ANITA M. ORENDT

EDUCATION

Ph. D. Physical Chemistry	University of Utah, Salt Lake City, UT	December 1987
B. S. Chemistry (ACS)	University of Pittsburgh, Pittsburgh, PA	April 1980

POSITIONS

Jul 2015 – present	Adjunct Associate Professor of Chemistry, Department of Chemistry, University of Utah
Oct 2013 – present	Assistant Director, Research Consulting & Faculty Engagement Center for High Performance Computing, University of Utah
Jul 2002 – Jul 2015	Adjunct Assistant Professor of Chemistry, Department of Chemistry, University of Utah
Nov 1999 – Oct 2013	Staff Scientist, Molecular Science Support Center for High Performance Computing, University of Utah
Sept 1992 - Aug 1994	Assistant Professor of Chemistry/Physics (half-time) Westminster College of Salt Lake City
Jan – Apr 1992	Adjunct Instructor of Chemistry Westminster College of Salt Lake City
Nov 1987 – Dec 1999	Post Doctoral Research Assistant, Department of Chemistry, University of Utah
Sept 1981 – Oct 1987	Graduate Research Assistant, Department of Chemistry, University of Utah
May – Sept 1980	Research Assistant, Department of Chemistry, University of Pittsburgh

RECENT TEACHING EXPERIENCE

Summer 2010	Lecturer for Math 5900 (Applications of Math in Science for HS MathTeachers); University of Utah
Summer 2008	Lecturer for General Chemistry (Chem 1220); University of Utah
Spring 2003	Lecturer for Physical Chemistry (Chem 3060 – Quantum Mechanics); University of Utah
Sprng 2002	Lecturer for Physical Chemistry (Chem 3060 – Quantum Mechanics); University of Utah
Fall 1999	Teaching Assistant for Physical Chemistry (Chem 3070 - Thermodynamics); also did 6 weeks of the class lectures; University of Utah

PROFESSIONAL SOCIETIES/ACTIVITIES/AWARDS

University of Utah, 2018 District Staff Excellence Award, August 2018
Open Science Grid (OSG) All-Hands Meeting 2018, Local Chair
PEARC (Practice & Experience in Advaned Research Computing) Conference Technical Program Reviewer, 2018, 2019
Rocky Mountain Advanced Computing Consortium (RMACC) HPC Symposium, Program Committee Member, 2017 – 2019
XSEDE Region 8 Campus Champion Leadership, 2016 – present
XSEDE14 Technical Program Reviewer, XSEDE14 Conference, July 2014
XSEDE Campus Champion, Oct 2013 – present
W.W. Epstein Outstanding Educator Award, April 2013, Given by UU Department of Chemistry Graduate Student Advisory Committee
W.W. Epstein Outstanding Educator Award, April 2010, Given by UU Department of Chemistry Graduate Student Advisory Committee

University of Utah ACS Student Affiliate Advisor, 2007 – 2013; recieved Honorable Mention Chapter award in 2008, 2009, 2010; Commendable 2012; Outstanding 2013
Workshop leader, Northern Utah Expanding Your Horizons Workshop, Ogden, UT, Nov 2007 – 2009
ACS Northwest Region Board, Salt Lake Section Director, 2007 – 2008
Chair of Local Salt Lake Section of ACS, 2007, 2009
Chair-Elect of Local Salt Lake Section of ACS, 2006, 2008
Guest Co-editor, *Magnetic Resonance in Chemistry*, Special Issue honoring David M. Grant on the Occasion of his 75th Birthday, appeared March 2006
Workshop Presenter, Science Day at the U, University of Utah, 2005 – 2007, 2011, 2013, 2014 – 2018
National Chemistry Week Coordinator for Salt Lake Local Section of ACS, 2003 – 2005
Member of American Chemical Society (ACS)

AWARDED GRANTS

XSEDE Allocation, Co-PI**,** First Principles Crystal Structure Prediction: Modified Genetic Algorithms and Quantum Espresso, Startup 4-1-2013; Research 10-01-2013

PRESENTATIONS

Co-Presenter, "Measuring the Impact of Facilitation Effort" , Practice & Experience in Advaned Research Computing (PEARC) 2018 Conference, Pittsburgh, PA, July 2018.
Co-Presenter, "HPC Carpentry", Rocky Mountain Advanced Computing Consortium (RMACC) HPC Symposium, Boulder, CO, August 2018.
Co-Presenter, "National Compute Resources for your Research", Rocky Mountain Advanced Computing Consortium (RMACC) HPC Symposium, Boulder, CO, August 2018.
Co-Moderator and Presenter, "Traning and Outreach Opportunities in HPC", Rocky Mountain Advanced Computing Consortium (RMACC) HPC Symposium, Boulder, CO, August 2017.
Co-Moderator and Presenter, "XSEDE Resources and the Campus Champion Program", Rocky Mountain Advanced Computing Consortium (RMACC) HPC Symposium, Boulder, CO, August 2017.
Co-Presenter, "Community of People: ACIREF", PEARC/ARCC Tutorial, Practice & Experience in Advanced Research Computing (PEARC) 17 Conference, New Orleans, LA, July 2017.
Co-Moderator, "XSEDE for Computational Research and the Campus Champion Program", Rocky Mountain Advanced Computing Consortium (RMACC) HPC Symposium, Fort Collins, CO, August 2016.
Co-Moderator, "Coordination of User Training and Support at RMACC Sites", Rocky Mountain Advanced Computing Consortium (RMACC) HPC Symposium, Fort Collins, CO, August 2016.
Tutorial Co-Presenter, "Facilitation: Best Practices on the Front Lines with Reserarchers", Advancing Research Computing on Campuses: Best Practices Workshp, Urbana, IL, March 2016.
Talk, Utah Valley University, November 2014.
Member of Panel Presenatation, Internet2 Joint Technology Exchange, Indianapolis, IN, October 2014.
Poster, 245th ACS National Meeting, New Orleans. LA, April 2013.
Talk, Material Science and Engineering Department Graduate Seminar Class, University of Utah, August 2012.
Poster, 243th ACS National Meeting, San Diego, CA, March 2012.
Two Talks and poster, 31st Oil Shale Symposium, Golden, CO, October 2011.
Talk, Crystal Structure Prediction 5th Blindtest Workshop, Cambridge Crystallographic Data Center, Cambridge, UK, September 2010.
Poster, 235th ACS National Meeting, New Orleans, LA, April 2008.
Talk, 38th Middle Atlantic Regional Meeting (MARM) of the American Chemical Society, Hershey, Pennsylvania; June 2006.
Research Presentation, Los Alamos National Laboratory, Los Alamos, New Mexico; March 1999.

Talk, EPRI Workshop on Chemical Characterization of Atmospheric Organic Aerosols in Support of Health Studies: Current Options and Future Prospects, EPRI, Palo Alto, California; April 1998.
Poster, 39th Annual Experimental NMR Conference, Asilomar, California; March 1998.
Poster, 38th Annual Experimental NMR Conference, Orlando, Florida; March 1997.
Poster, 37th Annual Experimental NMR Conference, Asilomar, California; March 1996.
Poster entitled "^{13}C Dipolar Spectrum of Matrix Isolated Benzyne"; Rocky Mountain Analytical Conference, Denver, Colorado; July 1995.
Poster, 36th Annual Experimental NMR Conference, Boston, Massachusetts; March 1995.
Poster, Sixth Annual Technical Meeting of the Consortium for Fossil Fuel Liquefaction, Wheeling, West Virginia; July 1992.
Poster, 33rd Annual Experimental NMR Conference, Asilomar, California; March 1992.
Poster, Fifth Annual Technical Meeting of the Consortium for Fossil Fuel Liquefaction, Lexington, Kentucky; August 1991.
Poster, Fourth Annual Technical Meeting of the Consortium for Fossil Fuel Liquefaction, Snowbird, Utah; August 1990.
Talk, 1989 International Chemical Congress of Pacific Basin Societies, Honolulu, Hawaii; December 1989.
Poster, Structure and Reactivity Symposium, Austin, Texas; March 1989.
Poster, 29th Annual Experimental NMR Conference, Rochester, New York; April 1988.
Poster, 26th Annual Experimental NMR Conference, Asilomar, California; April 1985.

PUBLICATIONS

77. A.M. Orendt and E. Shaw: "Measuring the Impact of Facilitation Effort" In Proceedings of Practice and Experience in Advanced Research Computing (PEARC'18). ACM, New York, NY, USA, 2018 . https://doi.org/10.1145/3219104.3219146

76. T. H Fletcher, R. J. Pugmire, M. S. Solum, C. L. Mayne, A. M. Orendt, J. C. Facelli: "Chemical and Structural Characterization of Oil Shale from the Green River Formation" in "Utah Oil Shale: Science, Technology, and Policy Perspectives" J. P. Spinti, Editor, CRC Press, Boca Raton, FL, **2017**, pages 87-118.

75. A. M. Reilly, et al: "Report on the sixth blind test of organic crystal structure prediction methods", *Acta Cryst. B: Structural Science, Crystal Engineering and Materials*, 72, **2016**, 439-459

74. Y. Zhang, X.-B. Li, A. M. Fleming, J. Dood, A. A. Beckstead, A. M. Orendt, C. J. Burrows, and B. Kohler: "UV-Induced Proton-Coupled Electron Transfer in Cyclic DNA Miniduplexes," *J. Am. Chem. Soc.*, 138, **2016**, 7395–7401

73. J. Zu, A.M. Fleming, A.M. Orendt, C.J. Burrows: "pH-Dependent equilibrium between 5-guanidinohydantoin and minoallantoin affects nucleotimde insertion opposite the DNA lesion", *J. Org. Chem.*, 81, **2016**, 351-9.

72. A.M. Lund, G.I. Pagola, A.M. Orendt, M.B. Ferraro, J.C. Facelli: "Crystal Structure Prediction from First Principles: The Crystal Structures of Glycine", *Chem. Phys. Lett*, 626, **2015**, 20-24.

71. A.M. Fleming, O. Alshykhly, A.M. Orendt, C.J. Burrows: "Computational studies of electronic circular dichroism spectra predict absolute configuration assignments for the guanine oxidation product 5-carboxamido-5-formamido-2-iminohydantoin", *Tetahedron Letters*, 56, **2015**, 3191-3196.

70. R. Jadulco, M. Koch, T. Kakule, E. Schmidt, A. Orendt, H. He, J. Janso, G. Carter, E. Larson, C. Pond, T. Matainaho, L. Barrows: "Isolation of Pyrrolocins A-C: cis- and trans-Decalin Tetramic Acid Antibiotics from an Endophytic Fungal-Derived Pathway", *Journal of Natural Products*, 77, **2014**, 2537 - 2544.

69. M.S. Solum, C.L. Mayne, A.M. Orendt, R.J. Pugmire, J. Adams, T.H. Fletcher: "Characterization of Macromolecular Structure Elements from a Green River Oil Shale, I. Extracts", *Energy & Fuels*, 28, **2014**, 453-465.

68. A.M. Fleming, A.M. Orendt, Y. He, J. Zhu, R. K. Dukor, C.J. Burrows: "Reconciliation of chemical, enzymatic, spectroscopic and computational data to assign the absolute configuration of the DNA base lesion spiroiminodihydantoin", *J. Am. Chem. Soc.*, 135, **2013**, 18191-18204.

67. A.M. Lund, A.M. Orendt, G.I. Pagola, M.B. Ferraro, J.C. Facelli: "Optimization of Crystal Structures of Archetypical Pharmaceutical Compounds: A plane wave DFT-D study using Quantum Espresso", *Crystal Growth & Design*, 13, **2013**, 2181−2189.

66. A.M. Orendt, I.S.O. Pimienta, S.R. Badu, M.S. Solum. R.J. Pugmire, J.C. Facelli, D.R. Locke, K.W. Chapman, P.J. Chupas, R.E. Winans: "Three Dimensional Structure of the Siskin Green River Oil Shale Kerogen Model: A Comparison between Calculated and Observed Properties", *Energy & Fuels*, 27(2), **2013**, 702-710.

65. S. Badu, I.S.O. Pimienta, A.M. Orendt, R.J. Pugmire, J.C. Facelli: "Modeling of Asphaltenes: Assessment of Sensitivity of ^{13}C SSNMR to Molecular Structure", *Energy & Fuels*, 26, **2012**, 2161-2167.

64. D.A. Bardwell, et al.,: "Towards crystal structure prediction of complex organic compounds – a report on the fifth blind test", *Acta. Cryst.*, B67, **2011**, 535-551.

63. K. Shahrokh, A.M. Orendt, G.S. Yost, T.E. Cheatham, III "Quantum Mechanically Derived AMBER-Compatible Heme Parameters for the Cytochrome P450 Catalytic Cycle", *J. Comp. Chem.*, 33, **2011**, 119-133.

62. M.D. Halling, A.M. Orendt, M. Strohmeier, M.S. Solum, V.M. Tsefrikas, T. Hirao, L.T. Scott, R.J. Pugmire, D.M. Grant, "Solid-State ^{13}C NMR Investigations of 4,7-Dihydro-1H-tricyclopenta[*def*,*jkl*,*pqr*]triphenylene (Sumanene) and Indeno[1,2,3-*cd*]fluoranthene: Buckminsterfullerene Moities", *Phys Chem Chem Phys*, 12, **2010**, 7934-7941.

61. M.C. Masiker, C.L. Mayne, B.J. Boone, A.M. Orendt, E.M. Eyring: "7Li NMR chemical shift titration and theoretical DFT calculation studies: solvent and anion effects on second-order complexation of 12-crown-4 and 1-aza-12-crown-4 with Lithium cation in several aprotic solvents", *Magnetic Resonance in Chemistry*, 48, **2010**, 94-100.

60. M.B. Ferraro, A.M. Orendt and J.C. Facelli: "Parallel Genetic Algorithms for Crystal Structure Prediction: Successes and Failures in Predicting Bicalutamide Polymorphs", ICIC 2009, LNCS 5754 proceedings, D.S. Huang et al, editors; Springer-Verlag Publishers, **2009**, 120-129.

59. U. Maran, D. Britt, C.B. Fox, J.M. Harris, A.M. Orendt, H. Conley, R. Davis, V. Hlady, P.J. Stang: "Self-Assembly of a Triangle-Shaped, Hexaplatinum-Incorporated, Supramolecular Amphiphile in Solution and at Interfaces", *Chemistry – A European Journal*, 15, **2009**, 8566-8577.

58. S. Kim, A.M. Orendt, M.B. Ferraro, J.C. Facelli: "Crystal Structure Prediction (CSP) of Flexible Molecules using Parallel Genetic Algorithms with a Standard Force Field", *J. Comp. Chem.*, 30, **2009**, 1973-1985.

57. A.M. Orendt and J.C. Facelli: "Chemical Shifts & Solid-State Molecular-Level Structure", *NMR Crystallography*, R.K. Harris, R.E. Wayslishen and M.J. Duer, editors; Wiley & Sons, **2009**, pages 99-111.

56. J.C. Facelli and A.M. Orendt: "Chemical Shifts: Basics", *NMR Crystallography*, R.K. Harris, R.E. Wayslishen and M.J. Duer, editors; Wiley & Sons, **2009**, pages 53-61.

55. U. Maran, H. Conley, M. Frank, A.M. Arif, A.M. Orendt, D. Britt, V. Hlady, R. Davis, P.J. Stang: "Giant Micelles of Organoplatinum(II) Gemini Amphiphiles", *Langmuir*, 24, **2008**, 5400-5410.

54. M. Krishnamurthy, K. Simon, A.M. Orendt, P.A. Beal: "Macrocyclic Helix-Threading Peptides for Targeting RNA", *Angew. Chem. Int. Ed.*, 46, **2007**, 7044.

53. A.M. Orendt and J.C. Facelli: "Solid State Effects on NMR Chemical Shifts", *Annual Reports of NMR Spectroscopy*; G.A. Webb, Editor; Elsevier Ltd; Volume 62, **2007**, pages 116-178.

52. Z. Ma, M.D. Halling, M.S. Solum, J.K. Harper, A.M. Orendt, J.C. Facelli, R.J. Pugmire, D.M. Grant A.W. Amick, L.T. Scott: "Ring Current Effects in a Crystal. Evidence from ^{13}C Chemical Shielding Tensors for Intermolecular Shielding and Molecular Magnetic Susceptibility in 4,7-di-t-butylacenaphthene versus 4,7-di-t-butylacenaphthylene ", *J. Phys. Chem.*, 111, **2007**, 2020.

51. A.M. Orendt, S.W. Roberts, J.D. Rainier: "The Role of Asynchronous Bond Formation in the Diastereoselective Epoxidation of Cyclic Enol Ethers-A Density Functional Theory Study", *J. Org. Chem.*, 71, **2006**, 5567.

50. I. Zharov, Z. Havlas, A.M. Orendt, D.H. Barich, D.M. Grant, J. Michl: "$CB_{11}Me_{11}$ Boronium Ylides: Carba-*closo*-dodecaboranes with a Naked Boron Vertex", *J. Am. Chem. Soc.*, 128, **2006**, 6089.

49. C. Chevallier, T.S. Bugni, X. Feng, M.K. Harper, A.M. Orendt, C.M. Ireland: "Tedanolide C: a potent new 18-membered ring cytotoxic macrolid isolated from the Papua New Guinea marine sponge *Ircinia* sp. ", *J. Org. Chem.*, 71, **2006**, 2510.

48. A.M. Orendt: "Revisiting the calculation of ^{13}C chemical shift tensors in cadmium acetate dihydrate with EIM and EIM/Cluster methods", *Magnetic Resonance in Chemistry*, 44, **2006**, 385.

47. A.M. Orendt B. Haymore, D. Richardson, S. Robb, A. Sanchez Alvarado, J.C. Facelli, "Design, Implementation, and Deployment of a Commodity Cluster for Periodic Comparisons of Gene Sequences" in *High Performance Computing: Paradigm and Infrastructure*; L.T. Yang and M. Guo, Editors; John Wiley and Sons; **2006**, pages 733-744.

46. N. DiFiori, A.M. Orendt, M.C. Caputo, M.B. Ferraro, J.C. Facelli: "Modeling Solid State Effects on NMR Chemical Shifts using Electrostatic models", *Magnetic Resonance in Chemistry*, 42, **2004**, S41-S47.

45. I. Zharov, T.-C. Weng, A.M. Orendt, D.H. Barich, J. Penner-Hahn, D.M. Grant, Z. Havlas, J. Michl: "Metal Cation – Methyl Interactions in $CB_{11}Me_{12}^-$ Salts of Me_3Ge^+, Me_3Sn^+, and Me_3Pb^+", *J. Am. Chem. Soc.*, 126, **2004**, 12033-12046.

44. T. Kameda, G. McGeorge, A.M. Orendt, D.M. Grant: "^{15}N Chemical Shifts of the Triclinic and Monoclinic Crystal Forms of Valinomycin", *J.Biomolecular NMR*, 29, **2004**, 281-288.

43. M.S. Solum, J.M. Veranth, Y.J. Jiang, A.M. Orendt, A.F. Sarofim, R.J. Pugmire: "The Study of Anthracene Aerosols by Solid State NMR and ESR", *Energy and Fuels,* 17, **2003**, 738-743.

42. J.S. Clawson, M. Strohmeier, D. Stueber, A.M. Orendt, D.H. Barich, B. Asay, M.A. Hiskey, R.J. Pugmire, D.M. Grant: "The ^{15}N Chemical Shift Tensors of β-HMX", *J. Phys. Chem. A,* 106, **2002**, 6352.

41. A.M. Orendt: "Fullerenes and Related Materials as Studied by Solid State NMR", in *Encyclopedia of NMR Supplement,* D.M. Grant and R.K. Harris, Editors, J. Wiley: London, **2002**, Volume 9, pap 551-558.

40. D. Stueber, A.M. Orendt, J.C. Facelli, D.M. Grant, R.W. Parry: "Carbonates, Thiocarbonates, and the Corresponding Monoalkyl Derivatives: 3. The ^{13}C Chemical Shift Tensors in Potassium Carbonate, Bicarbonate and Related MonoMethyl Derivatives", *Solid State NMR,* 22, **2002**, 29.

39. J.C. Facelli, B.K. Nakagawa, A.M. Orendt, R.J. Pugmire: "Cluster Analysis of ^{13}C Chemical Shift Tensor Principal Values in Polycyclic Aromatic Hydrocarbons", *J. Phys. Chem. A,* 105, **2001**, 7468.

38. M. Strohmeier, A.M. Orendt, D.W. Alderman, D.M. Grant: "Investigations of the Polymorphs of Dimethyl-3,6-Dichloro-2,5-Dihydroxyterephthalate by ^{13}C Solid-State NMR Spectroscopy", *J. Am. Chem. Soc.*, 123, **2001**, 1713.

37. D. Stueber, D. Patterson, C.L. Mayne, A.M. Orendt, D.M. Grant, R.W. Parry: "Carbonates, Thiocarbonates, and the Corresponding Mono Alkyl Derivatives.1.Their Preparation and Isotropic ^{13}C NMR Chemical Shifts", *Inorg. Chem.,* 40, **2001**, 1902.

36. D.H. Barich, A.M. Orendt, R.J. Pugmire, D.M. Grant: "Carbon-13 Shift Tensors in Polycyclic Aromatic Compounds. 9. Biphenylene", *J. Phys. Chem. A,* 104, **2000**, 8290.

35. A.M. Orendt, J.C. Facelli, S. Bai, A. Rai, M. Gossett, L.T. Scott, J. Boerio-Goates, R.J. Pugmire, D.M. Grant: "Carbon-13 Shift Tensors in Polycyclic Aromatic Compounds. 8. A Low-Temperature NMR Study of Coronene and Corannulene", *J. Phys. Chem. A,* 104, **2000**, 149.

34. A.M. Orendt, J.C. Facelli, D.M. Grant: "A Theoretical Study of the Acetate ^{13}C Chemical Shift Tensor in Cadmium Acetate Dihydrate", *Chem. Phys. Lett.*, 302, **1999**, 499.

33. A.M. Orendt, J.C. Facelli, Y.J. Jiang, D.M. Grant: "NMR at Cryogenic Temperatures: A ^{13}C NMR Study of Ferrocene", *J. Phys. Chem. A,* 102, **1998**, 7692.

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31. F. Liu, A.M. Orendt, D.W. Alderman, D.M. Grant: "Carbon-13 Chemical Shift Tensors in Pentaerythritol", *J. Am. Chem. Soc.,* 119, **1997**, 8981.

30. M. Strohmeier, A.M. Orendt, J.C. Facelli, M.S. Solum, R.J. Pugmire, R.J. Parry, D.M. Grant: "Solid state ^{15}N and ^{13}C NMR Study of Several Metal 5,10,15,20-Tetraphenylporphyrin Complexes", *J. Am. Chem. Soc.,* 119, **1997**, 7114.

29. J.C. Facelli, A.M. Orendt, Y.J. Jiang, R.J. Pugmire, D.M. Grant: "Carbon-13 Chemical Shift Tensors and Molecular Conformation of Anisole", *J. Phys. Chem.*, 100, **1996**, 8268.

28. A.M. Orendt, J.C. Facelli, J.G. Radziszewski, W.J. Horton, D.M. Grant, J. Michl: "^{13}C Dipolar NMR Spectrum of Matrix-Isolated *o*-Benzyne-*1,2-*$^{13}C_2$", *J. Am. Chem. Soc*., 118, **1996**, 846.

27. A.M. Orendt: "Chemical Shift Tensor Measurement in Solids", in *Encyclopedia of NMR*, D.M. Grant and R.K. Harris, Editors, J. Wiley: London, **1996**.

26. A.M. Orendt, R. Dunkel, W.J. Horton, R.J. Pugmire, D.M. Grant: "Computerized Analysis of 2D INADEQUATE Spectra to Assign Chemical Shifts in Aromatic Compounds", *Magn. Reson. in Chem*., 33, **1995**, 803.

25. J.C. Facelli, J.Z. Hu, A.M. Orendt, A.M. Arif, R.J. Pugmire, D.M. Grant: "Solid State ^{13}C NMR, X-ray, and Quantum Mechanical Studies of the Carbon Chemical Shift Tensors of *p*-Tolyl Ether", *J. Phys. Chem*., 98, **1994**, 12186.

24. J.Z. Hu, A.M. Orendt, D.W. Alderman, R.J. Pugmire, C. Ye, D.M. Grant: "Measurement of ^{13}C Chemical Shift Tensor Principal Values with a Magic Angle Turning Experiment", *Solid State NMR*, 3, **1994**, 181.

23. R.J. Pugmire, J.Z. Hu, D.W. Alderman, A.M. Orendt, C. Ye, D.M. Grant: "The Measurement of ^{13}C Chemical Shift Tensors in Complex Polycyclic Aromatic Compounds and Coals by an Extremely Slow Spinning MAS Experiment", *Prepr. Paper - Am. Chem. Soc. Div. Fuel Chem*., 39, **1994**, 42.

22. J.Z. Hu, A.M. Orendt, D.W. Alderman, C. Ye, R.J. Pugmire, D.M. Grant: "Improvements to the Magic Angle Hopping Experiment", *Solid State NMR*, 2, **1993**, 235.

21. R.J. Pugmire, J.Z. Hu, D.W. Alderman, A.M. Orendt, C. Ye, D.M. Grant: "The Measurement of ^{13}C Chemical Shift Tensors in Complex Polycyclic Aromatic Compounds and Coals by an Extremely Slow Spinning MAS Experiment", 1993 International Conference on Coal Science Proceedings, England.

20. R.H. Contreras, R.R. Biekofsky, D.G. de Kolawewski, A.M. Orendt, J.C. Facelli: "Effects of Electronic Resonance Interactions on Methoxy Group NMR Parameters. Theoretical and Experimental Study of Substituted 2-Methoxypyridines", *J. Phys. Chem*., 97, **1993**, 91.

19. A.M. Orendt, M.S. Solum, N.K. Sethi, C. D. Hughes, D. M. Grant, R. J. Pugmire: "Measurement of ^{13}C Chemical Shielding Anisotropy in Coals" in *Advances in Chemistry Series No. 229: Magnetic Resonance of Solid Carbonaceous Fuels*; R. E. Botto and Y. Sanada, Editors; ACS Publications: Washington, DC, **1993**, pp 419-439.

18. J.C. Facelli, A.M. Orendt, R.H. Contreras, M.F. Tufro, D.G. de Kolawewski: "Ab Initio and ^{17}O NMR Studies of the Substituent Effect on the Tautomeric Equilibrium in 6-X-(1-H)-2-Pyridones", *J. Phys. Chem*., 96, **1992**, 7895.

17. J.Z. Hu, R.J. Pugmire, A.M. Orendt, D.M. Grant, C. Ye: "Selective Saturation and Inversion of Multiple Resonances in High Resolution Solid State ^{13}C CP/MAS Experiments using Slow Spinning CP/MAS and Tailored DANTE Pulse Sequences", *Solid State NMR*, 1, **1992**, 185.

16. J. Z. Hu, R.J. Pugmire, A.M. Orendt, D.M. Grant, C. Ye: "Selective Saturation and Inversion of Multiple Resonances in High Resolution Solid State Carbon-13 CP/MAS Experiments", *Prepr. Paper - Am. Chem. Soc. Div. Fuel Chem*., 37, **1992**, 646.

15. A.M. Orendt, M.S. Solum, N.K. Sethi, R.J. Pugmire, D.M. Grant: "^{13}C NMR Techniques for Structural Studies of Coals and Coal Chars" in *Advances in Coal Spectroscopy*; H. L. C. Meuzelaar, Editor; Plenum Press: New York, **1992**, pp 215 - 254.

14. R.J. Pugmire, A.M. Orendt, J.C. Facelli, D.M. Grant: "Comparison of ^{13}C Chemical Shielding Anisotropy in Model Compounds and Coals with Theoretical Values", 1991 International Conference on Coal Science Proceedings, England, pg. 72.

13. A.M. Orendt, N.K. Sethi, J.C. Facelli, W.J. Horton, R.J. Pugmire, D.M. Grant: "^{13}C Chemical Shift Tensors in Aromatic Compounds. 4. Substituted Naphthalenes", *J. Am. Chem. Soc.*, 114, **1992**, 2832.

12. A.M. Orendt, R.R. Biekofsky, A.B. Pomilio, R. . Contreras, J.C. Facelli: "Ab Initio and ^{17}O NMR Study of Aromatic Compounds with Dicoordinate Oxygen Atoms. 2. Intramolecular Hydrogen Bonding in Hydroxy- and Methoxybenzene Derivatives", *J. Phys. Chem.*, 95, **1991**, 6179.

11. R.R. Biekofsky, A.B. Pomilio, R.H. Contreras, A.M. Orendt, J.C. Facelli: "Ab Initio and ^{17}O NMR Study of Aromatic Compounds with Dicoordinate Oxygen Atoms. 1. Methoxy- and Methylenedioxybenzene Derivatives", *J. Phys. Chem.*, 94, **1990**, 7418.

10. A.M. Orendt, J. Michl, J. Reiter: "On Triazoles. XIV. ^{15}N NMR Study of Substituted 5-Amino-1,2,4-triazoles", *Magn. Reson. in Chem.*, 27, **1989**, 1.

9. A.M. Orendt, J.C. Facelli, A.J. Beeler, K. Reuter, W.J. Horton, P. Cutts, D.M. Grant, J. Michl: "Low Temperature ^{13}C Magnetic Resonance in Solids. 8. Chemical Shielding Anisotropy of Olefinic Carbons", *J. Am. Chem. Soc.*, 110, **1988**, 3386.

8. A.M. Orendt, B.R. Arnold, J.G. Radziszewski, J.C. Facelli, K.D. Malsch, H. Strub, D.M. Grant, J. Michl: "^{13}C NMR of Cyclobutadiene-$^{13}C_2$ in an Argon Matrix: Interconversion of Valence Tautomers", *J. Am. Chem. Soc.*, 110, **1988**, 2648.

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