the Active Site of Methane Monooxygenase: The First Demonstration of Exogenous Ligand Binding to the Diiron Center," *J. Am. Chem. Soc.* **1992**, *114*, 8711-8713.
125. R. C. Holz, S. P. Salowe, C. K. Smith, G. C. Cuca, and L. Que, Jr., "EXAFS Evidence for a "Cysteine Switch" in the Activation of Prostromelysin," *J. Am. Chem. Soc.* **1992**, *114*, 9611-9614.
126. D. C. Crans, C. M. Simone, R. C. Holz, and L. Que, Jr., "Interaction of Porcine Uterine Fluid Purple Acid Phosphatase with Vanadate and Vanadyl Cation," *Biochemistry* **1992**, *31*, 11731-11739.
127. Y. Zang, T. E. Elgren, Y. Dong, and L. Que, Jr., "A High Potential Ferrous Complex and Its Conversion to an Alkylperoxoiron(III) Intermediate. A Lipoxygenase Model," *J. Am. Chem. Soc.* **1993**, *115*, 811-813.
128. H. G. Jang, M. P. Hendrich, and L. Que, Jr., "Insight into the $g \approx 16$ EPR Signals of Reduced Diiron-Oxo Proteins. Structure and Properties of $[\text{Fe}^{\text{II}}_2\text{BPMP}\{\text{O}_2\text{P}(\text{OC}_6\text{H}_5)_2\}_2]\text{Cl}$," *Inorg. Chem.* **1993**, *32*, 911-918.
129. Y. Dong, S. Ménage, B. A. Brennan, T. E. Elgren, H. G. Jang, L. L. Pearce, and L. Que, Jr., "Dioxygen Binding to Diferrous Centers. Models for Diiron-Oxo Proteins," *J. Am. Chem. Soc.* **1993**, *115*, 1851-1859.
130. A. E. True, R. C. Scarrow, C. R. Randall, R. C. Holz, and L. Que, Jr., "EXAFS Studies of Uteroferrin and Its Anion Complexes," *J. Am. Chem. Soc.* **1993**, *115*, 4246-4255.
131. C. R. Randall, Y. Zang, A. E. True, L. Que, Jr., J. M. Charnock, C. D. Garner, Y. Fujishima, C. J. Schofield and J. E. Baldwin, "X-ray Absorption Studies of the Ferrous Active Site of Isopenicillin N Synthase and Related Model Complexes," *Biochemistry* **1993**, *32*, 6664-6673.
132. L. Que, Jr., "Oxygen Activation at Nonheme Iron Centers" in "Bioinorganic Catalysis," J. Reedijk, ed.) Marcel Dekker, Inc., New York, **1993**, pp.347-395.
133. T. E. Elgren, M. P. Hendrich, and L. Que, Jr., "Azide Binding to the Diferrous Clusters of the R2 Protein of Ribonucleotide Reductase from *Escherichia coli*," *J. Am. Chem. Soc.* **1993**, *115*, 9291-9292.
134. Y. Zang, H. G. Jang, Y.-M. Chiou, M. P. Hendrich, L. Que, Jr., "Structures and Properties of Ferromagnetically Coupled Bis(μ -halo)diiron(II) Complexes," *Inorg. Chim. Acta* **1993**, *213*, 41-48.
135. R. A. Leising, J. Kim, M. A. Pérez, and L. Que, Jr., "Alkane Functionalization at (μ -Oxo)diiron(III) Centers," *J. Am. Chem. Soc.* **1993**, *115*, 9524-9530.
136. R. C. Holz, T. E. Elgren, L. L. Pearce, J. H. Zhang, C. J. O'Connor, and L. Que, Jr., "Spectroscopic and Electrochemical Properties of (μ -Oxo)diiron(III) Complexes Related to Diiron-Oxo Proteins. Structure of $[\text{Fe}_2\text{O}(\text{TPA})_2(\text{MoO}_4)](\text{ClO}_4)_2$," *Inorg. Chem.* **1993**, *32*, 5844-5850.

137. T. Kojima, R. A. Leising, S. Yan, and L. Que, Jr., "Alkane Functionalization at Nonheme Iron Centers. Stoichiometric Transfer of Metal-Bound Ligands to Alkane," *J. Am. Chem. Soc.* **1993**, *115*, 11328-11335.
138. Z. Wang, T. R. Holman, and L. Que, Jr., "Two-Dimensional ^1H NMR Studies of Paramagnetic Bimetallic Mixed-Metal Complexes" *Magnetic Resonance in Chemistry* **1993**, *31*, S78-S84.
139. L. M. T. Schnaith, R. S. Hanson, and L. Que, Jr., "Double-Stranded Cleavage of pBR322 by a Diiron Complex via a "Hydrolytic" Mechanism" *Proc. Natl. Acad. Sci. USA* **1994**, *91*, 569-573.
140. L.-J. Ming, J. B. Lynch, R. C. Holz, and L. Que, Jr., "One- and Two-Dimensional ^1H NMR Studies of the Active Site of Iron(II) Superoxide Dismutase from *Escherichia coli*" *Inorg. Chem.* **1994**, *33*, 83-87.
141. T. E. Elgren, L.-J. Ming, L. Que, Jr., "Spectroscopic Studies of Co(II)-Reconstituted Ribonucleotide Reductase R2 from *Escherichia coli*," *Inorg. Chem.* **1994**, *33*, 891-894.
142. C. A. Earhart, M. D. Hall, I. Michaud-Soret, L. Que, Jr., and D. H. Ohlendorf, "Crystallization of Catechol 1,2-Dioxygenase from *Pseudomonas arvilla C-1*" *J. Mol. Biol.* **1994**, *236*, 377-378.
143. Y. Zang, G. Pan, L. Que, Jr., B. Fox, and E. Münck, "First Diferric Complex with an $\text{Fe}_2(\mu\text{-O})(\mu\text{-OH})$ Core. Structure and Reactivity of $[\text{Fe}_2(\mu\text{-O})(\mu\text{-OH})(6\text{TLA})_2](\text{ClO}_4)_3$ " *J. Am. Chem. Soc.* **1994**, *116*, 3653-3654.
144. A. Ghosh, J. Almlöf, and L. Que, Jr. "Density Functional Theoretical Study of Oxo(porphyrinato)iron(IV) Complexes, Models of Peroxidase Compounds I and II" *J. Phys. Chem.* **1994**, *98*, 5576-5579.
145. E. Wilkinson, Y. Dong, and L. Que, Jr., "Modeling Hydrolysis at Dinuclear Iron Centers" *J. Am. Chem. Soc.* **1994**, *116*, 8394-8395.
146. S. Ménage, H. Fujii, M. P. Hendrich, and L. Que, Jr., "Carboxylatoiron(II) Aggregates: A Novel Fe^{II}_4 Complex with Threefold Symmetry" *Angew. Chem. Int. Ed. Engl.* **1994**, *33*, 1660-1662.
147. N. Kitajima, N. Tamura, H. Amagai, H. Fukui, Y. Moro-oka, Y. Mizutani, T. Kitagawa, R. Mathur, K. Heerwegh, C. A. Reed, C. R. Randall, L. Que, Jr., and K. Tatsumi, "Monomeric Carboxylate Ferrous Complexes as Models for the Dioxygen Binding Sites in Non-Heme Iron Proteins. The Reversible Formation and Characterization of μ -Peroxo Diferric Complexes" *J. Am. Chem. Soc.* **1994**, *116*, 9071-9085.
148. S. Mahapatra, J. A. Halfen, E. C. Wilkinson, L. Que, Jr., and W. B. Tolman, "Modeling Copper-Dioxygen Reactivity in Proteins: Aliphatic C-H Bond Activation by a New Dicopper(II)-Peroxo Complex" *J. Am. Chem. Soc.* **1994**, *116*, 9785-9786.
149. Y.-M. Chiou and L. Que, Jr., "A Model for α -Keto Acid Dependent Nonheme Iron Enzymes: Structure and Reactivity of $[\text{Fe}^{\text{II}}_2(\text{Me}_2\text{hdp})_2(\text{bf})](\text{ClO}_4)$ " *Angew. Chem. Int. Ed. Engl.* **1994**, *33*, 1886-1888.
150. L. Que, Jr., "Iron Proteins with Mononuclear Active Sites" in "Encyclopedia of Inorganic Chemistry," (R. B. King, ed.) Wiley, Chichester, **1994**, Vol. 4, pp. 1859-1871.
151. T. R. Holman, Z. Wang, M. P. Hendrich, and L. Que, Jr., "Structural and Spectroscopic Properties of Antiferromagnetically Coupled $\text{Fe}^{\text{III}}\text{Mn}^{\text{II}}$ and $\text{Fe}^{\text{II}}\text{Mn}^{\text{II}}$ Complexes" *Inorg. Chem.* **1995**, *34*, 134-139.

152. Y. Zang, Y. Dong, L. Que, Jr., K. Kauffmann, and E. Münck, "The First Bis(μ -oxo)diiron(III) Complex. Structure and Magnetic Properties of $[\text{Fe}_2(\mu\text{-O})_2(6\text{TLA})_2](\text{ClO}_4)_2$ " *J. Am. Chem. Soc.* **1995**, *117*, 1169-1170.
153. S. Ménage, E. C. Wilkinson, L. Que, Jr., and M. Fontecave, "Formation of an Alkylperoxoiron(III) Complex During Oxidations Catalyzed by μ -Oxodiiron(III) Complexes" *Angew. Chem. Int. Ed. Engl.* **1995**, *34*, 203-205.
154. Y. Zang and L. Que, Jr., "Structure and Reactivity of Fe(II)-SAr Complexes: Relevance to the Active Site of Isopenicillin N Synthase" *Inorg. Chem.* **1995**, *34*, 1030-1035.
155. C. R. Randall, L. Shu, Y.-M. Chiou, K. S. Hagen, M. Ito, N. Kitajima, R. J. Lachicotte, Y. Zang and L. Que, Jr., "X-ray Absorption Pre-Edge Studies of High Spin Iron(II) Complexes" *Inorg. Chem.* **1995**, *34*, 1036-1039.
156. Y. Dong, H. Fujii, M. P. Hendrich, R. A. Leising, G. Pan, C. R. Randall, E. C. Wilkinson, Y. Zang, L. Que, Jr., B. G. Fox, K. Kauffmann, and E. Münck, "A High Valent Nonheme Iron Intermediate. Structure and Properties of $[\text{Fe}_2(\mu\text{-O})_2(5\text{-Me-TPA})_2](\text{ClO}_4)_3$ " *J. Am. Chem. Soc.* **1995**, *117*, 2778-2792
157. G. Peng, J. van Elp, H. Jang, L. Que, Jr., W. H. Armstrong, and S. P. Cramer, "L-Edge X-ray Absorption and X-ray Magnetic Circular Dichroism of Oxygen-Bridged Dinuclear Iron Complexes" *J. Am. Chem. Soc.* **1995**, *117*, 2515-2519.
158. Y.-M. Chiou and L. Que, Jr., "Models for α -Keto Acid-Dependent Nonheme Iron Enzymes: Structures and Reactivity of $[\text{Fe}^{\text{II}}(\text{L})(\text{O}_2\text{CCOPh})](\text{ClO}_4)$ Complexes" *J. Am. Chem. Soc.* **1995**, *117*, 3999-4013.
159. M. Ormö, K. Regnström, Z. Wang, L. Que, Jr., M. Sahlin, and B.-M. Sjöberg, "Residues Important for Radical Stability in Ribonucleotide Reductase from Escherichia coli" *J. Biol. Chem.* **1995**, *270*, 6570-6576.
160. I. Michaud-Soret, K. K. Andersson, L. Que, Jr., and J. Haavik, "Resonance Raman Studies of Catecholate and Phenolate Complexes of Recombinant Human Tyrosine Hydroxylase" *Biochemistry* **1995**, *34*, 5504-5510.
161. L. Shu, Y.-M. Chiou, A. M. Orville, M. A. Miller, J. D. Lipscomb, and L. Que, Jr., "X-ray Absorption Spectroscopic Studies of the Fe(II) Active Site of Catechol 2,3-Dioxygenase. Implications for the Extradiol Cleavage Mechanism" *Biochemistry* **1995**, *34*, 6649-6659.
162. C. R. Randall and L. Que, Jr., "Functional Models for Metalloprotein in Dioxygen Metabolism" *Handbook of Metal-Ligand Interactions in Biological Fluids: Bioinorganic Chemistry* **1995**, *1*, 388-398.
163. Y. R. Boldt, M. J. Sadowsky, L. B. M. Ellis, L. Que, Jr., and L. P. Wackett, "A Manganese-Dependent Dioxygenase from *Arthrobacter globiformis* CM-2 Belongs to the Major Extradiol Dioxygenase Family" *J. Bacteriol.* **1995**, *177*, 1225-1232.
164. Y.-M. Chiou and L. Que, Jr., "Model Studies of α -Keto Acid-Dependent Nonheme Iron Enzymes: Nitric Oxide Adducts of $[\text{Fe}^{\text{II}}(\text{L})(\text{O}_2\text{CCOPh})](\text{ClO}_4)$ Complexes" *Inorg. Chem.* **1995**, *34*, 3270-3278.
165. Y.-M. Chiou and L. Que, Jr., "Structure of a Mononuclear Iron(II)-Catecholate Complex and Its Relevance to the Extradiol-Cleaving Catechol Dioxygenases" *Inorg. Chem.* **1995**, *34*, 3577-3578.

166. S. Mahapatra, J. A. Halfen, E. C. Wilkinson, G. Pan, C. J. Cramer, L. Que, Jr., and W. B. Tolman, "A New Intermediate in Copper Dioxygen Chemistry: Breaking the O-O Bond to Form a $\{\text{Cu}_2(\mu\text{-O})_2\}^{2+}$ Core" *J. Am. Chem. Soc.* **1995**, *117*, 8865-8866.
167. C. S. Haskin, N. Ravi, J. B. Lynch, E. Münck, and L. Que, Jr., "The Reaction of NO with the Reduced R2 Protein of Ribonucleotide Reductase from *E. coli*" *Biochemistry* **1995**, *34*, 11090-11098.
168. M. Lubben, A. Meetsma, E. C. Wilkinson, B. Feringa, and L. Que, Jr., "Nonheme Iron Centers in Oxygen Activation: Characterization of an Iron(III) Hydroperoxide Intermediate" *Angew. Chem. Int. Ed. Engl.* **1995**, *34*, 1512-1514.
169. Z. Wang and L. Que, Jr., "NMR Studies of Nonheme Iron Proteins" in *Nuclear Magnetic Resonance of Paramagnetic Molecules* (LaMar, G. N. Ed.) NATO ASI Series **1995**, *457*, 193-211.
170. J. Kim, E. Larka, E. C. Wilkinson, and L. Que, Jr., "An Alkylperoxoiron(III) Intermediate and Its Role in the Oxidation of Aliphatic C-H Bonds" *Angew. Chem. Int. Ed. Engl.* **1995**, *34*, 2048-2051.
171. L. Que, Jr., "Oxygen Activation at Nonheme Iron Centers" in *Active Oxygen In Biochemistry* (Valentine, J.V.; Foote, C. S.; Greenberg, A.; Liebman, J. F.; ed.) Blackie A & P: Glasgow, **1995**, SEARCH Series, Vol. 3; pp. 232-275.
172. K. E. Silva, T. E. Elgren, L. Que, Jr., and M. T. Stankovich, "Electron Transfer Properties of the R2 Protein of Ribonucleotide Reductase from *Escherichia coli*" *Biochemistry* **1995**, *34*, 14093-14103.
173. Y. Dong, L. Que, Jr., K. Kauffmann, and E. Münck, "An Exchange-Coupled Complex with Localized High-Spin Fe^{IV} and Fe^{III} Sites of Relevance to Cluster X of *Escherichia coli* Ribonucleotide Reductase" *J. Am. Chem. Soc.* **1995**, *117*, 11377-11378.
174. A. K. Whiting, Y. R. Boldt, M. P. Hendrich, L. P. Wackett, and L. Que, Jr., "A Manganese(II)-Dependent Extradiol-Cleaving Catechol Dioxygenase from *Arthrobacter globiformis* CM-2" *Biochemistry* **1996**, *35*, 160-170.
175. J. A. Halfen, S. Mahapatra, E. C. Wilkinson, S. Kaderli, V. G. Young, Jr., L. Que, Jr., A. D. Zuberbühler, and W. B. Tolman, "Reversible Cleavage and Formation of the Dioxygen O-O Bond Within a Dicopper Complex" *Science* **1996**, *271*, 1397-1400.
176. Y. Dong, S. Yan, V. G. Young, Jr., and L. Que, Jr., "Crystal Structure Analysis of a Synthetic Nonheme Diiron-O₂ Adduct: Insight into the Mechanism of Oxygen Activation" *Angew. Chem. Int. Ed. Engl.* **1996**, *35*, 618-620.
177. L. Que, Jr. and Y. Dong, "Modeling the Oxygen Activation Chemistry of Methane Monooxygenase and Ribonucleotide Reductase" *Acc. Chem. Res.* **1996**, *29*, 190-196.
178. A. Ghosh, J. E. Amlöf, and L. Que, Jr., "Electronic Structure of Non-Heme High-Valent Oxoiron Complexes With the Unprecedented $[\text{Fe}_2(\mu\text{-O})_2]^{3+}$ Core" *Angew. Chem. Int. Ed. Engl.* **1996**, *35*, 770-772.
179. J. A. Halfen, S. Mahapatra, E. C. Wilkinson, A. J. Gengenbach, V. G. Young, Jr., L. Que, Jr., and W. B. Tolman, "Synthetic Modeling of Nitrite Binding and Activation by Reduced Copper Proteins. Characterization of Copper(I)-Nitrite Complexes That Evolve Nitric Oxide" *J. Am. Chem. Soc.* **1996**, *118*, 763-776.

180. J. Kim, R. G. Harrison, C. Kim, and L. Que, Jr., "Fe(TPA)-Catalyzed Alkane Hydroxylation. Metal-Based Oxidation vs Radical Chain Autoxidation" *J. Am. Chem. Soc.* **1996**, *118*, 4373-4379.
181. J. Kim, Y. Dong, E. Larka, and L. Que, Jr., "Electrospray Ionization Mass Spectral Characterization of Transient Iron Species of Bioinorganic Relevance" *Inorg. Chem.* **1996**, *35*, 2369-2372.
182. L. Shu, Y. Liu, J. D. Lipscomb, and L. Que, Jr., "X-ray Absorption Spectroscopic Studies of the Methane Monooxygenase Hydroxylase Component from *Methylosinus trichosporium* OB3b" *J. Biol. Inorg. Chem.* **1996**, *1*, 297-304.
183. X. Wang, C. R. Randall, A. E. True, and L. Que, Jr., "X-ray Absorption Spectroscopic Studies of the FeZn Derivative of Uteroferrin" *Biochemistry* **1996**, *35*, 13946-13954.
184. L. Que, Jr. and R. Y.-N. Ho, "Dioxygen Activation by Enzymes of Mononuclear Non-Heme Iron Active Sites" *Chem. Rev.* **1996**, *96*, 2607-2624.
185. S. Yan, X. Pan, L. F. Taylor, J. H. Zhang, C. J. O'Connor, D. Britton, O. P. Anderson, and L. Que, Jr., "Diiron(III) Complexes of Some Relevance to the Purple Acid Phosphatases" *Inorg. Chim. Acta* **1996**, *243*, 1-8.
186. S. Mahapatra, J. A. Halfen, E. C. Wilkinson, G. Pan, X. Wang, V. G. Young, Jr., C. J. Cramer, L. Que, Jr., and W. B. Tolman, "Structural, Spectroscopic, and Theoretical Characterization of Bis(μ -oxo)dicopper Complexes, Novel Intermediates in Copper-Mediated Dioxygen Activation" *J. Am. Chem. Soc.* **1996**, *118*, 11555-11574.
187. L. Shu, J. Nesheim, K. Kauffmann, E. Münck, J. D. Lipscomb, and L. Que, Jr., "An Fe^{IV}₂O₂ Diamond Core Structure for the Key Intermediate Q of Methane Monooxygenase" *Science* **1997**, *275*, 515-518.
188. Y. R. Boldt, A. K. Whiting, M. L. Wagner, M. J. Sadowsky, L. Que, Jr., and L. P. Wackett, "Manganese(II) Active Site Mutants of 3,4-Dihydroxyphenylacetate 2,3-Dioxygenase from *Arthrobacter globiformis* strain CM-2" *Biochemistry* **1997**, *36*, 2147-2153.
189. T. Lehmann, L.-J. Ming, M. E. Rosen, and L. Que, Jr., "NMR Studies of the Paramagnetic Complex Fe(II)-Bleomycin" *Biochemistry* **1997**, *36*, 2807-2816.
190. A. K. Whiting, L. Que, Jr., R. E. Saari, R. P. Hausinger, M. A. Fredrick, and J. McCracken, "Metal Coordination Environment of a Cu(II)-Substituted α -Keto Acid-Dependent Dioxygenase That Degrades the Herbicide 2,4-D" *J. Am. Chem. Soc.* **1997**, *119*, 3413-3414.
191. C. Kim, Y. Dong and L. Que, Jr., "Modeling Nonheme Diiron Enzymes: Hydrocarbon Hydroxylation and Desaturation by a High-Valent Fe₂O₂ Diamond Core" *J. Am. Chem. Soc.* **1997**, *119*, 3635-3636.
192. Z. Wang, L. Martins, W. R. Ellis, Jr., and L. Que, Jr., "Proton NMR Studies of Myohemerythrin from *Thermite zostericola*" *J. Biol. Inorg. Chem.* **1997**, *2*, 56-64.
193. J. Kim, C. Kim, R. G. Harrison, E. C. Wilkinson, and L. Que, Jr., "Fe(TPA)-Catalyzed Alkane Hydroxylation Can Be a Metal-Based Oxidation" *J. Mol. Cat. A: Chem.* **1997**, *117*, 83-89.
194. G. Roelfes, M. Lubben, S. W. Leppard, E. P. Schudde, R. M. Hermant, R. Hage, E. C. Wilkinson, L. Que, Jr., and B. L. Feringa, "Functional Models for Iron-Bleomycin" *J. Mol. Cat. A: Chem.* **1997**, *117*, 223-227.

195. J. E. Bol, W. L. Driessen, R. Y. N. Ho, B. Maase, L. Que, Jr., and J. Reedjik, "Dioxygen Binding at Ambient Temperature: Formation of a Novel Peroxodicopper(II) Complex with an Azole Macrocyclic Ligand" *Angew. Chem. Int. Ed. Engl.* **1997**, *36*, 998-1000.
196. Y. Zang, J. Kim, Y. Dong, E. C. Wilkinson, E. H. Appelman, and L. Que, Jr., "Models for Nonheme Iron Intermediates: The Structural Basis for Tuning the Spin States of Fe(TPA) Complexes" *J. Am. Chem. Soc.* **1997**, *119*, 4197-4205.
197. M. Ito and L. Que, Jr., "Biomimetic Extradiol Cleavage of Catechols: Insights into the Enzyme Mechanism" *Angew. Chem. Int. Ed. Engl.* **1997**, *36*, 1342-1344.
198. C. Kim, K. Chen, J. Kim, and L. Que, Jr., "Stereospecific Alkane Hydroxylation with H₂O₂ Catalyzed by an Fe(II) TPA Complex" *J. Am. Chem. Soc.* **1997**, *119*, 5964-5965.
199. J. A. Halfen, B. A. Jazdzewski, S. Mahapatra, L. M. Berreau, E. C. Wilkinson, L. Que, Jr., and W. B. Tolman, "Synthetic Models of the Inactive Copper(II)-Tyrosinate and Active Copper(II)-Tyrosyl Radical Forms of Galactose and Glyoxal Oxidases" *J. Am. Chem. Soc.* **1997**, *119*, 8217-8227.
200. T. E. Elgren, A. M. Orville, K. A. Kelly, J. D. Lipscomb, D. H. Ohlendorf, L. Que, Jr., "Crystal Structure and Resonance Raman Studies of Protocatechuate 3,4-dioxygenase Complexed with 3,4-Dihydroxyphenylacetate" *Biochemistry* **1997**, *36*, 11504-11513.
201. H. Zheng and L. Que, Jr., "Cu(II)- α -Keto Acid Complexes as Structural Models of α -Keto Acid-Dependent Enzymes: Syntheses, Crystal Structure and Properties of [Cu(L) (benzoylformate)]X" *Inorg. Chim. Acta* **1997**, *263*, 301-307.
202. P. A. MacFaul, K. U. Ingold, D. D. M. Wayner, and L. Que, Jr., "A Putative Monooxygenase Mimic Which Functions via Well-Disguised Free Radical Chemistry" *J. Am. Chem. Soc.* **1997**, *119*, 10594-10598.
203. L. Que, Jr., "Oxygen Activation at Non-Heme Diiron Active Sites in Biology: Lessons from Model Complexes" *J. Chem. Soc., Dalton Trans.* **1997**, 3933-3940.
204. S. K. Mandal and L. Que, Jr., "Models for Amide Ligation in Nonheme Iron Enzymes" *Inorg. Chem.* **1997**, *36*, 5424-5425.
205. S. Mahapatra, S. Kaderli, A. Llobet, Y.-M. Neuhold, T. Palanché, J. A. Halfen, V. G. Young, Jr., T. A. Kaden, L. Que, Jr., A. D. Zuberbühler, and W. B. Tolman, "Binucleating Ligand Structural Effects on (μ -Peroxo)- and Bis(μ -oxo)dicopper Complex Formation and Decay: Competition between Arene Hydroxylation and Aliphatic C-H Bond Activation" *Inorg. Chem.* **1997**, *36*, 6343-6356.
206. Y. Dong, Y. Zang, L. Shu, E. C. Wilkinson, L. Que, Jr., K. Kauffmann, and E. Münck, "Models for Nonheme Diiron Enzymes. Assembly of a High-Valent Fe₂(μ -O)₂ Diamond Core from Its Peroxo Precursor" *J. Am. Chem. Soc.* **1997**, *119*, 12683-12684.
207. E. Hegg and L. Que, Jr., "The 2-His-1-Carboxylate Facial Triad. An Emerging Structural Motif in Mononuclear Non-Heme Iron(II) Enzymes" *Eur. J. Biochem.* **1997**, *250*, 625-629.
208. P. J. Riggs-Gelasco, L. Shu, S. Chen, D. Burdi, B. H. Huynh, L. Que, Jr., and J. Stubbe, "EXAFS Characterization of the Intermediate X Generated during the Assembly of the *E. coli* Ribonucleotide Reductase R2 Diferric-Tyrosyl Radical Cofactor" *J. Am. Chem. Soc.* **1998**, *120*, 849-860.

209. E. C. Wilkinson, Y. Dong, Y. Zang, H. Fujii, R. Fraczkiewicz, R. S. Czernuszewicz, and L. Que, Jr., "Raman Signature of the Fe₂O₂ "Diamond" Core" *J. Am. Chem. Soc.* **1998**, *120*, 955-962.
210. R. E. Norman, R. A. Leising, S. Yan, and L. Que, Jr., "Unexpected Assembly of a (μ-Oxo)(μ-formato)diiron(III) Complex from an Aerobic Methanolic Solution of Fe(III) and the TPA Ligand" *Inorg. Chim. Acta* **1998**, *273*, 393-396.
211. S. J. Lange and L. Que, Jr., "Oxygen Activating Nonheme Iron Enzymes" *Curr. Op. Chem. Biol.* **1998**, *2*, 159-172.
212. L. Que, Jr., "The High Valent Nonheme Fe₂O₂ Diamond Core: Comparisons with the Heme Ferryl" *Pure & Appl. Chem.* **1998**, *70*, 947-954.
213. L. Que, Jr., Y. Dong, L. Shu, and E. C. Wilkinson, "Spectroscopic Signatures of the Fe₂O₂ Diamond Core" *ACS Symp. Ser.* **1998**, *692*, 374-386.
214. X. Wang and L. Que, Jr., "Extended X-ray Absorption Fine Structure Studies of the Anion Complexes of FeZn Uteroferrin" *Biochemistry* **1998**, *21*, 7813-7821.
215. L. Shu, J. A. Broadwater, C. Achim, B. G. Fox, E. Münck, and L. Que, Jr., "EXAFS and Mössbauer Characterization of the Diiron(III) Site in Stearoyl-Acyl-Carrier-Protein (ACP) Δ⁹-Desaturase" *J. Biol. Inorg. Chem.* **1998**, *3*, 392-400.
216. K. E. Kauffmann, C. V. Popescu, Y. Dong, J. D. Lipscomb, L. Que, Jr., and E. Münck, "Mössbauer Evidence for Antisymmetric Exchange in a Diferric Synthetic Complex and Diferric Methane Monooxygenase" *J. Am. Chem. Soc.* **1998**, *120*, 8739-8746.
217. J. D. Lipscomb and L. Que, Jr., "MMO: P450 in Wolf's Clothing?" *J. Biol. Inorg. Chem.* **1998**, *3*, 331-336.
218. J. R. Hagadorn, L. Que, Jr., and W. B. Tolman, "A Bulky Benzoate Ligand for Modeling the Carboxylate-Rich Active Sites of Non-Heme Diiron Enzymes" *J. Am. Chem. Soc.* **1998**, *120*, 13531-13532.
219. R. Y. N. Ho, G. Roelfes, B. L. Feringa, and L. Que, Jr., "Raman Evidence for a Weakened O-O Bond in Mononuclear Low-Spin Iron(III) Hydroperoxides" *J. Am. Chem. Soc.* **1999**, *121*, 264-265.
220. M. A. Miller, F. T. Gobena, K. Kauffmann, E. Münck, L. Que, Jr., and M. T. Stankovich, "Differing Roles for the Diiron Clusters of Ribonucleotide Reductase from Aerobically Grown *Escherichia coli* in the Generation of the Y122 Radical" *J. Am. Chem. Soc.* **1999**, *121*, 1096-1097.
221. L. Que, Jr., "Oxygen Activation at Nonheme Iron Centers" in "Bioinorganic Catalysis," 2nd ed. (J. Reedijk and E. Bouwman, eds.) Marcel Dekker, Inc., New York, **1999**, pp.269-321.
222. E. L. Hegg, R. Y. N. Ho, and L. Que, Jr., "Oxygen Activation and Arene Hydroxylation by Functional Mimics of α-Keto Acid-Dependent Iron(II) Dioxygenases" *J. Am. Chem. Soc.* **1999**, *121*, 1972-1973.
223. H. Zheng, Y. Zang, Y. Dong, V. G. Young, Jr., and L. Que, Jr., "Complexes with Fe^{III}₂(μ-O)(μ-OH), Fe^{III}₂(μ-O)₂, and [Fe^{III}₃(μ-O)₃] Cores: Structures, Spectroscopy, and Core Interconversions" *J. Am. Chem. Soc.* **1999**, *121*, 2226-2235.
224. C. Duboc-Toia, S. Ménage, R. Y. N. Ho, L. Que, Jr., C. Lambeaux, and M. Fontecave, "Enantioselective Sulfoxidation as a Probe for a Metal-Based Mechanism in H₂O₂-Dependent Oxidations Catalyzed by a Diiron Complex" *Inorg. Chem.*, **1999**, *38*, 1261-1268.

225. G. Roelfes, M. Lubben, K. Chen, R. Y. N. Ho, A. Meetsma, S. Genseberger, R. M. Hermant, R. Hage, S. K. Mandal, V. G. Young, Jr., Y. Zang, H. Kooijman, A. L. Spek, L. Que, Jr., and B. L. Feringa, "Iron Chemistry of the Pentadentate Ligand That Generates a Metastable Fe^{III}-OOH Intermediate" *Inorg. Chem.* **1999**, *38*, 1929-1936.
226. H.-F. Hsu, Y. Dong, L. Shu, V. G. Young, Jr., and L. Que, Jr., "Crystal Structure of a Synthetic High-Valent Complex with an Fe₂(μ-O)₂ Diamond Core. Implications for the Core Structures of Methane Monooxygenase Intermediate Q and Ribonucleotide Reductase Intermediate X" *J. Am. Chem. Soc.* **1999**, *121*, 5230-5237.
227. A. M. Rocklin, D. L. Tierney, V. Kofman, N. M. W. Brunhuber, B. M. Hoffman, R. E. Christoffersen, N. O. Reich, J. D. Lipscomb, and L. Que, Jr., "Role for the Nonheme Fe(II) Center in the Biosynthesis of the Plant Hormone Ethylene" *Proc. Natl. Acad. Sci. USA* **1999**, *96*, 7905-7909.
228. S. J. Lange, H. Miyake, and L. Que, Jr., "Evidence for a Nonheme Fe(IV)=O Species in the Intramolecular Hydroxylation of a Phenyl Moiety" *J. Am. Chem. Soc.* **1999**, *121*, 6330-6331.
229. K. Chen and L. Que, Jr., "Evidence for the Participation of a High-Valent Iron-Oxo Species in Stereospecific Alkane Hydroxylation by a Nonheme Iron Catalyst" *Chem. Commun.* **1999**, 1375-1376.
230. K. Chen and L. Que, Jr., "cis-Dihydroxylation of Olefins by a Nonheme Iron Catalyst. A Functional Model for Rieske Dioxygenases" *Angew. Chem. Int. Ed.* **1999**, *38*, 2227-2229.
231. R. M. Davydov, J. Smieja, S. A. Dikanov, Y. Zang, L. Que, Jr., and M. K. Bowman, "EPR Properties of Mixed-Valent μ-Oxo and μ-Hydroxo Dinuclear Iron Complexes Produced by Radiolytic Reduction at 77 K" *J. Biol. Inorg. Chem.* **1999**, *4*, 292-301.
232. X. Wang, R. Y. N. Ho, A. K. Whiting, and L. Que, Jr., "Spectroscopic Characterization of a Ternary Phosphatase-Substrate-Fluoride Complex. Mechanistic Implications for Dinuclear Hydrolases" *J. Am. Chem. Soc.* **1999**, *121*, 9235-9236.
233. M. E. Branum and L. Que, Jr., "Double-strand DNA Hydrolysis by Dilanthanide Complexes" *J. Biol. Inorg. Chem.* **1999**, *4*, 593-600.
234. J. R. Hagadorn, L. Que, Jr., W. B. Tolman, I. Prisecaru, and E. Münck, "Conformational Tuning of Valence Delocalization in Carboxylate-Rich Diiron Complexes" *J. Am. Chem. Soc.* **1999**, *121*, 9760-9761.
235. R. Y. N. Ho, G. Roelfes, R. Hermant, R. Hage, B. L. Feringa, and L. Que, Jr., "Resonance Raman Evidence for the Interconversion between an [Fe^{III}-η¹-OOH]²⁺ and [Fe^{III}-η²-OO]²⁺ Species and Mechanistic Implications Thereof" *Chem. Commun.* **1999**, 2161-2162.
236. E. L. Hegg, A. K. Whiting, R. E. Saari, J. McCracken, R. P. Hausinger, and L. Que, Jr., "The Herbicide-Degrading α-Keto Acid-Dependent Enzymes TfdA: Metal Coordination Environment and Mechanistic Insights" *Biochemistry* **1999**, *38*, 16714-16726.
237. L. Que, Jr. and M. F. Reynolds, "Manganese(II)-Dependent Extradiol Cleaving Catechol Dioxygenases" *Metal Ions Biol. Sys.* **2000**, *37*, 505-525.
238. S. Itoh, M. Taki, H. Nakao, P. L. Holland, W. B. Tolman, L. Que, Jr., and S. Fukuzumi, "Aliphatic Hydroxylation by a Bis(μ-oxo)dicopper(III) Complex" *Angew. Chem. Int. Ed.* **2000**, *39*, 398-400.
239. P. L. Holland, C. J. Cramer, E. C. Wilkinson, S. Mahapatra, K. R. Rodgers, S. Itoh, M. Taki, S. Fukuzumi, L. Que, Jr., and W. B. Tolman, "Resonance Raman Spectroscopy as a

- Probe of the Bis(μ -oxo)dicopper Core" *J. Am. Chem. Soc.* **2000**, *122*, 792-802.
240. M. DiDonato, H.-F. Hsu, S. Narindrasorasak, L. Que, Jr., and B. Sarkar, "Copper-Induced Conformational Changes in the N-Terminal Domain of the Wilson Disease Copper-Transporting ATPase" *Biochemistry* **2000**, *39*, 1890-1896.
241. L. Que, Jr., "One Motif, Many Different Reactions" *Nat. Struct. Biol.* **2000**, *7*, 182-184.
242. T. E. Lehmann, M. L. Serrano, and L. Que, Jr., "Coordination Chemistry of Co(II)-Bleomycin: Its Investigation through NMR and Molecular Dynamics" *Biochemistry* **2000**, *39*, 3886-3898.
243. H. Zheng, S. J. Yoo, E. Münck, and L. Que, Jr., "The Flexible Fe₂(μ -O)₂ Diamond Core: A Terminal Iron(IV)-Oxo Species Generated from the Oxidation of a Bis(μ -oxo)diiron(III) Complex" *J. Am. Chem. Soc.* **2000**, *122*, 3789-3790.
244. S. K. Mandal, V. G. Young, Jr., and L. Que, Jr., "Polynuclear Carboxylate-Bridged Iron(II) Clusters: Synthesis, Structure, and Host-Guest Chemistry" *Inorg. Chem.* **2000**, *39*, 1831-1833.
245. V. L. MacMurdo, H. Zheng, and L. Que, Jr., "Model for the Cofactor Formation Reaction of *E. coli* Ribonucleotide Reductase. From a Diiron(II) Precursor to an Fe^{III}Fe^{IV} Species via a Peroxo Intermediate" *Inorg. Chem.* **2000**, *39*, 2254-2255.
246. G. Roelfes, M. Lubben, R. Hage, L. Que, Jr., and B. L. Feringa, "Catalytic Oxidation with a Non-Heme Iron Complex That Generates a Low-Spin Fe^{III}-OOH Intermediate" *Chem. Eur. J.* **2000**, *6*, 2152-2159.
247. M. Costas, K. Chen, and L. Que, Jr., "Biomimetic Nonheme Iron Catalysts for Alkane Hydroxylation" *Coord. Chem. Rev.* **2000**, *200-202*, 517-544.
248. J. A. Halfen, J. M. Uhan, D. C. Fox, M. P. Mehn, and L. Que, Jr., "Copper(II) Complexes of Pyridyl-Appended Diazacycloalkanes: Syntheses, Characterization, and Application to Catalytic Olefin Aziridination" *Inorg. Chem.* **2000**, *39*, 4913-4920.
249. G. Roelfes, M. E. Branum, L. Wang, L. Que, Jr., and B. L. Feringa, "Efficient DNA Cleavage with an Iron Complex Without Added Reductants" *J. Am. Chem. Soc.* **2000**, *122*, 11517-11518.
250. D.-H. Jo and L. Que, Jr., "Tuning the Regiospecificity of Cleavage in Fe(III)-Catecholate Complexes: Tridentate *Facial* vs. *Meridional* Ligands" *Angew. Chem. Int. Ed.* **2000**, *39*, 4284-4287.
251. J. R. Hagadorn, L. Que, Jr., and W. B. Tolman, "N-Donor Effects on Carboxylate Binding in Mononuclear Iron(II) Complexes of a Sterically Hindered Benzoate Ligand" *Inorg. Chem.* **2000**, *39*, 6086-6090.
252. Chavez, F. A.; Que, L., Jr.; Tolman, W. B., "Metal Ion Complexation by a New, Highly Sterically Hindered, Bowl-Shaped Carboxylate Ligand" *Chem. Commun.* **2001**, 111-112.
253. Branum, M. E.; Tipton, A. K.; Zhu, S.; Que, L., Jr., "Double-Strand Hydrolysis of Plasmid DNA by Dicerium Complexes" *J. Am. Chem. Soc.* **2001**, *123*, 1898-1904.
254. Kim, J.; Zang, Y.; Costas, M.; Harrison, R. G.; Wilkinson, E. C.; Que, L., Jr., "A Nonheme Iron(II) Complex That Models the Redox Cycle of Lipoyxygenase" *J. Biol. Inorg. Chem.* **2001**, *6*, 276-284.
255. Arakawa, H.; Aresta, M.; Armour, J. N.; Barteau, M. A.; Beckman, E. J.; Bell, A. T.; Bercaw, J. E.; Creutz, C.; Dinjus, E.; Eckert, J.; Fujita, E.; Gibson, D. H.; Goddard, W. A.;

- Goodman, D. W.; Keller, J.; Kubas, G. J.; Kung, H. H.; Lyons, J. E.; Manzer, L. E.; Marks, T. J.; Morokuma, K.; Nivholas, K. M.; Periana, R.; Que, L.; Rostrup-Nielsen, J.; Sachtler, W. M. H.; Schmidt, L. D.; Sen, A.; Somorjai, G. A.; Stair, P. C.; Stults, B. R.; Tumas, W., "Catalysis Research of Relevance to Carbon Management: Progress, Challenges, and Opportunities" *Chem. Rev.* **2001**, *101*, 953-996.
256. Que, L., Jr.; Watanabe, Y., "Oxygenase Pathways: Oxo, Peroxo and Superoxo" *Science* **2001**, *292*, 651-653.
257. Kryatov, S. V.; Rybak-Akimova, E. V.; MacMurdo, V. L.; Que, L., Jr., "A Mechanistic Study of the Reaction between a Diiron(II) Complex $[\text{Fe}^{\text{II}}_2(\mu\text{-OH})_2(6\text{-Me}_3\text{-TPA})_2]^{2+}$ and O_2 to Form a Diiron(III) Peroxo Complex" *Inorg. Chem.* **2001**, *40*, 2220-2228.
258. Ho, R. Y. N.; Mehn, M. P.; Hegg, E. L.; Liu, A.; Ryle, M. J.; Hausinger, R. P.; Que, L., Jr., "Resonance Raman Studies of the Iron(II)- α -Keto Acid Chromophore in Model and Enzyme Complexes" *J. Am. Chem. Soc.* **2001**, *123*, 5022-5029".
259. Liu, A.; Ho, R. Y. N.; Que, L., Jr.; Ryle, M. J.; Phinney, B. S.; Hausinger, R. P., "Alternative Reactivity of an α -Ketoglutarate-Dependent Iron(II) Oxygenase: Enzyme Self-Hydroxylation" *J. Am. Chem. Soc.* **2001**, *123*, 5126-5127.
260. Jo, D.-H.; Chiou, Y.-M.; Que, L., Jr., "Models for Extradiol Cleaving Catechol Dioxygenases: Syntheses, Structures, and Reactivities of Iron(II)-Monoanionic Catecholate Complexes" *Inorg. Chem.* **2001**, *40*, 3181-3190.
261. Miyake, H.; Chen, K.; Lange, S. J.; Que, L., Jr., "'Intermolecular' Trapping of a Nonheme $\text{Fe}(\text{IV})=\text{O}$ Intermediate" *Inorg. Chem.* **2001**, *40*, 3534-3538.
262. Chen, K.; Que, L., Jr., "Stereospecific Alkane Hydroxylation by Nonheme Iron Catalysts: Mechanistic Evidence for an $\text{Fe}^{\text{V}}=\text{O}$ Active Species" *J. Am. Chem. Soc.* **2001**, *123*, 6327-6337.
263. Costas, M.; Tipton, A. K.; Chen, K.; Jo, D.-H.; Que, L., Jr., "Modeling Rieske Dioxygenases. The First Example of Iron-Catalyzed Asymmetric *cis*-Dihydroxylation of Olefins" *J. Am. Chem. Soc.* **2001**, *123*, 6722-6723.
264. Lehnert, N.; Ho, R. Y. N.; Que, L., Jr.; Solomon, E. I., "Spectroscopic Properties and Electronic Structure of Low-spin $\text{Fe}(\text{III})$ -Alkylperoxo Complexes: Homolytic Cleavage of the O-O Bond" *J. Am. Chem. Soc.* **2001**, *123*, 8271-8290.
265. Halfen, J. A.; Fox, D. C.; Mehn, M. P.; Que, L., Jr., "Enhanced Reactivity of Copper Catalysts for Olefin Aziridination by Manipulation of Ancillary Ligand Denticity" *Inorg. Chem.* **2001**, *40*, 5060-5061.
266. Brennessel, W. W.; Brooks, N. R.; Mehn, M. P.; Que, L., Jr.; Young, V. G., Jr., "Hexakis(acetonitrile)iron(II) hexafluoroantimonate" *Acta Cryst.* **2001**, *E57*, m545-m546.
267. Lehnert, N.; Ho, R. Y. N.; Que, L., Jr.; Solomon, E. I., "Electronic Structure of High-spin $\text{Fe}(\text{III})$ -Alkylperoxo Complexes and its Relation to Low-spin Analogs: Reaction Coordinate of O-O Bond Homolysis" *J. Am. Chem. Soc.* **2001**, *123*, 12802-12816.
268. Costas, M.; Rohde, J.-U.; Stubna, A.; Ho, R. Y. N.; Quaroni, L.; Münck, E.; Que, L., Jr., "A Synthetic Model for the Putative $\text{Fe}^{\text{IV}}_2\text{O}_2$ Diamond Core of Methane Monooxygenase Intermediate Q" *J. Am. Chem. Soc.* **2001**, *123*, 12931-12932.
269. Chavez, F. A.; Ho, R. Y. N.; Pink, M.; Young, V. G., Jr.; Kryatov, S. V.; Rybak-Akimova, E. V.; Andres, H. P.; Münck, E.; Que, L., Jr.; Tolman, W. B., "Unusual Peroxo Intermediates in the Reaction of Dioxygen with Carboxylate-Bridged Diiron(II,II)

- Paddlewheel Complexes" *Angew. Chem. Int. Ed.* **2002**, *41*, 149-152.
270. Tolman, W. B.; Que, L., Jr., "Sterically Hindered Benzoates: A Synthetic Strategy for Modeling Dioxygen Activation at Metalloprotein Active Sites" *J. Chem. Soc., Dalton Trans.* **2002**, 653-660.
271. Chen, K.; Costas, M.; Que, L., Jr., "Spin State Tuning of Non-Heme Iron-Catalyzed Hydrocarbon Oxidations: Participation of Fe^{III}-OOH and Fe^V=O Intermediates" *J. Chem. Soc., Dalton Trans.* **2002**, 672-679.
272. Hummel, H.; Mekmouche, Y.; Duboc-Toia, C.; Ho, R. Y. N.; Que, L., Jr.; Schünemann, V.; Thomas, F.; Trautwein, A.; Lebrun, C.; Fontecave, M.; Ménage, S., "A New Diferric Peroxo Complex with an Unprecedented Spin Configuration: an S = 2 System Arising from an S = 5/2, 1/2 Pair" *Angew. Chem. Int. Ed.* **2002**, *41*, 617-620.
273. Mekmouche, Y.; Hummel, H.; Ho, R. Y. N.; Que, L., Jr.; Schünemann, V.; Thomas, F.; Trautwein, A. X.; Lebrun, C.; Gorgy, K.; Leprière, J.-C.; Collomb, M.-N.; Deronzier, A.; Fontecave, M.; Ménage, S., "Sulfide Oxidation by Hydrogen Peroxide Catalyzed by Iron Complexes: Two Metal Centers Are Better Than One." *Chem. Eur. J.* **2002**, *8*, 1196-1204.
274. Smoukov, S. K.; Quaroni, L.; Wang, X.; Doan, P. E.; Hoffman, B. M.; Que, L., Jr., "ENDOR Evidence for a Hydroxo-Bridge Nucleophile Involved in Catalysis by a Dinuclear Hydrolase." *J. Am. Chem. Soc.* **2002**, *124*, 2595-2603.
275. Chen, K.; Costas, M.; Kim, J.; Tipton, A. K.; Que, L., Jr., "Olefin *cis*-Dihydroxylation versus Epoxidation by Nonheme Iron Catalysts: Two Faces of an Fe^{III}-OOH Coin" *J. Am. Chem. Soc.* **2002**, *124*, 3026-3035.
276. DiDonato, M.; Zhang, J.; Que, L., Jr., Sarkar, B., "Zinc Binding to the N-Terminal Domain of the Wilson Disease Copper-Transporting ATPase: Implications for in vivo Metal Ion Mediated Regulation of ATPase Activity" *J. Biol. Chem.* **2002**, *277*, 13409-13414.
277. Que, L., Jr.; Tolman, W. B., "Bis(μ -oxo)dimetal "Diamond" Cores in Copper and Iron Complexes Relevant to Biocatalysis" *Angew. Chem. Int. Ed.* **2002**, *41*, 1114-1137.
278. Zhou, J.; Rocklin, A. M.; Lipscomb, J. D.; Que, L., Jr.; Solomon, E. I., "Spectroscopic Studies of 1-Aminocyclopropane-1-carboxylic Acid Oxidase: Molecular Mechanism and CO₂ Activation in the Biosynthesis of Ethylene" *J. Am. Chem. Soc.* **2002**, *124*, 4602-4609.
279. Ryu, J. Y.; Kim, J.; Costas, M.; Chen, K.; Nam, W.; Que, L., Jr., "High conversion of olefins to *cis*-diols by non-heme iron catalysts and H₂O₂" *Chem. Commun.* **2002**, 1288-1289.
280. Costas, M.; Que, L., Jr., "Ligand Topology Tuning of Iron-Catalyzed Hydrocarbon Oxidations" *Angew. Chem. Int. Ed.* **2002**, *41*, 2179-2181.
281. Zhu, S.; Brennessel, W. W.; Harrison, R. G.; Que, L., Jr., "Iron coordination chemistry of *N*-(bis(2-pyridyl)methyl)pyridine-2-carboxamide" *Inorg. Chim. Acta* **2002**, *337*, 32-38.
282. Lehnert, N.; Neese, F.; Ho, R. Y. N.; Que, L., Jr.; Solomon, E. I., "Electronic Structure and Reactivity of Low-spin Fe(III)-Hydroperoxo Complexes: Comparison to Activated Bleomycin" *J. Am. Chem. Soc.* **2002**, *124*, 10810-10822.
283. Bassan, A.; Blomberg, M. R. A.; Siegbahn, P. E. M.; Que, L., Jr., "A Density Functional Study of O-O Bond Cleavage for a Biomimetic Non-Heme Iron Complex Demonstrating an Fe^V Intermediate" *J. Am. Chem. Soc.* **2002**, *124*, 11056-11063.
284. Nam, W.; Choi, S. K.; Lim, M. H.; Rohde, J.-U.; Kim, I.; Kim, J.; Kim, C.; Que, L., Jr.,

- “Formation of Iodosylbenzene-Iron Porphyrin Intermediates in the Reactions of Oxoiron(IV) Porphyrin π -Cation Radicals and Iodobenzene” *Angew. Chem. Int. Ed.* **2003**, *42*, 109-111.
285. Reynolds, M. F.; Costas, M.; Ito, M.; Jo, D.-H.; Tipton, A. A.; Whiting, A. K., and Que, L., Jr., “4-Nitrocatechol as a Probe of a Mn(II)-Dependent Extradiol-Cleaving Catechol Dioxygenase (MndD). Comparison with Relevant Fe(II) and Mn(II) Model Complexes” *J. Biol. Inorg. Chem.* **2003**, *8*, 263-272.
286. Rohde, J.-U.; In, J. H.; Lim, M. H.; Brennessel, W. W.; Bukowski, M. R.; Stubna, A.; Münck, E.; Nam, W.; Que, L., Jr., "Crystallographic and Spectroscopic Evidence for a Nonheme Fe^{IV}=O Complex" *Science* **2003**, *299*, 1037-1039
287. Jensen, M. P.; Lange, S. J.; Mehn, M. P.; Que, E. L.; Que, L., Jr., "Biomimetic Aryl Hydroxylation Derived from Alkyl Hydroperoxide at a Nonheme Iron Center. Evidence for an Fe^{IV}=O Oxidant" *J. Am. Chem. Soc.* **2003**, *125*, 2113-2128.
288. Ryle, M. J.; Liu, A.; Muthukumar, R. B.; Ho, R. Y. N.; Koehntop, K. D.; McCracken, J.; Que, L., Jr.; Hausinger, R. P., "O₂- and α -Ketoglutarate-Dependent Tyrosyl Radical Formation in TauD, an α -Keto Acid-Dependent Non-Heme Iron Dioxygenase" *Biochemistry* **2003**, *42*, 1854-1862.
289. Lim, M. H.; Rohde, J.-U.; Stubna, A.; Bukowski, M. R.; Costas, M.; Ho, R. Y. N.; Münck, E.; Nam, W.; Que, L., Jr., "An Fe^{IV}=O Complex of a Tetradentate Tripodal Nonheme Ligand" *Proc. Natl. Acad. Sci. USA* **2003**, *100*, 3665-3670.
290. Ryle, M. J.; Koehntop, K. D.; Liu, A.; Que, L., Jr.; Hausinger, R. P., "Interconversion of two oxidized forms of taurine/ α -ketoglutarate dioxygenase, a non-heme iron hydroxylase: Evidence for bicarbonate binding" *Proc. Natl. Acad. Sci. USA* **2003**, *100*, 3790-3795.
291. Hagadorn, J. R.; Zahn, T. I.; Que, L., Jr.; Tolman, W. B., "Dicopper(I,I) and Delocalized Mixed-Valent Dicopper(I,II) Complexes of a Sterically Hindered Carboxylate Ligand" *J. Chem. Soc., Dalton Trans.* **2003**, 1790-1794.
292. Roelfes, G.; Vrajmisu, V.; Chen, K.; Ho, R. Y. N.; Rohde, J.-U.; Zondervan, C.; la Crois, R. M.; Schudde, E. P.; Lutz, M.; Spek, A. L.; Hage, R.; Feringa, B. L.; Münck, E.; Que, L., Jr., "End-on and Side-on Peroxo Derivatives of Non-Heme Iron Complexes with Pentadentate Ligands: Models for Putative Intermediates in Biological Iron/Dioxygen Chemistry" *Inorg. Chem.* **2003**, *42*, 2639-2653.
293. Skulan, A. J.; Hanson, M. A.; Hsu, H.-f.; Que, L., Jr.; Solomon, E. I., "Spectroscopic Study of [Fe₂O₂(5-Et₃-TPA)₂]³⁺: Nature of the Fe₂O₂ Diamond Core and Its Possible Relevance to High-Valent Binuclear Non-Heme Enzyme Intermediates" *J. Am. Chem. Soc.* **2003**, *125*, 7344-7356.
294. Mehn, M. P.; Fujisawa, K.; Hegg, E. L.; Que, L., Jr., "Oxygen Activation by Nonheme Iron(II) Complexes: α -Keto Carboxylate versus Carboxylate" *J. Am. Chem. Soc.* **2003**, *125*, 7828-7842.
295. Kaizer, J.; Costas, M.; Que, L., Jr., "A Dramatic Push Effect on the Homolysis of Fe^{III}(OOR) Intermediates To Form Nonheme Fe^{IV}=O Complexes" *Angew. Chem. Int. Ed.* **2003**, *42*, 3671-3673.
296. Fujita, M.; Costas, M.; Que, L., Jr., "Iron Catalyzed Olefin *cis*-Dihydroxylation by H₂O₂: Electrophilic versus Nucleophilic Mechanisms" *J. Am. Chem. Soc.* **2003**, *125*, 9912-9913.
297. Jensen, M. P.; Mehn, M. P.; Que, L., Jr., "Intramolecular Aromatic Amination through Iron-Mediated Nitrene Transfer" *Angew. Chem. Int. Ed.* **2003**, *42*, 4357-4360.

298. Skulan, A. J.; Hanson, M. A.; Hsu, H.-f.; Dong, Y.; Que, L., Jr.; Solomon, E. I., "EPR Spectroscopy of $[\text{Fe}_2\text{O}_2(5\text{-Et}_3\text{-TPA})_2]^{3+}$: Electronic Origin of the Unique Spin-Hamiltonian Parameters of the $\text{Fe}_2^{\text{III,IV}}\text{O}_2$ Diamond Core" *Inorg. Chem.* **2003**, *42*, 6489-6496.
299. Costas, M.; Cady, C. W.; Kryatov, S. V.; Ray, M.; Ryan, M. J.; Rybak-Akimova, E. V.; Que, L., Jr., "Role of Carboxylate Bridges in Modulating Nonheme Diiron(II)/ O_2 Reactivity" *Inorg. Chem.* **2003**, *42*, 7519-7530.
300. Buck, B.; Mascioni, A.; Que, L., Jr.; Veglia, G. "Dealkylation of Organotin Compounds by Biological Dithiols: Toward the Chemistry of Organotin Toxicity" *J. Am. Chem. Soc.* **2003**, *125*, 13316-13317.
301. Rohde, J.-U.; Bukowski, M. R.; Que, L., Jr., "Functional Models for Mononuclear Nonheme Iron Enzymes" *Curr. Op. Chem. Biol.* **2003**, *7*, 674-682.
302. Que, L., Jr.; Tolman, W. B., "Recurring Structural Motifs in Bioinorganic Chemistry", in *Bio-Coordination Chemistry* (Que, L., Jr.; Tolman, W. B., Eds.); Volume 8 of *Comprehensive Coordination Chemistry II* (McCleverty, J.; Meyer, T. J., Eds.) Elsevier, Amsterdam, 2003; pp 1-15.
303. Bukowski, M. R.; Zhu, S.; Koehntop, K. D.; Brennessel, W. W.; Que, L., Jr., "Characterization of an $\text{Fe}^{\text{III}}\text{-OOH}$ Species and Its Decomposition Product in a Bleomycin Model System" *J. Biol. Inorg. Chem.* **2004**, *9*, 39-48.
304. Kaizer, J.; Klinker, E. J.; Oh, N. Y.; Rohde, J.-U.; Song, W. J.; Stubna, A.; Kim, J.; Nam, W.; Münck, E.; Que, L., Jr., "Nonheme $\text{Fe}^{\text{IV}}\text{O}$ Complexes That Can Oxidize the C-H Bonds of Cyclohexane at Room Temperature" *J. Am. Chem. Soc.* **2004**, *126*, 472-473.
305. Costas, M.; Mehn, M. P.; Jensen, M. P.; Que, L., Jr., "Dioxygen Activation at Mononuclear Nonheme Iron: Enzymes, Intermediates, and Models" *Chem. Rev.* **2004**, *104*, 939-986.
306. Ghosh, A.; Tangen, E.; Gonzalez, E.; Que, L., Jr., "Models of High-Valent Intermediates of Nonheme Diiron Alkane Monooxygenases. Electronic Structure of a Bis(μ -oxo)diiron(IV) Complex with Locally Low-Spin Metal Centers" *Angew. Chem., Int. Ed.* **2004**, *43*, 834-838.
307. Bukowski, M. R.; Comba, P.; Limberg, C.; Merz, M.; Que, L., Jr.; Wistuba, T., "Bispidine ligand effects on iron/hydrogen peroxide chemistry" *Angew. Chem., Int. Ed.* **2004**, *43*, 1283-1287.
308. Rocklin, A. M.; Kato, K.; Liu, H.-w.; Que, L., Jr.; Lipscomb, J. D., "Mechanistic Studies of 1-aminocyclopropane-1-carboxylic Acid Oxidase: Single Turnover Reactions" *J. Biol. Inorg. Chem.* **2004**, *9*, 171-182.
309. Kryatov, S. V.; Chavez, F. A.; Reynolds, A. M.; Rybak-Akimova, E. V.; Que, L., Jr.; Tolman, W. B. "Mechanistic Studies on the Formation and Reactivity of Dioxygen Adducts of Diiron Complexes Supported by Sterically Hindered Carboxylates" *Inorg. Chem.* **2004**, *43*, 2141-2150.
310. Vetting, M. W.; Wackett, L. P.; Que, L., Jr.; Lipscomb, J. D.; Ohlendorf, D. H., "Crystallographic Comparison of Manganese and Iron Dependent Homoprotocatechuate 2,3-Dioxygenases" *J. Bacteriol.* **2004**, *186*, 1945-1958.
311. Stubna, A.; Jo, D.-H.; Costas, M.; Brennessel, W. W.; Andres, H.; Bominaar, E. L.; Münck, E.; Que, L., Jr. "A Structural and Mössbauer Study of Complexes with $\text{Fe}_2(\mu\text{-O}(\text{H}))_2$ Cores: Stepwise Oxidation from $\text{Fe}^{\text{II}}(\mu\text{-OH})_2\text{Fe}^{\text{II}}$ through $\text{Fe}^{\text{II}}(\mu\text{-OH})_2\text{Fe}^{\text{III}}$ to $\text{Fe}^{\text{III}}(\mu\text{-O})(\mu\text{-OH})\text{Fe}^{\text{III}}$ " *Inorg. Chem.* **2004**, *43*, 3067-3079

312. Decker, A.; Rohde, J.-U.; Que, L., Jr.; Solomon, E. I. "Spectroscopic and Quantum Chemical Characterization of the Electronic Structure and Bonding in a Non-Heme $\text{Fe}^{\text{IV}}=\text{O}$ Complex" *J. Am. Chem. Soc.* **2004**, *126*, 5378-5379.
313. Seo, M. S.; In, J.-H.; Kim, S. O.; Oh, N. Y.; Hong, J.; Kim, J.; Que, L., Jr.; Nam, W. "Direct Evidence for Oxygen-Atom Exchange between Nonheme Oxoiron(IV) Complexes and Isotopically Labeled Water" *Angew. Chem. Int. Ed.* **2004**, *43*, 2417-2420.
314. Zlateva, T.; Quaroni, L.; Que, L., Jr.; Stankovich, M. T., "Redox Studies of Subunit Interactivity in Aerobic Ribonucleotide Reductase from *Escherichia coli*," *J. Biol. Chem.* **2004**, *279*, 18742-18747.
315. Fujita, M.; Que, L., Jr., "In situ Formation of Peracetic Acid in Iron-Catalyzed Epoxidations by Hydrogen Peroxide in the Presence of Acetic Acid," *Adv. Synth. Catal.* **2004**, *346*, 190-194.
316. Que, L., Jr., The oxo/peroxo debate: a nonheme iron perspective. *J. Biol. Inorg. Chem.* **2004**, *9*, 684-690.
317. Liu, P.; Mehn, M. P.; Yan, F.; Zhao, Z.; Que, L., Jr.; Liu, H.-w., "Oxygenase Activity in the Self-Hydroxylation of (S)-2-Hydroxypropylphosphonic Acid Epoxidase Involved in Fosfomycin Biosynthesis," *J. Am. Chem. Soc.* **2004**, *126*, 10306-10312.
318. Koehntop, K. D.; Rohde, J.-U.; Costas, M.; Que, L., Jr., "XAS characterization of end-on and side-on peroxoiron(III) complexes of the neutral pentadentate N-donor ligand N-methyl-*N,N',N'*-tris(2 pyridylmethyl)ethane-1,2-diamine," *Dalton Trans.* **2004**, 3191-3198.
319. Mairata i Payeras, A.; Ho, R. Y. N.; Fujita, M.; Que, L., Jr., "The Reaction of $[\text{Fe}^{\text{II}}(\text{tpa})]$ with H_2O_2 in Acetonitrile and Acetone—Distinct Intermediates and Yet Similar Catalysis," *Chem. Eur. J.* **2004**, *10*, 4944 – 4953.
320. Rohde, J.-U.; Torelli, S.; Shan, X.; Lim, M. H.; Klinker, E. J.; Kaizer, J.; Chen, K.; Nam, W.; Que, L., Jr., "Structural Insights into Nonheme Alkylperoxoiron(III) and Oxoiron(IV) Intermediates by X-ray Absorption Spectroscopy," *J. Am. Chem. Soc.* **2004**, *126*, 16750-16761.
321. Kryatov, S. V.; Taktak, S.; Korendovych, I. V.; Rybak-Akimova, E. V.; Kaizer, J.; Torelli, S.; Shan, X.; Mandal, S.; MacMurdo, V.; Mairata i Payeras, A.; Que, L., Jr., "Dioxygen Binding to Complexes with $\text{Fe}^{\text{II}}(\mu\text{-OH})_2$ Cores: Steric Control of Activation Barriers and O_2 -Adduct Formation," *Inorg. Chem.* **2005**, *44*, 85-99.
322. Bassan, A.; Blomberg, M. R. A.; Siegbahn, P. E. M.; Que, L., Jr., "A Density Functional Study on a Biomimetic Non-Heme Iron Catalyst: Insights into Alkane Hydroxylation by a Formally $\text{HO-Fe}^{\text{V}}=\text{O}$ Oxidant," *Chem. Eur. J.* **2005**, *11*, 692-705.
323. Bukowski, M. R.; Halfen, H. L.; van den Berg, T. A.; Halfen, J. A.; Que, L., Jr., "Spin-State Rationale for the Peroxo-Stabilizing Role of the Thiolate Ligand in Superoxide Reductase," *Angew. Chem. Int. Ed.* **2005**, *44*, 584-587.
324. Shan, X.; Que, L., Jr., "Intermediates in the oxygenation of a nonheme diiron(II) complex, including the first evidence for a bound superoxo species," *Proc. Natl. Acad. Sci. USA* **2005**, *102*, 5340-5345.
325. Rohde, J.-U.; Que, L., Jr., "Axial Coordination of Carboxylate Activates the Non-heme $\text{Fe}^{\text{IV}}=\text{O}$ Unit," *Angew. Chem. Int. Ed.* **2005**, *44*, 2255-2258.
326. Koehntop, K. D.; Emerson, J. P.; Que, L., Jr., "The 2-His-1-carboxylate Facial Triad: A

- Versatile Platform for Dioxygen Activation by Mononuclear Nonheme Iron(II) Enzymes," *J. Biol. Inorg. Chem.* **2005**, *10*, 87-93.
327. Bassan, A.; Blomberg, M. R. A.; Siegbahn, P. E. M.; Que, L., Jr., "Two Faces of a Biomimetic Non-Heme HO-Fe^V=O Oxidant: Olefin Epoxidation versus cis-Dihydroxylation," *Angew. Chem. Int. Ed.* **2005**, *44*, 2939-2941.
328. Quiñero, D.; Morokuma, K.; Musaev, D. G.; Mas-Balleste, R.; Que, L., Jr., "Metal-Peroxo versus Metal-Oxo Oxidants in Non-Heme Iron-Catalyzed Olefin Oxidations: Computational and Experimental Studies on the Effect of Water," *J. Am. Chem. Soc.* **2005**, *127*, 6548-6549.
329. Klinker, E. J.; Kaizer, J.; Brennessel, W. W.; Woodrum, N. L.; Cramer, C. J.; Que, L., Jr., "Structures of Nonheme Oxoiron(IV) Complexes from X-ray Crystallography, NMR Spectroscopy, and DFT Calculations," *Angew. Chem. Int. Ed.* **2005**, *44*, 3690-3694.
330. Tierney, D. L.; Rocklin, A. M.; Lipscomb, J. D.; Que, L., Jr.; Hoffman, B. M., "ENDOR Studies of the Ligation and Structure of the Non-Heme Iron Site in ACC Oxidase," *J. Am. Chem. Soc.* **2005**, *127*, 7005-7013.
331. Kumar, D.; Hirao, H.; Que, L., Jr.; Shaik, S., "Theoretical Investigation of C-H Hydroxylation by (N4Py)Fe^{IV}=O²⁺: An Oxidant More Powerful than P450?," *J. Am. Chem. Soc.* **2005**, *127*, 8026-8027.
332. Jensen, M. P.; Costas, M.; Ho, R. Y. N.; Kaizer, J.; Mairata i Payeras, A.; Münck, E.; Que, L., Jr.; Rohde, J.-U.; Stubna, A., "High-Valent Nonheme Iron. Two Distinct Iron(IV) Species Derived from a Common Iron(II) Precursor," *J. Am. Chem. Soc.* **2005**, *127*, 10512-10525.
333. Sastri, C. V.; Park, M. J.; Ohta, T.; Jackson, T. A.; Stubna, A.; Seo, M. S.; Lee, J.; Kim, J.; Kitagawa, T.; Münck, E.; Que, L., Jr.; Nam, W., "Axial Ligand Substituted Nonheme Fe=O Complexes: Observation of Near UV LMCT Bands and Fe=O Raman Vibrations," *J. Am. Chem. Soc.* **2005**, *127*, 12494-12495.
334. Pestovsky, O.; Stoian, S.; Bominaar, E. L.; Shan, X.; Münck, E.; Que, L., Jr.; Bakac, A., "Aqueous Fe^{IV}=O: Spectroscopic Identification and Oxo Group Exchange," *Angew. Chem. Int. Ed.* **2005**, *44*, 6871-6874.
335. Taktak, S.; Flook, M.; Foxman, B. M.; Que, L., Jr.; Rybak-Akimova, E. V., "ortho-Hydroxylation of benzoic acids with hydrogen peroxide at a nonheme iron center," *Chem. Commun.* **2005**, 5301-5303.
336. Bukowski, M. R.; Koehntop, K. D.; Stubna, A.; Bominaar, E. L.; Halfen, J. A.; Münck, E.; Nam, W.; Que, L., Jr., "A Thiolate-Ligated Nonheme Oxoiron(IV) Complex Relevant to Cytochrome P450," *Science* **2005**, *310*, 1000-1002.
337. Oldenburg, P. D.; Shteinman, A. A.; Que, L., Jr., "Iron-Catalyzed Olefin cis-Dihydroxylation Using a Bio-Inspired N,N,O-Ligand," *J. Am. Chem. Soc.* **2005**, *127*, 15672-15673.
338. Oh, N. Y.; Seo, M. S.; Lim, M. H.; Consugar, M. B.; Park, M. J.; Rohde, J.-U.; Han, J.; Kim, K. M.; Kim, J.; Que, L., Jr.; Nam, W., "Self-hydroxylation of perbenzoic acids at a nonheme iron(II) center," *Chem. Commun.* **2005**, 5644-5646.
339. Emerson, J. P.; Wagner, M. L.; Reynolds, M. F.; Que, L., Jr.; Sadowsky, M. J.; Wackett, L. P., "The role of histidine 200 in MndD, the Mn(II)-dependent 3,4-dihydroxyphenylacetate 2,3-dioxygenase from *Arthrobacter globiformis* CM-2, a site-directed mutagenesis study," *J. Biol. Inorg. Chem.* **2005**, *10*, 751-760.

340. Farquhar, E. R.; Koehntop, K. D.; Emerson, J. P.; Que, L., Jr., "Post-translational self-hydroxylation: A probe for oxygen activation mechanisms in non-heme iron enzymes," *Biochem. Biophys. Res. Commun.* **2005**, *338*, 230-239.
341. Earhart, C. A.; Vetting, M. W.; Gosua, R.; Michaud-Soret, I.; Que, L., Jr.; Ohlendorf, D. H., "Structure of catechol 1,2-dioxygenase from *Pseudomonas arvilla*," *Biochem. Biophys. Res. Commun.* **2005**, *338*, 198-205.
342. Koehntop, K. D.; Marimanikkuppam, S.; Ryle, M. J.; Hausinger, R. P.; Que, L., Jr., "Self-hydroxylation of taurine/ α -ketoglutarate dioxygenase: evidence for more than one oxygen activation mechanism," *J. Biol. Inorg. Chem.* **2006**, *11*, 63-72.
343. Mehn, M. P.; Brown, S. D.; Paine, T. K.; Brennessel, W. W.; Cramer, C. J.; Peters, J. C.; Que, L., Jr., "High-spin and low-spin iron(II) complexes with facially-coordinated borohydride ligands," *Dalton Trans.* **2006**, 1347-1351.
344. Shan, X.; Que, L., Jr., High-valent nonheme iron-oxo species in biomimetic oxidations. *J. Inorg. Biochem.* **2006**, *100*, 421-433.
345. Paine, T. K.; Costas, M.; Kaizer, J.; Que, L., Jr., Oxoiron(IV) complexes of the tris(2-pyridylmethyl)amine ligand family: effect of pyridine α -substituents. *J. Biol. Inorg. Chem.* **2006**, *11*, 272-276.
346. Bukowski, M. R.; Comba, P.; Lienke, A.; Limberg, C.; Lopez de Laorden, C.; Mas-Ballesté, R.; Merz, M.; Que, L., Jr., Catalytic Epoxidation and 1,2-Dihydroxylation of Olefins with Bispidine-Iron(II)/H₂O₂ Systems, *Angew. Chem. Int. Ed.* **2006**, *45*, 3446-3449.
347. Jensen, M. P.; Que, E. L.; Shan, X.; Rybak-Akimova, E.; Que, L., Jr., Spectroscopic and kinetic studies of the reaction of [CuI(6-PhTPA)]⁺ with O₂. *Dalton Trans.* **2006**, 3523-3527.
348. Bautz, J.; Bukowski, M. R.; Kerscher, M.; Stubna, A.; Comba, P.; Lienke, A.; Münck, E.; Que, L., Jr., Formation of an Aqueous Oxoiron(IV) Complex at pH 2–6 from a Nonheme Iron(II) Complex and H₂O₂, *Angew. Chem. Int. Ed.* **2006**, *45*, 5681–5684.
349. Company, A.; Lamata, D.; Poater, A.; Sola, M.; Rybak-Akimova, E. V.; Que, L.; Fontrodona, X.; Parella, T.; Llobet, A.; Costas, M., O₂ Chemistry of Dicopper Complexes with Alkyltriamine Ligands. Comparing Synergistic Effects on O₂ Binding. *Inorg. Chem.* **2006**, *45*, 5239-5241. (PMCID: PMC2526348)
350. Rohde, J.-U.; Stubna, A.; Bominaar, E. L.; Münck, E.; Nam, W.; Que, L., Jr., Nonheme Oxoiron(IV) Complexes of Tris(2-pyridylmethyl)amine with *cis*-Monoanionic Ligands, *Inorg. Chem.* **2006**, *45*, 6435-6445.
351. Jackson, T. A.; Que, L., Jr., Structural and Functional Models for Oxygen Activating Nonheme Iron Enzymes. In *Concepts and Models in Bioinorganic Chemistry*, Kraatz, H.-B.; Metzler-Nolte, N., Eds. Wiley-VCH: Weinheim, 2006; pp 260-286.
352. Hirao, H.; Kumar, D.; Que, L., Jr.; Shaik, S., Two-State Reactivity in Alkane Hydroxylation by Non-Heme Iron-Oxo Complexes *J. Am. Chem. Soc.* **2006**, *128*, 8590-8606.
353. Bautz, J.; Comba, P.; Que, L., Jr., Spin-Crossover in an Iron(III)-Bispidine Alkylperoxide System, *Inorg. Chem.* **2006**, *45*, 7077-7082.
354. Mehn, M. P.; Brown, S. D.; Jenkins, D. M.; Peters, J. C.; Que, L., Jr., Vibrational Spectroscopy and Analysis of Pseudo-tetrahedral Complexes with Metal Imido Bonds,

- Inorg. Chem.* **2006**, *45*, 7417-7427.
355. Mas-Ballesté, R.; Fujita, M.; Hemmila, C., Que, L., Jr., Bio-inspired iron-catalyzed olefin oxidation. Additive effects on the *cis*-diol/epoxide ratio, *J. Mol. Catal. A: Chem.* **2006**, *251*, 49-53.
356. Oldenburg, P.; Que, L., Jr., Bio-inspired nonheme iron catalysts for olefin oxidation, *Catal. Today*, **2006**, *117*, 15-21.
357. Mas-Ballesté, R.; Que, L., Jr., Targeting Specific C-H Bonds for Oxidation, *Science* **2006**, *312*, 1885-1886
358. Mas-Ballesté, R.; Costas, M.; van den Berg, T.; Que, L., Jr., Ligand Topology Effects on Olefin Oxidations by Bio-Inspired [Fe^{II}(N₂Py₂)] Catalysts, *Chem. Eur. J.* **2006**, *12*, 7489-7500.
359. Friese, S. J.; Kucera, B. E.; Que, L., Jr.; Tolman, W. B., Self-Assembly of the 2-His-1-carboxylate Facial Triad in Mononuclear Iron(II) and Zinc(II) Models of Metalloenzyme Active Sites, *Inorg. Chem.* **2006**, *45*, 8003-8005
360. Klein, D. P.; Young, V. G., Jr.; Tolman, W. B.; Que, L., Jr., Mononitrosyl Iron Complexes Supported by Sterically Hindered Carboxylate Ligands, *Inorg. Chem.* **2006**, *45*, 8006-8008
361. Collins, M. J.; Ray, K.; Que, L., Jr., Electrochemical Generation of a Nonheme Oxoiron(IV) Complex, *Inorg. Chem.* **2006**, *45*, 8009-8011.
362. Klinker, E. J.; Jackson, T. A.; Jensen, M. P.; Stubna, A.; Juhász, G.; Bominaar, E. L.; Münck, E.; Que, L., Jr., A Tosylimido Analogue of a Nonheme Oxoiron(IV) Complex, *Angew. Chem. Int. Ed.* **2006**, *45*, 7394-7397.
363. Oldenburg, P. D.; Ke, C.-Y.; Tipton, A. A.; Shteinman, A. A.; Que, L., Jr., A Structural and Functional Model for Dioxygenases with a 2-His-1-carboxylate Triad, *Angew. Chem. Int. Ed.* **2006**, *45*, 7975-7978.
364. Tiago de Oliveira, F.; Chanda, A.; Banerjee, D.; Shan, X.; Mondal, S.; Que, L., Jr.; Bominaar, E. L.; Münck, E.; Collins, T. J., Chemical and Spectroscopic Evidence for an Fe^V-Oxo Complex. *Science* **2007**, *315*, 835-838.
365. Jensen, M. P.; Mairata i Payeras, A.; Fiedler, A. T.; Costas, M.; Kaizer, J.; Stubna, A.; Münck, E.; Que, L., Jr., Kinetic Analysis of the Conversion of Nonheme (Alkylperoxo)iron(III) Species to Iron(IV) Complexes, *Inorg. Chem.* **2007**, *46*, 2398-2408. (PMCID: PMC2526350)
366. Klotz, K. L.; Slominski, L. M.; Hull, A. V.; Gottsacker, V. M.; Mas-Ballesté, R.; Que, L., Jr.; Halfen, J. A., Non-heme iron(II) complexes are efficient olefin aziridination catalysts. *Chem. Commun.* **2007**, 2063-2065.
367. Company, A.; Gomez, L.; Mas-Balleste, R.; Korendovych, I. V.; Ribas, X.; Poater, A.; Parella, T.; Fontrodona, X.; Benet-Buchholz, J.; Sola, M.; Que, L., Jr.; Rybak-Akimova, E. V.; Costas, M., Fast O₂ Binding at Dicopper Complexes Containing Schiff-Base Dinucleating Ligands. *Inorg. Chem.* **2007**, *46*, 4997-5012. (PMCID: PMC2535575)
368. Rohde, J.-U.; Betley, T. A.; Jackson, T. A.; Saouma, C. T.; Peters, J. C.; Que, L., Jr., XAS Characterization of a Nitridoiron(IV) Complex with a Very Short Fe-N Bond. *Inorg. Chem.* **2007**, *46*, 5720-5726. (PMCID: PMC2535570)
369. Smith, A. L.; Day, C. S.; Que, L., Jr.; Zhou, Y.; Bierbach, U., Unexpected assembly of a novel triply bridged diiron(II) core by a bidentate Schiff base ligand. *Inorg. Chim. Acta* **2007**, *360*, 2824-2828.

370. Paine, T. K.; England, J.; Que, L., Jr., Iron-Catalyzed C2–C3 Bond Cleavage of Phenylpyruvate with O₂: Insight into Aliphatic C–C Bond-Cleaving Dioxygenases. *Chem. Eur. J.* **2007**, *13*, 6073–6081.
371. Que, L., Jr., The Road to Non-Heme Oxoferryls and Beyond. *Acc. Chem. Res.* **2007**, *40*, 493-500.
372. Shan, X.; Rohde, J.-U.; Koehntop, K. D.; Zhou, Y.; Bukowski, M. R.; Costas, M.; Fujisawa, K.; Que, L., Jr., X-ray Absorption Spectroscopic Studies of High-Spin Nonheme (Alkylperoxo)iron(III) Intermediates. *Inorg. Chem.* **2007**, *46*, 8410-8417.
373. Emerson, J. P.; Farquhar, E. R.; Que, L., Jr., Structural “Snapshots” along Reaction Pathways of Non-Heme Iron Enzymes. *Angew. Chem. Int. Ed.* **2007**, *46*, 8553-8556
374. Sastri, C. V.; Lee, J.; Oh, K.; Lee, Y. J.; Lee, J.; Jackson, T. A.; Ray, K.; Hirao, H.; Shin, W.; Halfen, J. A.; Kim, J.; Que, L., Jr.; Shaik, S.; Nam, W., Axial ligand tuning of a nonheme iron(IV)–oxo unit for hydrogen atom abstraction. *Proc. Natl. Acad. Sci. USA* **2007**, *104*, 19181-19186.
375. Xue, G.; Wang, D.; De Hont, R.; Fiedler, A. T.; Shan, X.; Münck, E.; Que, L., Jr., A Synthetic Precedent for the [Fe^{IV}₂(μ-O)₂] Diamond Core Proposed for Methane Monooxygenase Intermediate Q. *Proc. Natl. Acad. Sci. USA* **2007**, *104*, 20713-20718.
376. Company, A.; Gomez, L.; Guell, M.; Ribas, X.; Luis, J. M.; Que, L., Jr.; Costas, M., Alkane Hydroxylation by a Nonheme Iron Catalyst that Challenges the Heme Paradigm for Oxygenase Action. *J. Am. Chem. Soc.* **2007**, *129*, 15766-15767.
377. Mas-Ballesté, R.; Que, L., Jr., Iron-Catalyzed Olefin Epoxidation in the Presence of Acetic Acid: Insights into the Nature of the Metal-Based Oxidant. *J. Am. Chem. Soc.* **2007**, *129*, 15964-15972.
378. Decker, A.; Rohde, J.-U.; Klinker, E. J.; Wong, S. D.; Que, L., Jr.; Solomon, E. I., Spectroscopic and Quantum Chemical Studies on Low-Spin Fe^{IV}=O Complexes: Fe-O Bonding and Its Contributions to Reactivity. *J. Am. Chem. Soc.* **2007**, *129*, 15983-15996 (PMCID: PMC2547486)
379. Hirao, H.; Que, L., Jr.; Nam, W.; Shaik, S., A Two-State Reactivity Rationale for Counterintuitive Axial Ligand Effects on the CH Activation Reactivity of Nonheme Fe^{IV}O Oxidants. *Chem. Eur. J.* **2008**, *14*, 1740-1756.
380. Suzuki, K.; Oldenburg, P. D.; Que, L., Jr., Iron-Catalyzed Asymmetric Olefin *cis*-Dihydroxylation with 97 % Enantiomeric Excess *Angew. Chem. Int. Ed.* **2008**, *47*, 1887-1889.
381. Zhou, Y.; Shan, X.; Mas-Ballesté, R.; Bukowski, M. R.; Stubna, A.; Chakrabarti, M.; Slominski, L.; Halfen, J. A.; Münck, E.; Que, L., Jr., Contrasting *cis* and *trans* Effects on the Reactivity of Nonheme Oxoiron(IV) Complexes *Angew. Chem. Int. Ed.* **2008**, *47*, 1896-1899.
382. Ray, K.; Lee, S. M.; Que, L., Jr., “Iron-oxidation-state-dependent O–O bond cleavage of meta-chloroperbenzoic acid to form an iron(IV)-oxo complex” *Inorg. Chim. Acta* **2008**, *361*, 1066-1069 (doi: 10.1016/j.ica.2007.07.039; PMCID: PMC2352149)
383. Friese, S. J.; Kucera, B. E.; Young, V. G., Jr.; Que, L., Jr.; Tolman, W. B., Iron(II) Complexes of Sterically Bulky α -Ketocarboxylates. Structural Models for α -Ketoacid-Dependent Nonheme Iron Halogenases *Inorg. Chem.* **2008**, *47*, 1324-1331.
384. Mas-Ballesté, R.; Fujita, M.; Que, L., Jr., High-valent iron-mediated *cis*-

- hydroxyacetoxylation of olefins. *Dalton Trans.* **2008**, 1828-1830.
385. Krzystek, J.; England, J.; Ray, K.; Ozarowski, A.; Smirnov, D.; Que, L., Jr.; Telser, J., Determination by High-Frequency and -Field EPR of Zero-Field Splitting in Iron(IV) Oxo Complexes: Implications for Intermediates in Nonheme Iron Enzymes *Inorg. Chem.* **2008**, *47*, 3483-3485.
386. Company, A.; Palavicini, S.; Garcia-Bosch, I.; Mas-Ballesté, R.; Que, L., Jr.; Rybak-Akimova, E. V.; Casella, L.; Ribas, X.; Costas, M., Tyrosinase-Like Reactivity in a $\text{Cu}^{\text{III}}_2(\mu\text{-O})_2$ Species. *Chem. Eur. J.* **2008**, *14*, 3535-3538.
387. Chanda, A.; Shan, X.; Chakrabarti, M.; Ellis, W. C.; Popescu, D. L.; Tiago de Oliveira, F.; Wang, D.; Que, L., Jr.; Collins, T. J.; Münck, E.; Bominaar, E. L., (TAML) $\text{Fe}^{\text{IV}}=\text{O}$ Complex in Aqueous Solution: Synthesis and Spectroscopic and Computational Characterization. *Inorg. Chem.* **2008**, *47*, 3669-3678.
388. Shan, X.; Que, L., Jr., Unexpected kinetic complexity in the formation of a nonheme oxoiron(IV) complex. *Chem. Commun.* **2008**, 2209-2011.
389. Emerson, J. P.; Kovaleva, E. G.; Farquhar, E. R.; Lipscomb, J. D.; Que, L., Jr., Swapping metals in Fe- and Mn-dependent dioxygenases: Evidence for oxygen activation without a change in metal redox state. *Proc. Natl. Acad. Sci. USA* **2008**, *105*, 7347-7352 (doi: 10.1073/pnas.0711179105; PMC2396700)
390. Thibon, A.; England, J.; Martinho, M.; Young, V. G., Jr.; Frisch, J. R.; Guillot, R.; Girerd, J.-J.; Münck, E.; Que, L., Jr.; Banse, F., Proton- and Reductant-Assisted Dioxygen Activation by a Nonheme Iron(II) Complex to Form an Oxoiron(IV) Intermediate. *Angew. Chem. Int. Ed.* **2008**, *47*, 7064-7067 (doi: 10.1002/anie.200801832; PMC2652675)
391. Oldenburg, P., D.; Mas-Balleste', R.; Que, L., Jr., Bio-Inspired Iron-Catalyzed Olefin Oxidations: Epoxidation Versus *cis*-Dihydroxylation in *Mechanisms in Homogeneous and Heterogeneous Epoxidation Catalysis*, Oyama, S. T., Ed.; Elsevier: Amsterdam, 2008, pp. 452-469.
392. Que, L., Jr.; Tolman, W. B., Biologically inspired oxidation catalysis. *Nature* **2008**, *455*, 333-340 (doi:10.1038/nature07371)
393. Jackson, T. A.; Rohde, J.-U.; Seo, M. S.; Sastri, C. V.; DeHont, R.; Stubna, A.; Ohta, T.; Kitagawa, T.; Münck, E.; Nam, W.; Que, L., Jr., Axial Ligand Effects on the Geometric and Electronic Structures of Nonheme Oxoiron(IV) Complexes. *J. Am. Chem. Soc.* **2008**, *130*, 12394-12407 (doi:10.1021/ja8022576; PMCID: PMC2574688)
394. Ray, K.; England, J.; Fiedler, A. T.; Martinho, M.; Münck, E.; Que, L., Jr., An Inverted and More Oxidizing Isomer of $[\text{Fe}^{\text{IV}}(\text{O})(\text{tmc})(\text{NCCH}_3)]^{2+}$. *Angew. Chem. Int. Ed.* **2008**, *47*, 8068-8071 (doi:10.1002/anie.200802219; PMCID: PMC2656284)
395. Gunderson, W. A.; Zatsman, A. I.; Emerson, J. P.; Farquhar, E. R.; Que, L., Jr.; Lipscomb, J. D.; Hendrich, M. P., EPR Detection of Intermediates in the Enzymatic Cycle of an Extradiol Dioxygenase. *J. Am. Chem. Soc.* **2008**, *130*, 14465-14467. (doi: 10.1021/ja8052255; PMC2806810).
396. Bell, C. B., III; Wong, S. D.; Xiao, Y.; Klinker, E. J.; Tenderholt, A. L.; Smith, M. C.; Rohde, J.-U.; Que, L., Jr.; Cramer, S. P.; Solomon, E. I., A Combined NRVS and DFT Study of $\text{Fe}^{\text{IV}}=\text{O}$ Model Complexes: a Diagnostic Method for the Elucidation of Non-Heme Iron Enzyme Intermediates. *Angew. Chem. Int. Ed.* **2008**, *47*, 9071-9074 (doi: 10.1002/anie.200803740; PMC2662738)
397. Fiedler, A. T.; Shan, X.; Mehn, M. P.; Kaizer, J.; Torelli, S.; Frisch, J. R.; Kodera, M.;

- Que, L., Jr., Spectroscopic and Computational Studies of (μ -Oxo)(μ -1,2-Peroxo)diiron(III) Complexes of Relevance to Nonheme Diiron Oxygenase Intermediates *J. Phys. Chem. A* **2008**, *112*, 13037-13044 (doi:10.1021/jp8038225; PMC2736334)
398. Xue, G.; Fiedler, A. T.; Martinho, M.; Münck, E.; Que, L., Jr., Insights into the P-to-Q Conversion in the Catalytic Cycle of Methane Monooxygenase from a Synthetic Model System. *Proc. Natl. Acad. Sci. USA* **2008**, *105*, 20615-20620 (doi:10.1073/pnas.0808512105; PMC2634879)
399. Feng, Y.; Ke, C.-y.; Xue, G.; Que, L., Jr., Bio-inspired arene *cis*-dihydroxylation by a non-haem iron catalyst modeling the action of naphthalene dioxygenase. *Chem. Commun.* **2009**, 50-56 (DOI: 10.1039/b817222f) (designated as a HOT paper by journal)
400. Klinker, E. J.; Shaik, S.; Hajime, H.; Que, L., Jr., Two-State Reactivity Model Explains Unusual Kinetic Isotope Effect Patterns in C-H Bond Cleavage by Nonheme Oxoiron(IV) Complexes *Angew. Chem. Int. Ed.* **2009**, *48*, 1291-1295 (DOI: 10.1002/anie.200804029; PMC2832851)
401. Mukherjee, A.; Martinho, M.; Bominaar, E. L.; Münck, E.; Que, L., Jr., Shape-Selective Interception by Hydrocarbons of the O₂-Derived Oxidant of a Biomimetic Nonheme Iron Complex *Angew. Chem. Int. Ed.* **2009**, *48*, 1780-1783. (DOI:10.1002/anie.200805342; PMC2719302)
402. Company, A.; Feng, Y.; Güell, M.; Ribas, X.; Luis, J. M.; Que, L., Jr.; Costas, M., Olefin-Dependent Discrimination Between Two Nonheme HO-Fe^V=O Tautomeric Species in Catalytic H₂O₂ Epoxidations. *Chem. Eur. J.* **2009**, *15*, 3356-3362. (DOI:10.1002/chem.200802597) (designated as VIP by journal)
403. Wang, D.; Farquhar, E. R.; Stubna, A.; Münck, E.; Que, L., Jr., A Diiron(IV) Complex That Cleaves Strong C-H and O-H Bonds. *Nature Chem.* **2009**, *1*, 145-150 (doi:10.1038/nchem.162; PMC2744316) (highlighted in *Nature*, April 3, 2009 issue and *C&ENews*, April 6, 2009 issue)
404. England, J.; Martinho, M.; Farquhar, E. R.; Frisch, J. R.; Bominaar, E. L.; Münck, E.; Que, L., Jr., A Synthetic High-Spin Oxoiron(IV) Complex: Generation, Spectroscopic Characterization, and Reactivity. *Angew. Chem. Int. Ed.* **2009**, *48*, 3622-3626 (DOI: 10.1002/anie.200900863; PMC2719303) (designated as VIP by journal)
405. Martinho, M.; Xue, G.; Fiedler, A.T.; Que, L., Jr. ; Bominaar, E.; Münck, E., Mössbauer and DFT Study of the Ferromagnetically Coupled Diiron(IV) Precursor to a Complex with an Fe^{IV}₂O₂ Diamond Core. *J. Am. Chem. Soc.* **2009**, *131*, 5823-5830 (DOI: 10.1021/ja8098917; PMC2675788)
406. Frisch, J. R.; Vu, V. V.; Martinho, M.; Münck, E.; Que, L., Jr., Characterization of Two Distinct Adducts in the Reaction of a Nonheme Diiron(II) Complex with O₂. *Inorg. Chem.* **2009**, *48*, 8325-8336 (DOI: 10.1021/ic900961k; PMC19610611)
407. Johansson, A. J.; Noack, H.; Siegbahn, P. E. M.; Xue, G.; Que, L., Jr., Observed enhancement of the reactivity of a biomimetic diiron complex by the addition of water - mechanistic insights from theoretical modeling. *Dalton Trans.* **2009**, 6741-6750 (DOI: 10.1039/b907263b; PMC2829260).
408. Vu, V. V.; Emerson, J. P.; Martinho, M.; Kim, Y. S.; Münck, E.; Park, M. H.; Que, L., Jr., Human deoxyhypusine hydroxylase, an enzyme involved in regulating cell growth, activates O₂ with a nonheme diiron center. *Proc. Natl. Acad. Sci. USA* **2009**, *106*, 14814-14819 (doi:10.1073/pnas.0904553106; PMC2736468).

409. Fielder, A. T.; Que, L., Jr., Reactivities of Fe(IV) Complexes with Oxo, Hydroxo, and Alkylperoxo Ligands: An Experimental and Computational Study. *Inorg. Chem.* **2009**, *48*, 11038-11047 (DOI: 10.1021/ic901391y; PMC2789986)
410. Makhlynets, O. V.; Das, P.; Taktak, S.; Flook, M.; Mas-Ballesté, R.; Rybak-Akimova, E. V.; Que, L., Jr., Iron-promoted *ortho*- and/or *ipso*-hydroxylation of benzoic acids with H₂O₂. *Chem. Eur. J.* **2009**, *15*, 13171-13180 (DOI: 10.1002/chem.200901296).
411. Li, F., England, J., and Que, L., Jr., Near-Stoichiometric Conversion of H₂O₂ to Fe^{IV}=O at a Non-Heme Iron(II) Center. Insights into the O-O Bond Cleavage Step. *J. Am. Chem. Soc.* **2010**, *132*, 2134-2135 (DOI: 10.1021/ja9101908; PMC2823852)
412. Paine, T. K.; Paria, S.; Que, L., Jr., Oxidative Decarboxylation of α -Hydroxy Acids by a Functional Model of the Nonheme Iron Oxygenase, CloR. *Chem. Commun.* **2010**, 1830-1832 (DOI: 10.1039/B925389K; PMC 20198223).
413. Garcia-Bosch, I.; Company, A.; Frisch, J. R.; Torrent-Sucarrat, M.; Cardellach, M.; Gamba, I.; Güell, M.; Casella, L.; Que, L., Jr.; Ribas, X.; Luis, J. M.; Costas, M., O₂ Activation and Selective Phenolate *ortho*-Hydroxylation by an Unsymmetric Dicopper - 1:1-Peroxido Complex. *Angew. Chem. Int. Ed.* **2010**, *49*, 2406-2409 (DOI: 10.1002/anie.200906749; PMC3328305).
414. Mukherjee, A.; Cranswick, M. A.; Chakrabarti, M.; Paine, T. K.; Fujisawa, K.; Münck, E.; Que, L., Jr., Oxygen Activation at Mononuclear Nonheme Iron Centers: A Superoxo Perspective. *Inorg. Chem.* **2010**, *49*, 3618-3628 (DOI: 10.1021/ic901891n; PMC20380464).
415. Janardanan, D.; Wang, Y.; Schyman, P.; Que, L., Jr.; Shaik, S., The Fundamental Role of Exchange-Enhanced Reactivity in C-H Activation by *S* = 2 Oxo Iron(IV) Complexes. *Angew. Chem. Int. Ed.* **2010**, *49*, 3342-3346 (DOI: 10.1002/anie.201000004; PMC20358569).
416. Xue, G.; De Hont, R.; Münck, E.; Que, L., Jr., Million-fold activation of the [Fe₂(μ -O)₂] diamond core for C-H bond cleavage. *Nature Chem.* **2010**, *2*, 400-405 (DOI: 10.1038/nchem.586; PMC2859466).
417. Wang, D.; Zhang, M.; Bühlmann, P.; Que, L., Jr., Redox Potential and C-H Bond Cleaving Properties of a Nonheme Fe^{IV}=O Complex in Aqueous Solution. *J. Am. Chem. Soc.* **2010**, *132*, 7638-7644 (DOI: 10.1021/ja909923w; PMC20476758)
418. Torres Martin de Rosales, R.; Faiella, M.; Farquhar, E.; Que, L., Jr.; Andreozzi, C.; Pavone, V.; Maglio, O.; Nistri, F.; Lombardi, A., Spectroscopic and metal-binding properties of DF3: an artificial protein able to accommodate different metal ions. *J. Biol. Inorg. Chem.* **2010**, *15*, 717-728 (DOI: 10.1007/s00775-010-0639-9; PMC2915772).
419. England, J.; Guo, Y.; Farquhar, E. R.; Young, V. G., Jr.; Münck, E.; Que, L., Jr., The Crystal Structure of a High-Spin Oxoiron(IV) Complex and Characterization of Its Self-Decay Pathway. *J. Am. Chem. Soc.* **2010**, *132*, 8635-8644 (DOI: 10.1021/ja100366c; PMC2903234).
420. De Hont, R. F.; Xue, G.; Hendrich, M. P.; Que, L., Jr.; Bominaar, E. L.; Münck, E., Mössbauer, Electron Paramagnetic Resonance, and Density Functional Theory Studies of Synthetic *S* = 1/2 Fe^{III}-O-Fe^{IV}=O Complexes. Superexchange-Mediated Spin Transition at the Fe^{IV}=O Site. *Inorg. Chem.* **2010**, *49*, 8310-8322 (DOI: 10.1021/ic100870v; PMC2957120).
421. Das, P.; Que, L., Jr., Iron Catalyzed Competitive Olefin Oxidation and *ipso*-Hydroxylation

- of Benzoic Acids: Further Evidence for an $\text{Fe}^{\text{V}}=\text{O}$ Oxidant. *Inorg. Chem.* **2010**, *49*, 9479-9485 (DOI: 10.1021/ic101144s).
422. McDonald, A. R.; Bukowski, M. R.; Farquhar, E. R.; Jackson, T. A.; Koehntop, K. D.; Seo, M. S.; Hont, R. F. D.; Stubna, A.; Halfen, J. A.; Münck, E.; Nam, W.; Que, L., Jr., Sulfur versus Iron Oxidation in an Iron–Thiolate Model Complex. *J. Am. Chem. Soc.* **2010**, *132*, 17118-17129 (DOI: 10.1021/ja1045428; PMC21070030).
423. Oldenburg, P. D.; Feng, Y.; Pryjomska-Ray, I.; Ness, D.; Que, L., Jr., Olefin *cis*-Dihydroxylation with Bio-Inspired Iron Catalysts. Evidence for an $\text{Fe}^{\text{II}}/\text{Fe}^{\text{IV}}$ Catalytic Cycle. *J. Am. Chem. Soc.* **2010**, *132*, 17713-17723 (DOI: 10.1021/ja1021014).
424. Company, A.; Prat, I.; Frisch, J. R.; Mas-Ballesté, R.; Güell, M.; Juhász, G.; Ribas, X.; Münck, E.; Luis, J. M.; Que, L., Jr.; Costas, M., Modeling the *cis*-Oxo-Labile Binding Site Motif of Non-Heme Iron Oxygenases: Water Exchange and Oxidation Reactivity of a Non-Heme Iron(IV)-Oxo Compound Bearing a Tripodal Tetradentate Ligand. *Chem. Eur. J.* **2011**, *17*, 1622-1634 (DOI : 10.1002/chem.201002297; PMC3097279).
425. Fielding, A. J.; Kovaleva, E. G.; Farquhar, E. R.; Lipscomb, J. D.; Que, L., Jr., A Hyperactive Cobalt-Substituted Extradiol-Cleaving Catechol Dioxygenase. *J. Biol. Inorg. Chem.* **2011**, *16*, 341-355 (DOI 10.1007/s00775-010-0732-0; PMC3192431).
426. Farquhar, E. R.; Emerson, J. P.; Koehntop, K. D.; Reynolds, M. F.; Trmčić, M.; Que, L., Jr., In vivo self-hydroxylation of an iron-substituted manganese-dependent extradiol cleaving catechol dioxygenase. *J. Biol. Inorg. Chem.* **2011**, *16*, 589-597 (PMC3177297).
427. Wong, S. D.; Bell, C. B., III; Liu, L. V.; Kwak, Y.; England, J.; Zhao, J.; Que, L., Jr.; Solomon, E. I., Nuclear Resonance Vibrational Spectroscopy on the $\text{Fe}^{\text{IV}}=\text{O}$ $S = 2$ nonheme site in TMG₃tren: Experimentally-calibrated Insights into Reactivity. *Angew. Chem. Int. Ed.* **2011**, *50*, 3215–3218 (10.1002/anie.201007692; PMC3085250).
428. England, J.; Farquhar, E. R.; Guo, Y.; Cranswick, M. A.; Ray, K.; Münck, E.; Que, L., Jr., Characterization of a Tricationic Trigonal Bipyramidal Iron(IV) Cyanide Complex, with a Very High Reduction Potential, and Its Iron(II) and Iron(III) Congeners. *Inorg. Chem.* **2011**, *50*, 2885–2896 (10.1021/ic102094d; PMC3065519).
429. Li, F.; Meier, K. K.; Cranswick, M. A.; Chakrabarti, M.; Van Heuvelen, K. M.; Münck, E.; Que, L., Jr., Characterization of a High-Spin Nonheme $\text{Fe}^{\text{III}}-\text{OOH}$ Intermediate and Its Quantitative Conversion to an $\text{Fe}^{\text{IV}}=\text{O}$ Complex. *J. Am. Chem. Soc.* **2011**, *133*, 7256-7259 (10.1021/ja111742z; PMC3097042).
430. Vu, V.; Makris, T.; Lipscomb, J. D.; Que, L., Jr., Active site structure of a β -hydroxylase in antibiotic biosynthesis. *J. Am. Chem. Soc.* **2011**, *133*, 6938-6941 (10.1021/ja201822v; PMC3096070).
431. Hirao, H.; Li, F.; Que, L., Jr.; Morokuma, K. Theoretical Study of the Mechanism of Oxoiron(IV) Formation from H_2O_2 and a Nonheme Iron(II) Complex: O–O Cleavage Involving Proton-Coupled Electron Transfer. *Inorg. Chem.* **2011**, *50*, 6637-6648. (10.1021/ic200522r; PMC3136038).
432. England, J.; Guo, Y.; van Heuvelen, K. M.; Cranswick, M. A.; Rohde, G. T.; Bominaar, E. L.; Münck, E.; Que, L., Jr., A More Reactive Trigonal Bipyramidal High-Spin Oxoiron(IV) Complex with a *cis*-Labile Site. *J. Am. Chem. Soc.* **2011**, *133*, 11880–11883 (10.1021/ja2040909; PMC3150404).
433. Feng, Y.; England, J.; Que, L., Jr., Iron-Catalyzed Olefin Epoxidation and *cis*-Dihydroxylation by Tetraalkylcyclam Complexes: the Importance of *cis*-Labile Sites. *ACS*

- Catal.* **2011**, *1*, 1035–1042 (10.1021/cs200292h)
434. McDonald, A. R.; Que, L., Jr., Iron–oxo complexes: Elusive iron(V) species identified. *Nature Chem.* **2011**, *3*, 761–762 (10.1038/nchem.1153)
435. Xue, G.; Pokutsa, A.; Que, L., Jr., Substrate-Triggered Activation of a Synthetic [Fe₂(μ-O)₂] Diamond Core for C–H Bond Cleavage. *J. Am. Chem. Soc.* **2011**, *133*, 16657–16667 (DOI: 10.1021/ja207131g; PMC3192255).
436. Chandrasekaran, P.; Stieber, S. C. E.; Collins, T. J.; Que, L., Jr.; Neese, F.; DeBeer, S., Prediction of high-valent iron K-edge absorption spectra by time-dependent Density Functional Theory. *Dalton Trans.* **2011**, *40*, 11070–11079 (10.1039/c1dt11331c, PMC3242413).
437. Paria, S.; Que, L., Jr.; Paine, T. K., Oxidative Decarboxylation of Benzilic Acid by a Biomimetic Iron(II) Complex: Evidence for an Iron(IV)–Oxo–Hydroxo Oxidant from O₂. *Angew. Chem. Int. Ed.* **2011**, *50*, 11129–11132 (10.1002/anie.201103971).
438. Fielding, A. J.; Lipscomb, J. D.; Que, L. Jr., Characterization of an O₂ Adduct of an Active Cobalt-Substituted Extradiol-Cleaving Catechol Dioxygenase. *J. Am. Chem. Soc.* **2012**, *134*, 796–799 (10.1021/ja2095365, PMC3262093).
439. Do, L. H.; Xue, G.; Que, L., Jr.; Lippard, S. J., Evaluating the Identity and Diiron Core Transformations of a (μ-Oxo)diiron(III) Complex Supported by Electron-Rich Tris(pyridyl-2-methyl)amine Ligands. *Inorg. Chem.* **2012**, *51*, 2393–2402 (10.1021/ic202379b, PMC3288163).
440. Li, F.; Chakrabarti, M.; Dong, Y.; Kauffmann, K.; Bominaar, E. L.; Münck, E.; Que, L., Jr., Structural, EPR and Mössbauer Characterization of (μ-Alkoxo)(μ-Carboxylato)Diiron(II,III) Model Complexes for the Active Sites of Mixed-valent Diiron Enzymes. *Inorg. Chem.* **2012**, *51*, 2917–29–29 (10.1021/ic2021726; PMC3298377).
441. McDonald, A. R.; Guo, Y.; Vu, V. V.; Bominaar, E. L.; Münck, E.; Que, L., Jr., A Mononuclear Carboxylate-Rich Oxoiron(IV) Complex: a Structural and Functional Mimic of TauD Intermediate ‘J’ *Chem. Sci.* **2012**, *3*, 1680–1683 (10.1039/C2SC01044E; **PMC in process**).
442. Mas-Ballesté, R.; McDonald, A. R.; Reed, D.; Usharani, D.; Schyman, P.; Milko, P.; Shaik, S.; Que, L., Jr., Intramolecular Gas Phase Reactions of Synthetic Non-heme Oxoiron(IV) Ions: Proximity and Spin-State Reactivity Rules. *Chem. Eur. J.* **2012**, in press.
443. Van Heuvelen, K. M.; Fiedler, A. T.; Shan, X.; De Hont, R. H.; Meier, K. K.; Bominaar, E. L.; Münck, E.; Que, L., Jr., One-electron oxidation of an oxoiron(IV) complex to form an [O=Fe^V=NR] center. *Proc. Nat. Acad. Sci. USA* **2012**, early edition.
444. Huo, L.; Fielding, A. J.; Chen, Y.; Li, T.; Iwaki, H.; Hosler, J. P.; Chen, L.; Hasegawa, Y.; Que, L., Jr.; Liu, A., Evidence for a Dual Role of an Active Site Histidine in α-Amino-β-Carboxymuconate-ε-Semialdehyde Decarboxylase. *Biochemistry* **2012**, *51*, just accepted.

Books

- Que, L., Jr. (Ed.) "Metal Cluster in Proteins" Volume 372 of *ACS Symposium Series*, 1988.
- Que, L., Jr. (Ed.), "Physical Methods in Bioinorganic Chemistry. Spectroscopy and Magnetism" University Science Books, Mill Valley, CA, 2000.
- Que, L., Jr.; Tolman, W. B. (Eds.), "Bio-Coordination Chemistry", Volume 8 of "Comprehensive Coordination Chemistry II" (McCleverty, J.; Meyer, T. J., Eds.) Elsevier, Amsterdam, 2004.

Patents

1. B. L. Feringa, M. Lubben, R. M. Hermant, R. S. Twisker, and L. Que, Jr., "Bleach Activation" U.S. Patent Number 5,580,485, December 3, 1996.
2. A.C.M. Appel; R.F. Carina; M.G.J Delroisse; B.L. Feringa, J.J Girerd, R. Hage; R. Kalmeijer; C.F Martens; J.C.J. Peelen; L. Que; T. Swarthoff; D. Tetard; D. Thornthwaite; L. Tiwari; R. Thijssen; R.S. Twisker; S.M. Veerman; G. van der Voet, "Composition and method for bleaching a substrate", WO0012667.
3. A.C.M. Appel; R.F. Carina; M.G.J Delroisse; B.L. Feringa, J.J Girerd, R. Hage; R. Kalmeijer; C.F Martens; J.C.J. Peelen; L. Que; R.G. Smith; T. Swarthoff; D. Tetard; D. Thornthwaite; L. Tiwari; R. Thijssen; R.S. Twisker; S.M. Veerman; G. van der Voet, "Method of treating a textile", WO0012808.
4. L. Que, Jr., C. Kim, J. Kim, and Y. Zang, "Iron Complexes for Bleach Activation and Stereospecific Oxidation" U.S. Patent Number 5,850,086, December 15, 1998.
5. M.E. Branum, B.L. Feringa, G. Roelfes, L. Que Jr, "Pentadentate complexes for DNA cleavage", GB patent appl. C 3907, Filing date 22/4/1999.
6. L. Que, Jr., C. Kim, J. Kim, and Y. Zang, "Iron Complexes for Bleach Activation and Stereospecific Oxidation" U.S. Patent Number 6,107,528, August 22, 2000.
7. L. Que, Jr., R. S. Hanson, L. M. T. Schnaith, "Nucleotide Cleaving Agents and Method" U.S. Patent Number 6,143,879, November 7, 2000.

Invited Lectures at Meetings Since 1984

XXIII International Conference on Coordination Chemistry, Boulder, CO, 8/84
 American Chemical Society National Meeting, Philadelphia, PA, 8/84
 Pacific Basin Chemical Congress, Honolulu, HI, 12/84
 2nd International Conference on Bioinorganic Chemistry, Algarve, Portugal, 4/85
 American Chemical Society National Meeting, Miami Beach, FL, 4/85
 NATO/NSF Workshop on Bioinorganic Chemistry, Noordwijkerhout, Netherlands, 7/85
 SUNY Albany EXAFS Minisymposium, Albany, NY, 4/87
 American Chemical Society Great Lakes Regional Meeting, Columbus, OH, 6/87
 3rd International Symposium on Dioxygen Activation, Tsukuba, Japan, 7/87
 American Chemical Society National Meeting, New Orleans, LA, 8/87
 International Conference on Magnetic Resonance in Biology, Madison, WI, 8/88
 XXVI International Conference on Coordination Chemistry, Porto, Portugal, 8/88
 Pacific Spectroscopy Conference, San Francisco, CA, 10/88
 Gordon Conference on "Metals in Biology", 1/89
 American Society for Biochemistry and Molecular Biology National Meeting,
 San Francisco, CA, 2/89
 4th International Conference on Bioinorganic Chemistry, Cambridge, MA, 7/89
 Gordon Conference on "Inorganic Chemistry", New Hampshire, 8/89
 Pacific Basin Chemical Congress, Honolulu, HI, 12/89
 Royal Society of Chemistry National Meeting, Belfast, Northern Ireland, 4/90
 Roussel-UCLAF Table Ronde on "Nonporphyrinic Iron Oxidation Enzymes", Paris, France, 6/90
 American Chemical Society National Meeting, Washington, DC, 8/90
 International Symposium on Oxygenases and Active Oxygen, Kyoto, Japan, 12/90
 Gordon Conference on "Metals in Biology", 1/91
 1st European Symposium of Enzymes in Deoxyribonucleotide Synthesis, Grenoble, France, 4/91
 5th International Conference on Bioinorganic Chemistry, Oxford, England, 8/91 **25**
 Keystone Conference on the "Inorganic Chemistry/Molecular Biology Interface", Lake Tahoe,
 CA, 3/92
 American Chemical Society National Meeting, San Francisco, CA, 4/92
 5th International Symposium on Dioxygen Activation, College Station, TX, 3/93
 76th CSC Conference, Sherbrooke, Quebec, 6/93
 ICBC6, 6th International Conference on Bioinorganic Chemistry, San Diego, CA, 8/93
 Gordon Conference on "Metals in Biology", Ventura, CA, 1/94
 American Chemical Society National Meeting, San Diego, CA, 3/94
 Unilever Corporation Symposium on "Biomimetic Catalysis", England, 4/94

American Chemical Society Midwest & Great Lakes Joint Regional Meeting, Ann Arbor, MI,
6/94

NATO NMR Workshop, Sintra, Portugal, 6/94

Georgia Bioinorganic Workshop, Athens, GA, 8/94

American Chemical Society National Meeting, Washington, DC, 8/94

University of Minnesota Molecular Biophysics Symposium, Minneapolis, MN, 11/94

University of Minnesota Chemistry Departmental Minisymposium, Minneapolis, MN, 11/94

American Chemical Society National Meeting, Anaheim, CA, 4/95

Florida Catalysis Conference, 4/95

ESF Conference on Protein Radicals, Stockholm, Sweden, 9/95

Pacific Basin Chemical Congress, Honolulu, HI, 12/95

55th Okazaki Conference on Bioinorganic Chemistry, Okazaki, Japan, 2/96

6th International Symposium on Dioxygen Activation, Noordwijkerhout, Netherlands, 4/96

1996 Conference on Oxygen Intermediates in Nonheme Metallobiochemistry, Minneapolis, MN,
6/96

EUROBIC3, 3rd European Biological Inorganic Chemistry Conference, Noordwijkerhout,
Netherlands, 8/96 (plenary lecture)

6th European Inorganic Chemistry Conference, Denmark, 9/96

Gordon Conference on "Metals in Biology", Ventura, CA, 1/97 (keynote lecture)

American Chemical Society National Meeting, San Francisco, 4/97 **50**

ICBIC8, 8th International Conference on Biological Inorganic Chemistry, Yokohama, Japan,
7/97

Dalton Discussions II on Bioinorganic Chemistry, Norwich, England, 9/97 (keynote lecture)

Unilever International Research Workshop, Merseyside, UK, 7/98

Ferritin Workshop, Sheffield, UK, 7/98

American Chemical Society National Meeting, Boston, 8/98

33rd International Conference on Coordination Chemistry, Florence, Italy, 8/98 (plenary lecture)

Riken Conference on Bioinorganic Chemistry, Tokyo, Japan, 4/99

DOE Carbon Management Workshop, Santa Fe, NM, 5/99

American Chemical Society National Meeting, New Orleans, LA, 8/99

EUROBIC5, 5th European Conf. on Biological Inorganic Chemistry, Toulouse, France, 7/2000

International Symposium on New Horizons of Coordination Chemistry Towards the 21st
Century, Kusatsu, Japan, 9/2000

Pacificchem 2000, Honolulu, HI, 12/2000

American Chemical Society National Meeting, San Diego, CA, 4/2001

NRSC-Catalysis/GBB Workshop on Bio-inspired Man-Made Catalysis, The Netherlands, 6/2001

Gordon Conference on Inorganic Chemistry, Newport, RI, 7/2001

10th International Conference on Bioinorganic Chemistry (ICBIC10), Florence, Italy, 8/2001
Korean Chemical Society National Meeting, Pusan, South Korea, 10/2001
Dalton Discussions IV, Kloster Banz, Germany, 1/2002 (keynote lecturer)
American Chemical Society National Meeting, Orlando, FL, 4/2002
Chemical Society of Canada National Meeting, Vancouver, BC, 6/2002
ACS Great Lakes Regional Meeting, Minneapolis, MN, 6/2002
Activation of Dioxygen and Homogeneous Catalysis ADHOC-2002, Atlanta, GA, 6/2002
(keynote speaker)
Inorganic Reaction Mechanisms Gordon Research Conference, Ventura, CA, 2/2003
Annual FASEB Conference, San Diego, CA, 4/2003
Texas A&M Epoxidation Symposium, College Station, TX, 5/2003 **75**
11th International Conference on Bioinorganic Chemistry (ICBIC11), Cairns, Australia, 7/2003
(plenary lecturer)
Taiwan Bioinorganic Symposium 2003, Hsinchu, Taiwan 10/2003
American Chemical Society National Meeting, Anaheim, CA, 3/2004
8th International Symposium on Applied Bioinorganic Chemistry, Hong Kong, China, 4/2004
(plenary lecturer)
36th International Conference on Coordination Chemistry, Merida, Mexico, 7/2004
2nd Asian Bioinorganic Conference, Goa, India, 12/2004 (plenary lecturer)
Metals in Biology Gordon Research Conference, Ventura, CA, 1/2005
Activation of Dioxygen and Homogeneous Catalysis ADHOC-2005, Köln, Germany, 7/2005
(keynote speaker)
12th International Conference on Bioinorganic Chemistry (ICBIC12), Ann Arbor, MI, 8/2005
5th World Congress on Oxidation Catalysis, Sapporo, Japan, 9/2005 (plenary lecturer)
SORST International Symposium on Homogeneous Oxidation Catalysis, Osaka, Japan 10/2005
(plenary lecturer)
Pacifichem 2005, Symposium on Oxygen Activation by Nonheme Metal Centers, Honolulu, HI,
12/2005
ACS Spring '06 National Meeting, Solomon Award Symposium, Atlanta, GA, 3/2006
ACS Spring '06 National Meeting, Wieghardt Award Symposium, Atlanta, GA, 3/2006
ACS Spring '06 National Meeting, Symposium on Dinuclear, Cluster, and Polynuclear
Chemistry: Frontiers in the New Millenium, Atlanta, GA, 3/2006
Conference to Celebrate the 50th Anniversary of Oxygenases, Kyoto, Japan 4/2006
ACS Fall '06 National Meeting, Symposium on Radical Metal Complex Chemistry, 9/2006
2nd IMBG International Meeting, Grenoble, France 9/2006 (plenary lecturer)
ACS Spring '07 National Meeting, Münck Bader Award Symposium, Chicago, IL, 3/2007

- ACS Spring '07 National Meeting, Symposium on Exploring and Exploiting Nature with Biomimetics, Chicago, IL, 3/2007
- 13th International Conference on Bioinorganic Chemistry (ICBIC13), Vienna, Austria, 7/2007 (keynote lecturer)
- ACS Fall '07 National Meeting, Conference on Mechanism in Homogeneous and Heterogeneous Catalytic Epoxidation, Boston, MA, 8/2007 (keynote lecturer)
- Metals in Biology Gordon Research Conference, Ventura, CA, 1/2008
- ACS Spring '08 National Meeting, Alfred Bader Award address, New Orleans, LA, 4/2008
- 38th Int'l Conference on Coordination Chemistry, Jerusalem, 7/2008 (plenary lecturer)
- 100 (16 plenary + keynote)**
- ACS Fall '08 National Meeting, Pfizer Award symposium in honor of Carsten Krebs, Philadelphia, PA, 8/2008
- ACS Spring '09 National Meeting, F. A. Cotton Award symposium in honor of Kenneth Karlin, Salt Lake City, UT, 3/2009
- 44th EuCHEM Conference on Stereochemistry (Bürgenstock Conference), Brunnen, Switzerland, 5/2009
- ICBIC14, 14th International Conference on Bioinorganic Chemistry, Nagoya, Japan, 7/2009
- 42nd IUPAC Conference, Glasgow, Scotland, 8/2009 (**keynote** lecturer)
- ACS Spring '10 National Meeting, Alfred Bader Award symposium in honor of Joan Valentine, San Francisco, CA, 3/2010
- EUROBIC10, 10th European Conf. on Biological Inorganic Chemistry, Thessaloniki, Greece, 6/2010 (**plenary** lecturer)
- ACS Fall '10 National Meeting, Symposia on 'Metals in Biology' and 'Ligand Design and Metal Behavior', Boston, MA, 8/2010.
- ASBIC5, 5th Asian Conf. on Biological Inorganic Chemistry, Kaohsiung, Taiwan 11/2010 (**keynote** lecturer)
- Pacificchem 2010, Symposium on Oxygen Activation and Oxidation Catalysis, Honolulu, HI, 12/2010
- Metals in Biology Gordon Research Conference, Ventura, CA, 1/2011
- Brazilian Chemical Society Annual Meeting, Florianopolis, Brazil, 5/2011 (**plenary** lecturer)
- ACS Spring '12 National Meeting, Symposium on 'Geometric and Electronic Structure Contributions to Reactivity', San Diego, CA, 3/2012
- Activation of Dioxygen and Homogeneous Catalysis ADHOC-2012, Jerusalem, Israel, 9/2012 (**plenary** lecturer)
- CECAM workshop on Spin States in Biochemistry and Inorganic Chemistry, Zaragoza, Spain, 9/2012 (invited lecturer)

IX International Conference on Mechanisms of Catalytic Reactions, St. Petersburg, Russia,
10/2012 (**plenary** lecturer)
ACS Spring '13 National Meeting, Symposium on 'C–H Bond Activation', New Orleans, LA,
4/2013

Invited Seminars Since 1984

Kyoto University, 1/84
Osaka University, 1/84
Iowa State University, 2/84
Lawrence University, 11/84
University of Michigan, 2/85
University of British Columbia, 3/85
Washington State University, 3/85
St. Olaf College, 10/85
Exxon Research and Engineering, 10/85
Princeton University, 10/85
San Francisco State University, 1/86
University of California at Berkeley, 1/86
Georgetown University, 2/86
Colorado State University, 3/86
University of Colorado, 4/86
Massachusetts Institute of Technology, 5/86
Oxford University, 7/86
University of California at San Diego, 9/86
University of South Carolina, 2/87
University of Wisconsin-Milwaukee, 3/87
University of Wisconsin-Madison, 4/87
Northwestern University, 5/87
University of Iowa, 6/87
Ruhr-Universität-Bochum, 7/87
University of Wisconsin-Eau Claire, 9/87
Proctor & Gamble, 12/87
University of California at San Diego, 1/88
University of Southern California, 2/88
California Institute of Technology, 4/88
University of California at Davis, 4/88

University of California at Berkeley, 4/88
University of California at Los Angeles, 5/88
E.I. duPont de Nemours, Inc., 10/88
University of Massachusetts at Amherst, 10/88
University of Louisville, 3/89
University of Illinois at Urbana-Champaign, 3/89
Carnegie-Mellon University, 4/89
Amoco Technology Corporation, 4/89
University of Milan, 5/89
University of Florence, 5/89
Oregon Graduate Center, 6/89
University of Alabama at Tuscaloosa, 3/90
Emory University, 3/90
Indiana-Purdue University at Indianapolis, 3/90
University of Washington, 10/90
Nagoya University, 12/90
Tokyo Institute of Technology, 12/90
Washington State University, 2/91
Haverford College, 3/91
Carleton College, 4/91
Johns Hopkins University, 4/91
Harvard/MIT Inorganic Colloquium, 10/91
Amoco Corporation, 11/91
Ateneo de Manila University, 12/91
Wesleyan University, 2/92
Université Paris Sud, 4/92
Université Joseph Fourier, Grenoble, France, 5/92
Université Paris V, 5/92
University of Stockholm, 5/92
Swedish Agricultural University, 5/92
University of Umeå, 5/92
Indiana University, 4/93
University of Wisconsin, 5/93
Chinese University of Hong Kong, 7/93
Ateneo de Manila University, 7/93
University of the Philippines, Diliman, 7/93
De La Salle University, Manila, 7/93

University of Santo Tomas, Manila, 7/93
 University of the Philippines, Los Baños, 7/93
 University of the Philippines, Diliman, 7/93
 Tsinghua University, China, 9/93
 Nankai University, China, 9/93
 Nanjing University, China, 10/93
 University of Georgia, 12/93
 University of Delaware, 12/93
 Pennsylvania State University, 1/94
 University of Utah, 2/94
 Utah State University, 2/94
 University of South Florida, 3/94
 Columbia University, 4/94
 Boston College, 5/94
 Notre Dame, 9/94
 University of Nebraska, 9/94
 North Dakota State University, 10/94
 University of Leiden, The Netherlands, 11/94
 Unilever, Vlaardingen, The Netherlands, 11/94
 University of Groningen, The Netherlands, 11/94
 University of Toronto, 12/94
 Syntex Corporation, Palo Alto, CA, 2/95
 Stanford University, 2/95
 University of California Santa Cruz, 2/95
 University of Pennsylvania, 3/95
 Princeton University, 3/95
 CENG (CEA-Grenoble), 7/95
 Université Paris-Sud, 7/95
 University of Houston, 10/95
 Texas A & M, 10/95
 Georgia Tech, 11/95
 University of California Davis, 11/95
 University of California Berkeley, 12/95
 University of Illinois at Chicago, 2/96
 University of Colorado at Boulder, 3/96
 Colorado State University, 3/96
 University of Regina, 5/96

75

100

Boston University, 10/96
Leiden University, 11/96
Groningen University, 11/96
DSM Co., 11/96
Nijmegen University, 11/96
University of Utrecht, 11/96
University of Amsterdam, 11/96
New York University, 12/96
University of Southern California, 2/97
Purdue University, 4/97
Northwestern University Summer Inorganic Lectureship, 6/97
University of Illinois at Urbana-Champaign, 10/97
State University of New York Stony Brook, 11/97
Unilever Research Laboratories US, 11/97
Calvin College, 2/98
Hope College, 2/98
Emory University, 3/98
University of Wisconsin Madison, 4/98
University of Wisconsin Eau Claire, 9/98
Chinese University of Hong Kong, 10/98
Hong Kong University of Science and Technology, 10/98
University of Florida, 12/98
University of Florida, 9/99
University of Wisconsin La Crosse, 10/99
Michigan State University, 10/99
University of Chicago, 1/2000
University of Oklahoma, 11/2000
Colorado State University, 3/2001
University of Colorado, 3/2001
Boston College, 4/2001
Seoul National University, 10/2001
Korea University, 10/2001
College of St. Catherine, 11/2001
University of Erlangen-Nürnberg, 1/2002
University of Rochester, 2/2002
University of Wisconsin Madison, 3/2002
College of Saint Benedict, 10/2002

Carnegie Mellon University, 10/2002
University of California, San Diego, 4/2003
University of Texas, Austin, 5/2003
Carnegie Mellon University, 5/2003
University of Groningen, 6/2003
National Chung Kung University, 9/2003
Tamkang University, 10/2003
Academia Sinica, 10/2003
Stockholm University, 11/2003 150
Universita Autonoma Barcelona, 12/2003
California Institute of Technology, 1/2004
Vanderbilt University, 2/2004
University of Delaware, 5/2004
Iowa State University, 10/2004
Harvard/MIT Inorganic Colloquium, 1/2005
University of Heidelberg (3 lectures) 4/2005
University of Washington (Cady Lectureship, 2 lectures), 5/2005
Max Planck Institut für Bioorganische Chemie (6 lectures), 6/2005
University of Illinois at Urbana-Champaign, 10/2005
Yale University, 11/2005
Tsukuba University, 2/2006
Sendai University, 2/2006
Takasago Corporation, 2/2006
Kyushu University 2/2006
Kanazawa University 2/2006
Université Paris-Sud, 9/2006
Stanford University (student invited), 3/2007
Columbia University, 4/2007
University of Wyoming (5 lectures), 6/2007
Nanjing University (2 lectures), 10/2007
Fudan University, Shanghai, China, 10/2007
Canadian Light Source, Saskatoon, SK, Canada, 11/2007
Northwestern University, 2/2008
Cornell University, Baker Symposium, 4/2008 175
University of Chicago, 4/2008
Ateneo de Manila University, 6/2008
Carnegie Mellon University, 10/2008

University of Utrecht, Netherlands, 11/2008
 University of Groningen, Netherlands, 11/2008
 University of Geneva, Switzerland 1/2009
 University of Basel, Switzerland, 1/2009
 University of Bern, Switzerland, 1/2009
 University of Neuchatel, Switzerland, 1/2009
 University of Minnesota, Duluth, 4/2009
 University of California Berkeley (student invited), 5/2009
 Marquette University (Habermann Distinguished Lecture), 9/2009
 UCLA, 10/2009
 U of Tennessee, Knoxville, 11/2009
 University of California Santa Cruz, 1/2010
 University of California Davis, 1/2010
 University of Houston, 4/2010
 Ohio State University, 5/2010
 University of Michigan (Moses Gomberg Lecturer), 9/2010
 University of Houston (student invited), 10/2010
 Kaohsiung Medical University, 11/2010
 Hope College (student invited), 2/2011
 Technical University Berlin, 3/2011
 Humboldt University Berlin, 3/2011
 Georgia Tech, 4/2011
 Emory University, 4/2011
 Universidade Federal do Rio de Janeiro, 5/2011
 University of Montana, October 2011 (postponed)
 Florida State University, October 2011 (postponed)
 Drexel University, November 2011
 Pennsylvania State University December 2011 (postponed)
 University of Toronto, February 2012 (postponed)
 Harvard University (student invited) April 2012
 Brown University, April 2012
 University of Manchester, May 2012
 University of Nottingham, May 2012
 Oxford University, May 2012
 Queen Mary University of London, May 2012
 Caltech, December 2012
 UCLA, December 2012

University of Wisconsin, January 2013

University of Arizona, February 2013