

October 26, 2009

**PUBLICATIONS (190+ external, unclassified)**

1. "The Structure Implication in Metalloporphyrins of the 1590 cm<sup>-1</sup> Anomalously Polarized Resonance Raman Line," Felton, R. H.; Yu, N.-T.; O'Shea, D. C.; Shelnett, J. A., *J. Am. Chem. Soc.* **96**, 3675 (1974).
2. "Resonance Raman Spectra of Manganese(III) Etioporphyrin I," Shelnett, J. A.; O'Shea, D. C.; Yu, N.-T.; Cheung, L. D.; Felton, R. H., *J. Chem. Phys.* **64**, 1156 (1976).
3. "Effects of Jahn-Teller Instability and Excited State Nuclear Distortion on Resonance Raman Excitation Profiles: Theory and Experiment," Shelnett, J. A.; Yu, N.-T.; Chang, R. C. C.; Cheung, L. D.; Felton, R. H., in "Proceedings of the Fifth International Conference on Raman Spectroscopy," (eds. E. Schmid, *et al.*), Freiburg, p. 336, H. F. Schulz Publ., Freiburg, 1976).
4. "Effects of Jahn-Teller Instability and Excited State Nuclear Distortion on Resonance Raman Excitation Profiles of Copper Tetraphenylporphyrin," Shelnett, J. A.; O'Shea, D. C., *Biophys. J.* **17**, 252a (1977).
5. "Resonance Raman Spectra of Metalloporphyrins. Effects of Jahn-Teller Instability and Nuclear Distortion on Excitation Profiles of Stokes Fundamentals," Shelnett, J. A.; Cheung, L. D.; Chang, R. C. C.; Yu, N.-T.; Felton, R. H., *J. Chem. Phys.* **66**, 3387 (1977).
6. "Solid-Phase Epitaxy of Implanted Silicon by CW Ar Ion Laser Irradiation," with Williams, J. S.; Brown, W. L.; Leamy, H. J.; Poate, J. M.; Rodgers, J. W.; Rousseau, D. L.; Rozgonyi, G. A.; Shelnett, J. A.; Sheng, T. T., *Appl. Phys. Letts.* **33**, 542 (1978).
7. "Resonance Raman Spectra of Copper Tetraphenylporphyrin: Effects of Strong Vibronic Coupling on Excitation Profiles and the Absorption Spectrum," Shelnett, J. A.; O'Shea, D. C., *J. Chem. Phys.* **69**, 5361 (1978).
8. "An Electronic Interaction Model for Hemoglobin Cooperativity: I. Evidence from Raman Difference Spectroscopy," Rousseau, D. L.; Shelnett, J. A.; Friedman, J. M.; Simon, S. R., in "Hemoglobin and Oxygen Binding" Ho, C., ed. (Elsevier: New York) 1982.
9. "An Electronic Interaction Model for Hemoglobin Cooperativity: II. The Elements of the Model," Shelnett, J. A.; Rousseau, D. L.; Friedman, J. M.; Simon, S. R., *Biophys. J.* **25**, 39a (1979).
10. "Resonance Raman Spectroscopy of Copper Tetraphenylporphyrin Isolated in a Nitrogen Matrix," O'Shea, D. C.; Yang, J. L.; Shelnett, J. A., *Biophys. J.* **25**, 149a (1979).
11. "Protein Influence on the Heme in Cytochrome c: Evidence from Raman Difference Spectroscopy," Shelnett, J. A.; Rousseau, D. L.; Dethmers, J. K.; Margoliash, E., *Proc. Natl. Acad. Sci. USA* **76**, 3865 (1979).
12. "Protein-Heme Interaction in Hemoglobin: Evidence from Raman Difference Spectroscopy," Shelnett, J. A.; Rousseau, D. L.; Friedman, J. M.; Simon, S. R., *Proc. Natl. Acad. Sci. USA* **76**, 4409 (1979).
13. "Interference Between Intra- and Inter-Manifold Couplings in Resonance Raman Spectra of Metalloporphyrins," Zgierski, M. Z.; Shelnett, J. A.; Pawlikowski, M., *Chem. Phys. Lett.* **68**, 262 (1979).
14. "Charge Transfer Stabilization of Hemoglobin Structures," Rousseau, D. L.; Shelnett, J. A.; Friedman, J. M.; Henry, E. R.; Simon, S. R., *Biophys. J.* **32**, 83 (1980).
15. Liquid and Solid Phase Regrowth of Si by Laser Irradiation and Thermally Assisted Flash Annealing," Poate, J. M.; Bean, J. C.; Brown, W. L.; Cohen, R. L.; Feldman, L. C.; Leamy, H. J.; Rodgers, J. W.; Rousseau, D. L.; Rozgonyi, G. A.; Shen, T. T.; Shelnett, J. A.; West, K. W.; Williams, J. S., *Radiation Effects* **48**, 167 (1980).

16. "The Raman Excitation Spectra and Absorption Spectrum of a Metalloporphyrin in an Environment of Low Symmetry," Shelnett, J. A., *J. Chem. Phys.* **72**, 3948 (1980).
17. "Methemoglobin Imidazole: Evidence Against an IHP-Induced Change in Quaternary Structure," Rousseau, D. L.; Shelnett, J. A.; Simon, S. R., *FEBS Letts.* **111**, 235 (1980).
18. "Raman Difference Spectroscopy of Tertiary and Quaternary Structure Changes in Methaemoglobins," Rousseau, D. L.; Shelnett, J. A.; Henry, E. R.; Simon, S. R., *Nature* **285**, 49 (1980).
19. "A Charge Transfer Mechanism for Cooperative O<sub>2</sub> Binding in Hemoglobin," Shelnett, J. A., Proc. of the 7th Intl. Conference on Raman Spectroscopy, ed. W. F. Murphy, (North-Holland, 1980) p. 516.
20. "Raman Difference Spectroscopic Studies of Tertiary and Quaternary Structure Changes in Methemoglobins," Henry, E. R.; Rousseau, D. L.; Shelnett, J. A.; Simon, S. R., *Fed. Proc.* **39**, 1889 (1980).
21. "Raman Difference Spectroscopy from Deoxyhemoglobins as a Probe of the Energetics of Cooperativity" with Rousseau, D. L.; Simon, S. R., *Fed. Proc.* **39**, 1890 (1980).
22. "Conformation Differences Among Cytochromes  $\underline{c}$  that Influence the Properties of the Heme," Shelnett, J. A.; Rousseau, D. L.; Dethmers, J.; Margoliash, E., *Fed. Proc.* **39**, 2150 (1980).
23. "A Simple Interpretation of Raman Excitation Spectra of Metalloporphyrins," Shelnett, J. A., *J. Chem. Phys.* **74**, 6644-6657 (1981).
24. "The Structure of Molecular Complexes of Copper Uroporphyrin with Aromatic Heterocycles," Shelnett, J. A., *J. Am. Chem. Soc.* **103**, 4275-4277 (1981).
25. "Protein Influences on Porphyrin Structure in Cytochrome c: Evidence from Raman Difference Spectroscopy," Shelnett, J. A.; Rousseau, D. L.; Dethmers, J.; Margoliash, E., *Biochemistry* **20**, 6485-6497 (1981).
26. "Quaternary Transformation-Induced Changes at the Heme in Deoxyhemoglobins," Ondrias, M. R.; Rousseau, D. L.; Shelnett, J. A.; Simon, S. R., *Biochemistry* **21**, 3428 (1982).
27. "Metal Effects on Metalloporphyrin  $\pi$ - $\pi$  Charge-Transfer Complexes with Aromatic Heterocycles," Shelnett, J. A., *J. Am. Chem. Soc.* **105**, 774 (1983).
28. "Metal Effects on Metalloporphyrins and on Their  $\pi$ - $\pi$  Charge-Transfer Complexes with Aromatic Acceptors: Urohemin Complexes," Shelnett, J. A., *Inorg. Chem.* **22**, 2535 (1983).
29. "Molecular Complexes of Copper Uroporphyrin with Aromatic Acceptors," Shelnett, J. A., *J. Phys. Chem.* **87**, 605 (1983).
30. "Raman Difference Spectroscopy of Heme-Linked Ionizations in Cytochrome  $\underline{c}$  Peroxidase," Shelnett, J. A.; Satterlee, J. D.; Erman, J. E., *J. Biol. Chem.* **258**, 2168 (1983).
31. "Unusual Coordination and Metal Ligand Geometry of a Vanadyl Porphyrin in Aqueous Solution," Shelnett, J. A.; Dobry, M. M., *J. Phys. Chem.* **87**, 3012 (1983).
32. "Raman Spectroscopic Study of Scandium in Sodium Silicate Glasses," Nelson, C.; Tallant, D. R.; Shelnett, J. A., *J. Non-Cryst. Sol.* **68**, 87, (1984).
33. "Correlations Between Core Size and Wavelength of the  $\alpha$  Band for Nonhyper Metalloporphyrins," Shelnett, J. A.; Ondrias, M. R., *Inorg. Chem.* **23**, 1175 (1984).
34. "Photoreduction of Methyl Viologen Sensitized by Dihydroxy Tin(IV) Uroporphyrins," Shelnett, J. A., *J. Am. Chem. Soc.* **105**, 7179 (1983).

35. "Core Expansion and Electronic Structure of the Porphyrin in Neutral pH Form of Copper Cytochrome  $c$ " Shelnett, J. A.; Straub, K. D.; Rentzepis, P. M.; Gouterman, M.; Davidson, E. R., *Biochemistry* **23**, 3946 (1984).
36. "Chloroquine Interaction with Ferric Uroporphyrin in Solution," with Satterlee, J. D.; Constantinidis, I., *Inorg. Chim. Acta* **79**, 172 (1983).
37. "A Resonance Raman Study of *Ambystroma Tigrinum* Hemoglobins: Evidence for Intraspecies Hemepocket Variations," Ondrias, M. R.; Carson, S. D.; Wood, S. C.; Shelnett, J. A., *Comp. Biochem. Physiol.* **79B**, 637 (1984).
38. "Electronic Structure of Metallouroporphyrins and Their  $\pi$ - $\pi$  Dimers," Shelnett, J. A., *J. Phys. Chem.* **88**, 4988 (1984).
39. "Aggregation of Uroporphyrins I and its Metal Derivatives in Aqueous Solution: Raman Difference Spectroscopy and Absorption Spectroscopy," Shelnett, J. A.; Dobry, M. M.; Satterlee, J. D., *J. Phys. Chem.* **88**, 4980 (1984).
40. "Studies of Urohemin in Aqueous Solution: Thermodynamics of Self- Association and Electronic Properties of Two Species Detected by Proton NMR Spectroscopy." Satterlee, J. D.; Shelnett, J. A., *J. Phys. Chem.* **88**, 5487 (1984).
41. "Electronic Structure of the Porphyrin Ring in an Electrostatically Bound  $\pi$ - $\pi$  Complex: Methylviologen-Metallouroporphyrin Complexes," Shelnett, J. A.; *J. Phys. Chem.* **88**, 6121 (1984).
42. "Substituent Effects on the Electronic Structure of Metalloporphyrins: A Quantitative Analysis in Terms of Four-Orbital Model Parameters," Shelnett, J. A.; Ortiz, V., *J. Phys. Chem.* **89**, 4733 (1985).
43. "Characterization of pH Dependent Axial Ligation Changes of Monomer and Dimer Forms of Iron (III) Uroporphyrin I in Aqueous Solution," Satterlee, J. D.; Shelnett, J. A., *Inorg. Chim. Acta* **106**, 165 (1985).
44. "Raman Spectroscopy of Polymers of Metal-Protoporphyrin Free Acids on Metal Electrodes," Shelnett, J. A.; Ginley, D. S., *J. Phys. Chem.* **89**, 5473 (1985).
45. "Heme-linked Ionizations in Horseradish Peroxidase Detected by Raman Difference Spectroscopy," Shelnett, J. A.; Alden, R. G.; Ondrias, M. R., *J. Biol. Chem.* **261**, 1720 (1986).
46. "Heme-linked Ionizations of Myeloperoxidase Detected by Raman Difference Spectroscopy: A Comparison with Plant and Yeast Peroxidases," Stump, R. F.; Deanin, G. G.; Oliver, J. M.; Shelnett, J. A., *Biophys. J.* **51**, 605 (1987).
47. "Synthesis and Vibrational Characterization of Polymeric Copper-Coproporphyrin," Shelnett, J. A.; Ginley, D. S., *J. Polym. Sci. Part A, Chem.* **24**, 1717 (1986).
48. "Four- and Five-Coordinate Species in Nickel-Reconstituted Hemoglobin and Myoglobin: Raman Identification of the Ni- Histidine Stretching Mode," Shelnett, J. A.; Alston, K.; Yamamoto, T.; Ho, J.-T.; Yu, N.-T.; Rifkind, J. M., *Biochemistry* **25**, 620 (1986).
49. "Resonance Raman Investigation of Transient Photo-induced Ligation Changes in Nickel Octaethyl Porphyrin," Findsen, E. W.; Shelnett, J. A.; Ondrias, M. R.; Friedman, J. M., *Chem. Phys. Lett.* **126**, 465 (1986).
50. "Raman Spectroscopy of Boron Carbides and Related Boron-Containing Materials," Morosin, B.; Emin, D.; Mullendore, A.; Slack, G.; Wood, C., in "Boron-Rich Solids," eds. Emin, D.; Aselage, T.; Beckel, C. L.; Howard, I. A.; Wood, C. (American Institute of Physics: New York) 1986, p. 312.
51. "Axial Coordination in Nickel Porphyrins and Nickel- Reconstituted Heme Proteins Investigated by Raman-Difference and Transient-Raman Spectroscopy," Shelnett, J. A.; Alston, K.; Findsen, E. W.; Ondrias, M. R.; Rifkind, J. M., in "Porphyrins: Excited States and Dynamics", eds.

- Gouterman, M.; Rentzepis, P. M.; Straub, K. D., ACS Symposium Series, Vol. 321 (American Chemical Society: Washington) 1986, Chpt. 16.
52. "Axial Ligand Dynamics of Nickel-Protoporphyrin Reconstituted Hemoglobin and Myoglobin", Findsen, E. W.; Alston, K.; Shelnett, J. A.; Ondrias, M. R., *J. Am. Chem. Soc.* **108**, 4009 (1986).
53. "Resonance Raman Investigation of Transient Photoinduced Ligation Changes in Nickel Porphyrin" Findsen, E. W.; Ondrias, M. R.; Shelnett, J. A.; Friedman, J. M., in "Porphyrins: Excited States and Dynamics", eds. Gouterman, M.; Rentzepis P. M.; Straub, K. D., ACS Symposium Series, Vol. 321 (American Chemical Society: Washington) 1986, Chpt. 18.
54. "Small Bipolaronic Hopping in Boron Carbides" Emin, D.; Samara, G. A.; Azevedo, L. J.; Venturini, E. L.; Madden, H. H.; Nelson, G. C.; Shelnett, J. A.; Morosin, B.; Moss, M., *J. Less-Common Met.* **117**, 415 (1986).
55. "Raman Spectroscopy of Carboranes and Polycarboranesiloxanes" Shelnett, J. A., in "Microbeam Analysis - 1986," eds. Romig, A. D.; Chambers, F. W., San Francisco Press: San Francisco, 1986, p. 35.
56. "Axial Coordination in Nickel and Vanadium Porphyrins: Transient and Difference Raman Spectroscopy" Shelnett, J. A.; Findsen, E. W.; Ondrias, M. R.; Alston, K., in "Metal Complexes in Fossil Fuels", eds. R. H. Filby; J. F. Branthaver, ACS Symposium Series, Vol. 344, American Chemical Society; Washington, 1987, Chpt. 24.
57. "Axial Ligation-induced Structural Changes in Nickel Corphinoids Related to Coenzyme F<sub>430</sub> Detected by Raman Difference Spectroscopy", Shelnett, J. A., *J. Am. Chem. Soc.* **109**, 4169 (1987).
58. "Photodynamics of Ni-Porphyrins in Non-coordinating Solvents: Characterization of d-d Excited States Using Transient Raman Spectroscopy," Findsen, E. W.; Shelnett, J. A.; Ondrias, M. R., *J. Phys. Chem.* **97**, 307 (1988).
59. "Method for Improving Product Yields in an Anionic Metalloporphyrin-based Artificial Photosynthesis System," Shelnett, J. A., *Bioinvention* **5**, 63 (1986).
60. "A New Crystalline Form of Octaethylporphinatonicel(II). Effects of  $\pi$ - $\pi$  Interactions on Molecular Structure and Resonance Raman Spectra" Brennan, T. D.; Scheidt, W. R.; Shelnett, J. A., *J. Am. Chem. Soc.* **110**, 3919 (1988).
61. "Axial Coordination in Nickel Porphyrins and Nickel-Reconstituted Heme Proteins Investigated by Raman-Difference and Transient-Raman Spectroscopy" Shelnett, J. A.; Alston, K.; Findsen, E. W.; Ondrias, M. R.; Rifkind, J. M., in "Proceedings of the Tenth International Conference on Raman Spectroscopy," eds. Peticolas, W. L.; Hudson, B. H. (University Printing Department, University of Oregon: Eugene, OR) p. 1-15, 1986.
62. "Characterization of the Photodynamic Behavior of Nickel Porphyrins in Non-coordinating Solvent Using Transient Raman Spectroscopy," with Findsen, E. W.; Ondrias, M. R., in "Proceedings of the Tenth International Conference on Raman Spectroscopy," eds. Peticolas, W. L.; Hudson, B. H. (University Printing Department, University of Oregon: Eugene, OR) p. 18-12, 1986.
63. "Resonance Raman Spectroscopic Investigation of Axial Coordination in Methyl Reductase and its Nickel Tetrapyrrole Cofactor F<sub>430</sub>," Shiemke, A. K.; Scott, R. A.; Shelnett, J. A., *J. Am. Chem. Soc.* **110**, 1645 (1988).
64. "The Photodynamics of a Nickel-Corphanoid Model of F<sub>430</sub>," Crawford, B. A.; Findsen, E. W.; Ondrias, M. R.; Shelnett, J. A., *Inorg. Chem.* **27**, 1846 (1988).
65. "A Resonance Raman Study of the Binding of Methanol and Ethanol to Ferrihemoglobin," Muhoberac, B. B.; Shelnett, J. A.; Ondrias, M. R., *FEBS Lett.* **228**, 310 (1988).

66. "Nickel Site of Methane Catalysis in the Methyl Reductase Enzyme," Shelnut, J. A., Fuel Chemistry Division Preprints, Vol. 32, eds. Ratcliffe, C. T.; Suuberg, E. M. (American Chemical Society: Washington) p. 272, 1987.
67. "The Testing of Catalysts for Alkane Activation," Stohl, F. V.; Shelnut, J. A.; Granoff, B.; Trudell, D. E., Fuel Chemistry Division Preprints, Vol. 32, eds. Ratcliffe, C. T.; Suuberg, E. M. (American Chemical Society: Washington) p. 280, 1987.
68. "Multiple Four-Coordinate Forms in a Nickel Hydrocorphinato Related to Cofactor F<sub>430</sub> of Methylreductase," Shelnut, J. A., *J. Phys. Chem.* **93**, 6283 (1989).
69. "Sensitization and Photoredox Reactions of Zn(II)- and Sb(V)(O)(Cl)-Uroporphyrins in Aqueous Media," Kalyanasundaram, K.; Shelnut, J. A.; Gratzel, M., *Inorg. Chem.* **27**, 2820 (1988).
70. "Computer-Aided Molecular Design of Alkane-Activation Catalysts," Shelnut, J. A.; Stohl, F. V.; Granoff, B., Fuel Chem. Div. Preprints, Vol. 33, ed. Ghate, M. R., American Chemical Society: Washington, p. 479, 1988.
71. "The Design of Methane Activation Catalysts," Stohl, F. V.; Shelnut, J. A.; Granoff, B., in "Proceedings 9th International Congress on Catalysis" Vol. 2, eds. M. J. Phillips; M. Ternan (Chemical Institute of Canada: Ottawa) pg. 982, 1988.
72. "Ruffling of Nickel(II) Octaethylporphyrin in Solution," Alden, R. G.; Crawford, B. A.; Ondrias, M. R.; Shelnut, J. A., in Proc. 11<sup>th</sup> International Conf. on Raman Spectroscopy, 1988.
73. "Ruffling of Nickel(II) Octaethylporphyrin in Solution," Alden, R. G.; Crawford, B. A.; Doolen, R.; Ondrias, M. R., Shelnut, J. A., *J. Am. Chem. Soc.* **111**, 2070 (1989).
74. "Synthesis and Spectroscopic Characterization of Bis-Pocket Porphyrins: Tetrakis(2',6'-Dinitrophenyl)Porphyrin and Catalytic Activity of a Manganese(III) Chloride Derivative in Alkane Oxidation," Quintana, C. A.; Assink, R. A.; Shelnut, J. A., *Inorg. Chem.* **28**, 3421 (1989).
75. "Structural and Spectroscopic Characterization of Exogenous Ligand Binding to Isolated Cofactor F<sub>430</sub> and its Isomeric Derivatives" Shiemke, A. K.; Kaplan, W. A.; Hamilton, C. L.; Shelnut, J. A.; Scott, R. A., *J. Biol. Chem.* **264**, 7276 (1989).
76. "Coordination Chemistry of Cofactor F<sub>430</sub>: Axial Ligation Equilibrium between Square-Planar and Bis-Aquo Species in Aqueous Solution" Shiemke, A. K.; Scott, R. A.; Shelnut, J. A., *J. Biol. Chem.* **264**, 11236 (1989).
77. "Photochemically-Driven Biomimetic Oxidation of Alkanes and Olefins" Shelnut, J. A.; Trudell, D. E., *Tetrahedron Lett.* **30**, 5231 (1989).
78. "Influences of  $\pi$ - $\pi$  Complex Formation, Dimerization, and Binding to Hemoglobin on the Planarity of Nickel Porphyrins" Alden, R. G.; Ondrias, M. R.; Shelnut, J. A., *J. Am. Chem. Soc.* **112**, 691 (1990).
79. "Computer Aided Molecular Design of Methane Activation Catalysts" Shelnut, J. A., Advances in Catalytic Technologies, Seminar Proceedings and Audio Cassette Package, Catalytica, Mountain View, CA, December (1988)
80. "Photochemically-Driven Biomimetic Oxidation of Alkanes and Olefins" Shelnut, J. A.; Trudell, D. E., Fuel Chem. Div. Preprints, **34**, 1402 (1989).
81. "Excited State Transient of Vanadyl Uroporphyrin I Detected Using Resonance Raman Spectroscopy" Alden, R. G.; Sparks, L. D.; Ondrias, M. R.; Crawford, B. A.; Shelnut, J. A., *J. Phys. Chem.* **94**, 1440 (1990).
82. "Transient Raman Difference Spectroscopy of Nickel(II)-Uroporphyrin  $\pi$ - $\pi$  Complexes" Crawford, B. A.; Ondrias, M. R.; Shelnut, J. A., *J. Phys. Chem.* **94**, 6647 (1990).

83. "Photochemically-Driven Biomimetic Oxidation of Alkanes and Olefins" Shelnett, J. A., in "Novel Materials in Heterogeneous Catalysis" ACS Symposium Series, No. 437, American Chemical Society: Washington, DC, Chpt. 24, 1990.
84. "Tetracycloalkenyl-*meso*-Tetraphenylporphyrins as Models for the Effect of Non-Planarity on the Light Absorption Properties of Photosynthetic Chromophores" Medforth, C.; Berber, M. D.; Smith, K. M.; Shelnett, J. A., *Tetrahedron Lett.* **31**, 3719 (1990).
85. "Biomimetic Oxidation of Alkanes and Olefins Using O<sub>2</sub> and Light" Shelnett, J. A. in *Methane Activation, Conversion and Utilization* Preprints, PACIFICHEM'89, Honolulu, Hawaii, 40 (1989).
86. "The Effects of  $\pi$ - $\pi$  Interaction on the Molecular Structure and Resonance Raman Spectra of Crystalline Copper(II) Octaethylporphyrin" Sparks, L. D.; Scheidt, W. R.; Shelnett, J. A., *Inorg. Chem.* **31**, 2191 (1991).
87. "Relationships between Structural Parameters and Raman Frequencies for Some Planar and Nonplanar Nickel(II) Porphyrins" Shelnett, J. A.; Medforth, C. J.; Berber, M. D.; Barkigia, K. M.; Smith, K. M., *J. Am. Chem. Soc.* **113**, 4077 (1990).
88. "Non-planar Distortion Modes for Highly Substituted Porphyrins" Medforth, C. J.; Senge, M. O.; Smith, K. M.; Sparks, L. D.; Shelnett, J. A., *J. Am. Chem. Soc.*, **114**, 9859-9869 (1992).
89. "Metal Dependence of the Non-Planar Distortion of Octaalkyltetraphenylporphyrins" Sparks, L. D.; Medforth, C. J.; Park, M.-S.; Chamberlain, J. R.; Ondrias, M. R.; Senge, M. O.; Smith, K. M.; Shelnett, J. A., *J. Am. Chem. Soc.* **115**, 581-592 (1992).
90. "Raman Spectroscopic Characterization of Isomers of Metal N-Phenyl Protoporphyrin IX Dimethylesters" Sparks, L. D.; Chamberlain, J. R.; Hsu, P. Y.-F.; Ondrias, M. R.; Swanson, B.; Ortiz de Montellano, P.; Shelnett J. A., *Inorg. Chem.*, **32**, 3153-3161 (1993). SAND92-2303J or 2271J.
91. "Computer Modeling Opportunities in Catalysis Research" Carlson, G. A.; Shelnett, J. A., Massively Parallel Computing Res. Lab. Research Bulletin. SAND91-2121J.
92. "Enhancement of Solar Photocatalytic Detoxification by Adsorption of Porphyrins onto TiO<sub>2</sub>" Majumder, S. A.; Prairie, M. R.; Ondrias, M. R.; Shelnett, J. A., *Solar Engineering-Vol. 1*, **1992**, Eds. Stine, W.; Kreider, J.; Watanabe, K., ASME: New York, pp. 9-14. SAND91-1856C.
93. "Molecular Design of Substrate Binding Sites" Shelnett, J. A.; Hobbs, J. D., Fuel Chemistry Division Preprints, Vol. 37 (American Chemical Society: Washington), 332-339 (1992).
94. "Resonance Raman Spectroscopy of Non-Planar Nickel Porphyrins" Shelnett, J. A.; Hobbs, J. D.; Majumder, S. A.; Sparks, L. D.; Medforth, C. J.; Senge, M. O.; Smith, K. M.; Miura, M.; Quirke, J. M. E., *J. Raman Spectrosc.* **23**, 523-529 (1992).
95. "A Planar Dodecasubstituted Porphyrin" Senge, M. O.; Medforth, C. J.; Sparks, L. D.; Shelnett, J. A.; Smith, K. M., *Inorg. Chem.*, **32**, 1716-1723 (1993). SAND92-1766J.
96. "Enhancing Solar Photocatalytic Detoxification by Adsorption of Porphyrins onto TiO<sub>2</sub>" Ondrias, M. R.; Majumder, S. A.; Prairie, M. R.; Shelnett, J. A., 1st Intl. Conf. on Environmentally Conscious Manufacturing, Sante Fe, NM, 9/18-20/91. SAND91-2164C.
97. "Recent Developments in Solar Photocatalysis for Water Detoxification" Prairie, M. R.; Majumder, S. A.; Evans, L. R.; Martinez, S. L.; Shelnett, J. A. Proc. AIChE Proc., Miami Beach, FL, 11/1-6/92. SAND92-1476C.
98. "Structural Heterogeneity and Coordination Chemistry of Nickel(II) Octaethyl-*meso*-Nitro-Porphyrins" Hobbs, J. D.; Majumder, S. A.; Luo, L.; Sickelsmith, G. A.; Quirke, J. M. E.; Medforth, C. J.; Smith, K. M.; Shelnett, J. A., *J. Am. Chem. Soc.* **116**, 3261-3270 (1994). SAND93-2176J.

99. "Macrocycle and Substituent Vibrational Modes of Nonplanar Ni(II) Octaethyl-tetraphenylporphyrin from its Resonance Raman, Near-Infrared-Excited FT Raman, and FT-IR Spectra and Deuterium Isotope Shifts" Stichternath, A.; Schweitzer-Stenner, R.; Dreybrodt, W.; Mak, R. S. W.; Li, X.-Y.; Sparks, L. D.; Shelnett, J. A.; Medforth, C. J.; Smith, K. M. *J. Phys. Chem.* **97**, 3701-3708 (1993). SAND92-2252J.
100. "Synthesis and Spectroscopic Studies of Octaacetic Acid Tetraphenylporphyrins" Miura, M.; Majumder, S. A.; Hobbs, J. D.; Renner, M. W.; Furenlid, L. R.; Shelnett, J. A., *Inorg. Chem.* **33**, 6078-6085 (1994). SAND92-1992J.
101. "Solution Conformations of Dodeca-substituted Cobalt(II) Porphyrins" Medforth, C. J.; Hobbs, J. D.; Rodriguez, M. R.; Abraham, R.; Smith, K. M.; Shelnett, J. A., *Inorg. Chem.* **34**, 1333 (1995).
102. "Correlations between Raman Frequencies and Structure for Planar and Nonplanar Metalloporphyrins" Sparks, L. D.; Anderson, K. K.; Medforth, C. J.; Smith, K. M.; Shelnett, J. A. *Inorg. Chem.* **33**, 2297-2302 (1994).
103. "Conserved Non-Planar Heme Distortions in Cytochromes *c*" Hobbs, J. D.; Shelnett, J. A. *J. Protein Chem.*, **14**, 19-25 (1994).
104. "The Planar-Nonplanar Conformational Equilibrium in Metal Derivatives of Octaethylporphyrin and Meso-Nitro-Octaethylporphyrin" Anderson, K. K.; Hobbs, J. D.; Luo, L.; Stanley, K. D.; Quirke, J. M. E.; Shelnett, J. A. *J. Am. Chem. Soc.*, **115**, 12346-12352 (1993).
105. "Light Hydrocarbon Gas Conversion Using Halogenated Iron Dodeca-phenylporphyrin Catalysts" Showalter, M. Erkkila, K., Shelnett, J. A. In Coal Liquefaction and Gas Conversion, Proceed., Vol. I, U. S. DOE, PETC, Pittsburgh, PA. p. 249-263, (1993).
106. "Conformational Study of 2,3,5,7,8,12,13,17,18-Decaalkylporphyrins" Medforth, C. J.; Senge, M. O.; Forsyth, T. P.; Hobbs, J. D.; Shelnett, J. A.; Smith, K. M., *Inorg. Chem.* **33**, 3865-3872 (1994).
107. "Novel Ligand Orientations in Pyridine and Imidazole Complexes of a Highly Substituted Nonplanar Porphyrin, and Implications for the Design of Porphyrins as Regio- and Stereo-Specific Oxidation Catalysts" Medforth, C. J.; Muzzi, C. M.; Smith, K. M.; Abraham, R. J.; Hobbs, J. D.; Shelnett, J. A., *Perkin II* **1994**, 1843-1844 (1994).
108. "Computer-Aided Design of Molecular Catalysts for Alkane Oxidation Using Dodeca-substituted Iron Porphyrins" Shelnett, J. A.; Martinez, S.; Erkkila, K., Indirect Liq. Contractors' Rev. Conf., Pittsburgh, PA, 9/22-24/92. SAND92-2303C.
109. "An Unusual Near-Eclipsed Porphyrin Ring Orientation in Two Crystalline Forms of (m-Oxo)bis[*octaethylporphinato*]iron(III)]. Structural and Molecular Mechanics Studies" Cheng, B.; Hobbs, J. D.; Debrunner, P. G.; Erlebaacher, J.; Shelnett, J. A.; Scheidt, W. R., *Inorg. Chem.* **34**, 102-110 (1995).
110. "Ruffling in a Series of Nickel(II) *Meso*-Tetrasubstituted Porphyrins as a Model for the Conserved Ruffling of the Heme of Cytochrome *c*" Jentzen, W.; Hobbs, J. D.; Song, X.; Simpson, M. C.; Taylor, K. K.; Ema, T.; Nelson, N. Y.; Medforth, C. J.; Smith, K. M.; Veyrat, M.; Mazzanti, M.; Ramasseul, R.; Marchon, J.-C.; Takeuchi, T.; Goddard III, W. A.; Shelnett, J. A., *J. Am. Chem. Soc.* **117**, 11085-11097 (1995).
111. "Conformational Properties of Nickel(II) Octaethylporphyrin in Solution. 1. Resonance Excitation Profiles and Temperature Dependence of Structure-Sensitive Raman Lines" Jentzen, W.; Unger, E.; Karvounis, G.; Shelnett, J. A.; Dreybrodt, W.; Reinhard Schweitzer-Stenner, *J. Phys. Chem.* **100**, 14184-14191 (1996)
112. "Planar Solid-State and Solution Structures of (Porphinato)nickel(II) As Determined by X-ray Diffraction and Resonance Raman Spectroscopy" Jentzen, W.; Turswska-Tyrk, I.; Scheidt, W. R.; Shelnett, J. A. *Inorg. Chem.* **35**, 3559-3567 (1996).

113. "Isolation and Characterization of Vibrational Spectra of Individual Heme Active Sites in bc<sub>1</sub> Complexes from *Rhodobacter capsulatus*" Gao, F.; Qin, H.; Simpson, M. C.; Shelnett, J. A.; Knaff, D. B.; Ondrias, M. R., *Biochemistry*, **35**, 12812-12819 (1996).
114. "Representation of Nonplanar Conformers of Nickel(II) 5,15-Di-Substituted Porphyrins in Terms of Displacements along Low-Frequency Normal Coordinates of the Macrocycle" Song, X.-Z.; Jentzen, W.; Jia, S.-L.; Jaquinod, L.; Nurco, D. J.; Medforth, C. J.; Smith, K. M.; Shelnett, J. A. *J. Am. Chem. Soc.* **118**, 12975-12988 (1996).
115. "NMR Studies of Nonplanar Porphyrins. Part 2. Effect of Nonplanar Conformational Distortions on the Porphyrin Ring Current" Medforth, C. J.; Muzzi, C. M.; Shea, K. M.; Smith, K. M.; Abraham, R. J.; Jia, S.-L.; Shelnett, J. A. *J. Chem. Soc., Perkin Trans. 2*, 839-844 (1997).
116. "Synthesis and Physical Characterization of Novel Heme-based Model Systems for Photoinitiated Electron Transfer. II. Direct Ruthenation of Microperoxidase-11" Fan, B.; Simpson, M. C.; Shelnett, J. A.; Martinez, L.; Falcon, R.; Pastuszyn, A. J.; Ondrias, M. R. *Inorg. Chem.* **18**, 3847-3853 (1997).
117. "Synthesis and Physical Characterisation of Novel Heme-based Model Systems for Photoinitiated Electron Transfer. I. Complexation of RuProHis Bifunctional peptide and microperoxidase-11" Fan, B.; Fontenot, D. L.; Larsen, R. W.; Simpson, M. C.; Shelnett, J. A.; Falcon, R.; Martinez, L.; Niu, S.; Zhong, S.; Niemczyk, T.; Ondrias, M. R. *Inorg. Chem.* **18**, 3839-3846 (1997).
118. "Conservation of the Conformation of the Porphyrin Macrocycle in Hemoproteins" Jentzen, W.; Ma, J.-G.; Shelnett, J. A. *Biophys. J.* **74**, 753-763 (1998).
119. "Metal-Dependence of the Contributions of Low-Frequency Normal Coordinates to the Sterically-Induced Distortions of Meso-Di-Alkyl-Substituted Porphyrins" Song, X.-Z.; Jaquinod, L.; Jentzen, W.; Nurco, D. J.; Jia, S.-L.; Khoury, R. G.; Ma, J.-G.; Medforth, C. J.; Smith, K. M.; Shelnett, J. A., *Inorg. Chem.* **37**, 2009-2019 (1998).
120. "A Pyridine-Sensitive Molecular Venus Flytrap. Ligand-Triggered Atropisomerization of a Zinc Chiroporphyrin" Mazzanti, M.; Marchon, J.-C.; Shang, M.; Scheidt, W. R.; Jia, S.-L.; Shelnett, J. A. *J. Am. Chem. Soc.* **119**, 12400-12401 (1997).
121. "NMR Studies of Nonplanar Porphyrins. Part 1. Axial Ligand Orientations in Highly Nonplanar Porphyrins" Medforth, C. J.; Muzzi, C. M.; Shea, K. M.; Smith, K. M.; Abraham, R. J.; Jia, S.-L.; Shelnett, J. A. *J. Chem. Soc., Perkin Trans. 2*, 833-837 (1997).
122. "Langmuir-Blodgett Films of Stearic Acid Containing Octakis((methoxycarbonyl)-methyl)- meso-tetrakis(((icosanyloxy)carbonyl)phenyl)-porphyrin" Song, X.; Miura, M.; Xu, X.; Taylor, K. K.; Majumder, S. A.; Hobbs, J. D.; Cesarano, J.; Shelnett, J. A., *Langmuir*, **12**, 2019-2027 (1996).
123. "Structural Characterization of Synthetic and Protein-Bound Porphyrins in Terms of the Lowest-Frequency Normal Coordinates of the Macrocycle" Jentzen, W.; Song, X.-Z.; Shelnett, J. A. *J. Phys. Chem. B* **101**, 1684-1699 (1997).
124. "Axial Coordination and Conformational Heterogeneity of Nickel(II) Tetraphenylporphyrin Complexes with Nitrogenous Bases" Jia, S.-L.; Jentzen, W.; Shang, M.; Song, X.-Z.; Ma, J.-G.; Scheidt, W. R.; Shelnett, J. A. *Inorg. Chem.* **37**, 4402-4412 (1998).
125. "Comparative Analysis of the Conformations of Symmetrically and Asymmetrically Deca- and Undeca-substituted Porphyrins Bearing meso-alkyl or Aryl Groups" Senge, M. O.; Medforth, C. J.; Forsyth, T. P.; Lee, D. A.; Olmstead, M. M.; Jentzen, W.; Pandey, R. K.; Shelnett, J. A.; Smith, K. M. *Inorg. Chem.* 1149-1163 (1997).
126. "Planar and Nonplanar Conformations of (Meso-Tetraphenylporphinato)nickel(II) in Solution as Inferred from Solution and Solid-State Raman Spectroscopy" Jentzen, W.; Unger, E.; Song, X.-Z.; Turowska-Tyrk, I.; Schweitzer-Stenner, R.; Dreybrodt, W.; Scheidt, W. R.; Shelnett, J. A. *J. Phys. Chem.* **101**, 5789-5798 (1997).

127. "Application of Matrix-Assisted Laser Desorption/Fourier Transform Mass Spectrometry to the Analysis of Planar Porphyrins and Highly Substituted Nonplanar Porphyrins" Green, M. K.; Medforth, C. J.; Muzzi, C. M.; Nurco, D. J.; Shea, K. M.; Smith, K. M.; Lebrilla, C. B.; Shelnut, J. A. *Eur. Mass Spectrom.* **3**, 439-451 (1997).
128. "Raman Dispersion Spectroscopy on the Highly Saddled Nickel(II)-Octaethyltetraphenylporphyrin Reveals the Symmetry of Non-planar Distortions and the Vibronic Coupling Strength of Normal Modes" Schweitzer-Stenner, R.; Stichernath, A.; Dreybrodt, W.; Jentzen, W.; Song, X.-Z.; Shelnut, J. A.; Nielsen, O. F.; Medforth, C. J.; Smith, K. M. *J. Chem. Phys.* **107**, 1794-1815 (1997).
129. "Electron Transfer Photosensitized by a Tin Lipoporphyrin in Solution, Micelles, and at Water-Organic Solvent Interfaces" Song, X.-Z.; Jia, S.-L.; Miura, M.; Ma, J.-G.; Shelnut, J. A. *J. Photochem. Photobiol. A: Chem.* **113**, 233-241 (1998).
130. "Substituent-Induced Perturbation Symmetries and Distortions of Meso-Tert-Butylporphyrins" Song, X.-Z.; Jentzen, W.; Jaquinod, L.; Khoury, R. G.; Medforth, C. J.; Jia, S.-L.; Ma, J.-G.; Smith, K. M.; Shelnut, J. A. *Inorg. Chem.* **37**, 2117-2128 (1998).
131. "Protein-Induced Changes in the Nonplanarity of the Porphyrin in Nickel Cytochrome c Probed by Resonance Raman Spectroscopy" Ma, J.-G.; Laberge, M.; Song, X.-Z.; Jentzen, W.; Jia, S.-L.; Vanderkooi, J. M.; Shelnut, J. A. *Biochemistry* **37**, 5118-5128 (1998).
132. "Picosecond to Microsecond Photodynamics of a Nonplanar Nickel Porphyrin: Solvent Dielectric and Temperature Effects" Drain, C. M.; Gentemann, S.; Roberts, J. A.; Nelson, N. Y.; Medforth, C. J.; Jia, S.-L.; Simpson, M. C.; Smith, K. M.; Fajer, J.; Shelnut, J. A.; Holten, D. *J. Am. Chem. Soc.* **120**, 3781-3791 (1998).
133. "Nonplanar Porphyrins and their Significance in Proteins" Shelnut, J. A.; Song, X.-Z.; Ma, J.-G.; Jia, S.-L.; Jentzen, W.; Medforth, C. J. *Chem. Soc. Rev.* **27**, 31-41 (1998).
134. "The Structural Origin of Nonplanar Heme Distortions in Tetraheme Ferricytochromes  $c_3$ " Ma, J.-G.; Zhang, J.; Franco, R.; Jia, S.-L.; Moura, I.; Moura, J. J. G.; Kroneck, P. M. H.; Shelnut, J. A. *Biochemistry*, **37**, 12431-12442 (1998).
135. "Polarized Raman Dispersion Spectroscopy Probes Planar and Non-planar Distortions of Ni(II) Porphyrins with Different Peripheral Substituents" Lemke, C.; Dreybrodt, W.; Shelnut, J. A.; Quirke, J. M. E.; Schweitzer-Stenner, R., *J. Raman Spectrosc.* **29**, 945-953 (1998).
136. "Conformational Diversity in (Octaethylporphinato)(trichloroacetato)iron(III) Derivatives" Neal, T. J.; Cheng, B.; Ma, J.-G.; Shelnut, J. A.; Schulz, C. E.; Scheidt, W. R., *Inorg. Chim. Acta*, **291**, 49-59 (1999).
137. "Synthesis and Electrochemical Studies of a Series of Fluorinated Dodecaphenylporphyrins" Kadish, K. M.; Van Caemelbecke, E.; D'Souza, F.; Lin, M.; Nurco, D. J.; Medforth, C. J.; Forsyth, T. P.; Krattinger, B.; Smith, K. M.; Fukuzumi, S.; Nakanishi, I.; Shelnut, J. A., *Inorg. Chem.* **38**, 2188-2198 (1999).
138. "Resonance Raman Investigation of Nickel Microperoxidase-11" Ma, J.-G.; Vanderkooi, J. M.; Zhang, J.; Jia, S.-L.; Shelnut, J. A., *Biochemistry* **38**, 2787-2795 (1999).
139. "The Quantum Mixed-Spin Heme State of Barley Peroxidase: A Paradigm for Class III Peroxidases" Howes, B. D.; Schiodt, C. B.; Welinder, K. G.; Marzocchi, M. P.; Ma, J.-G.; Zhang, J.; Shelnut, J. A.; Smulevich, G., *Biophys. J.* **77**, 478-492 (1999).
140. "Novel Dodecaarylporphyrins: Synthesis and Dynamic Properties" Muzzi, C. M.; Medforth, C. J.; Voss, L.; Cancilla, M.; Lebrilla, C.; Ma, J.-G.; Shelnut, J. A.; Smith, K. M. *Tetrahedron Lett.* **40**, 6159-6162 (1999).

141. "Synthesis and unusual properties of the first 2,3,7,8,12,13,17,18-octabromo-5,10,15,20-tetraalkylporphyrin" Nelson, N. Y.; Medforth, C. J.; Nurco, D. J.; Jia, S.; Shelnett, J. A.; Smith, K. M. *Chem. Commun.* 2071-2072 (1999).
142. "Molecular Simulations and Normal-Coordinate Structural Analysis of Porphyrins and Heme Proteins" Shelnett, J. A., *The Porphyrin Handbook: Vol 7: Theoretical and Physical Characterization*, Eds. Kadish, K. M.; Smith, K. M.; Guillard, R. (Academic Press: New York) Chpt. 50, 167-223 (2000).
143. "Porphyrin Interactions with Wild Type and Mutant Mouse Ferrochelatase" Franco, R.; Ma, J.-G.; Lu, Y.; Ferreira, G. C.; Shelnett, J. A., *Biochemistry*, **39**, 2517-2529 (2000).
144. "Synthesis and Characterization of a Chiral Nonplanar Porphyrin" Muzzi, C. M.; Medforth, C. J.; Smith, K. M.; Jia, S.-L.; Shelnett, J. A. *Chem. Commun.* 131 (2000).
145. "Using Cytochrome  $c_3$  To Make Elemental Selenium Nanowires" Abdelouas, A.; Gong, W. L.; Lutze, W.; Franco, R.; Moura, I.; Shelnett, J. A. *Chem. Mater.* **12**, 1510-1512 (2000).
146. "Molecular Simulations of Porphyrins and Heme Proteins" Shelnett, J. A., *J. Porphyrins Phthalocyanines*, **4**, 386-389 (2000).
147. "Molecular Dynamics Simulations of Carbonmonoxy Myoglobin and Calculations of Heme Circular Dichroism" Woody, R. W.; Kiefl, C. Sreerama, N.; Lu, Y.; Qiu, Y.; Shelnett, J. A. in *Insulin and Related Proteins – from Structure to Function and Pharmacology*, Federwisch, M.; Dieken, M. L., Eds. (Kluwer Academic Publishers, Dordrecht, The Netherlands), 2000.
148. "Normal-Coordinate Structural Decomposition and the Vibronic Spectra of Porphyrins" Shelnett, J. A. *J. Porphyrins Phthalocyanines*, **5**, 300-311 (2001).
149. "Conformational Distortions of Metalloporphyrins with Electron Withdrawing  $\text{NO}_2$  Substituents at Different *meso* Positions. A Structural Analysis by Polarized Resonance Raman Dispersion Spectroscopy and Molecular Mechanics Calculations" Schweitzer-Stenner, R.; Lemke, C.; Haddad, R.; Qiu, Y.; Shelnett, J. A.; Quirke, J. M. E.; Dreybrodt, W., *J. Phys. Chem. A* **105**, 6680-6694 (2001).
150. "Conformational Analysis of the Non-Planar Deformations of Cobalt Porphyrin Complexes in the Cambridge Structural Database" Cullen, D. L.; Desai, L. V.; Shelnett, J. A.; Zimmer, M., *Struct. Chem.* **12**, 127-136 (2001).
151. "Shear-induced Mechanochromism in Polydiacetylene Monolayers" Burns, A. R.; Carpick, R. W.; Sasaki, D. Y.; Shelnett, J. A., Haddad, R., *Tribology Lett.* **10**, 89-96 (2001).
152. "Calcium-Dependent Conformation of a Heme and Fingerprint Peptide of the Di-Heme Cytochrome *c* Peroxidase from *Paracoccus pantotrophus*" Pauleta, S. R.; Lu, Y.; Goodhew, C. F.; Moura, I.; Pettigrew, G. W.; Shelnett, J. A., *Biochemistry* **40**, 6570-6579 (2001).
153. "Self-assembly of Mesoscopically Ordered Chromatic Polydiacetylene/silica nanocomposites Using Polymerizable Surfactants as Structure Directing Monomers" Lu, Y.; Yang, Y.; Lu, M.; Huang, J.; Fan, H.; Haddad, R.; Lopez, G.; Burns, A. R.; Sasaki, D. Y.; Shelnett, J. A.; Brinker, C. J., *Nature*, **410**, 913-917 (2001).
154. "Vibrational Analysis of Metalloporphyrins with Electron Withdrawing  $\text{NO}_2$ -Substituents at Different *meso* Positions." Lemke, C.; Schweitzer-Stenner, R.; Shelnett, J. A.; Quirke, J. M. E.; Dreybrodt, W., *J. Phys. Chem. A* **105**, 6668-6679 (2001).
155. "Ligand-induced Heme Ruffling and Bent NO Geometry in Ultra-high Resolution Structures of Nitrophorin 4" Roberts, S. A.; Weichsel, A.; Qiu, Y.; Shelnett, J. A.; Walker, F. A.; Montfort, W. R., *Biochemistry* **40**, 11327-11337 (2001).
156. "Heme Distortions in Sperm Whale Carbonmonoxy Myoglobin. Correlations between Rotational Strengths and Heme Deformations MD-Generated Structures" Kiefl, C.; Sreerama, N.; Lu, Y.; Qiu, Y.; Shelnett, J. A.; Woody, R. W., *J. Am. Chem. Soc.* **124**, 3384-3394 (2002).

157. "Binding of Protoporphyrin IX and Metal Derivatives to the Active Site of Wild-Type Mouse Ferrochelatase at Low Porphyrin-to-Protein Ratios" Lu, Y.; Sousa, A.; Franco, R.; Mangravita, A.; Ferreira, G. C.; Moura, I.; Shelnett, J. A. *Biochemistry* **41**, 8253-8262 (2002).
158. "Molecular Structures and Magnetic Properties of Chloroiron(III) Complexes of the 2,3-diethyl- (detpp), 2,3,7,8-tetraethyl- (*cis*-tetpp), 2,3,12,13-tetraethyl- (*trans*-tetpp), and 2,3,7,8,12,13-hexaethyl- (hetpp)-5,10,15,20-tetraphenylporphyrin Complexes" Weiss, R.; Fischer, J.; Bulach, V.; Shelnett, J. A. *C. R. Chimie*, **5**, 405-416 (2002).
159. "Structure and Mixed Spin State of the Chloroiron(III) Complex of 2,3,7,8,12,13,17,18-octaphenyl-5,10,15,20-tetraphenylporphyrin, Fe(dpp)Cl" Weiss, R.; Fischer, J.; Bulach, V.; Schunemann, V.; Gerdan, M.; Trautwein, A. X.; Shelnett, J. A.; Gros, C.; Tabard, A.; Cuillard, R. *Inorg. Chim. Acta*, **337**, 223-232 (2002).
160. "Influence of Electronic and Structural Effects on the Oxidative Behavior of Nickel Porphyrins" Kadish, K. M.; Lin, M.; Van Caemelbecke, E.; De Stefano, G.; Medforth, C. J.; Nurco, D. J.; Nelson, N. Y.; Krattinger, B.; Muzzi, C. M.; Jaquinod, L.; Xu, Y.; Shyr, D. C.; Smith, K. M.; Shelnett, J. A., *Inorg. Chem.* **41**, 6673-6687 (2002).
161. "Twisting the Porphyrin Ring to Enhance Epoxidation Enantioselectivity" Gazeau, S.; Pécaut, J.; Haddad, R.; Shelnett, J. A.; Marchon, J.-C., *Eur. J. Inorg. Chem.* 2956-2960 (2002).
162. "Unusual Aryl-Porphyrin Rotational Barriers in Peripherally Crowded Porphyrins" Medforth, C. J.; Haddad, R.; Muzzi, C. M.; Dooley, N. R.; Jaquinod, L.; Shyr, D. C.; Nurco, D. J.; Olmstead, M. M.; Smith, K. M.; Ma, J.-G.; Shelnett, J. A., *Inorg. Chem.* **42**, 2227-2241, (2003).
163. "Origin of the Red Shifts in the Optical Absorption Bands of Nonplanar Tetraalkylporphyrins" Haddad, R. E.; Gazeau, S.; Pécaut, J.; Marchon, J.-C.; Medforth, C. J.; Shelnett, J. A., *J. Am. Chem. Soc.* **125**, 1253-1268 (2003).
164. "Functional Nanocomposites Prepared by Self-Assembly and Polymerization of Diacetylene Surfactants and Silicic Acid" Yang, Y.; Lu, Y.; Lu, M.; Huang, J.; Haddad, R. E.; Xomeritakis, G.; Liu, N.; Malanoski, A. P.; Sturmayer, D.; Fan, H.; Sasaki, D. Y.; Assink, R. A.; Shelnett, J. A.; van Swol, F.; Lopez, G. P.; Burns, A. P.; Brinker, C. J., *J. Am. Chem. Soc.* **125**, 1269-1277 (2003).
165. "Controlled Synthesis of 2-D and 3-D Dendritic Platinum Nanostructures" Song, Y.; Yang, Y.; Medforth, C. J.; Pereira, E.; Singh, A. K.; Xu, H.; Jiang, Y.; Brinker, C. J.; van Swol, F.; Shelnett, J. A., *J. Am. Chem. Soc.* **126**, 625-635 (2004).
166. "Synthesis of Peptide-Nanotube Platinum-Nanoparticle Composites" Song, Y.; Challa, S. R.; Medforth, C. J.; Qiu, Y.; Watt, R. K.; van Swol, F.; Shelnett, J. A., *Chem. Commun.* 1044-1045 (2004).
167. "Porphyrin Nanotubes from Ionic Self-Assembly" Wang, Z.; Medforth, C. J.; Shelnett, J. A., *J. Am. Chem. Soc.* **126**, 15954-15955 (2004).
168. "Self-metallization of photocatalytic porphyrin nanotubes" Wang, Z.; Medforth, C. J.; Shelnett, J. A., *J. Am. Chem. Soc.* **126**, 16720-16721 (2004).
169. "Energetics and Structural Consequences of Axial Ligand Coordination in Nonplanar Nickel Porphyrins" Song, Y.; Haddad, R. E.; Jia, S.-L.; Hok, S.; Olmstead, M. M.; Nurco, D. J.; Schore, N. E.; Zhang, J.; Ma, J.-G.; Smith, K. M.; Gazeau, S.; Pécaut, J.; Marchon, J.-C.; Medforth, C. J.; Shelnett, J. A., *J. Am. Chem. Soc.* **127**, 1179-1192 (2005).
170. "The conserved active-site loop residues of ferrochelatase induce porphyrin conformational changes necessary for catalysis" Shi, Z.; Franco, R.; Haddad, R.; Shelnett, J.A.; Ferreira, G.C.; *Biochemistry*, **45**, 2904-2912 (2006).
171. "Synthesis of Platinum Nanocages Using Liposomes Containing Photocatalyst Molecules" Garcia, R. M.; Dorin, R. M.; Wang, H.; Qiu, Y.; Shelnett, J. A., *Angew. Chem., Int. Ed.* **45**, 8126-8130. (2006).

172. “Interfacial synthesis of dendritic platinum nanoshells templated on oil nanodroplets stabilized in water by a photocatalytic lipoporphyrin” Wang, H.; Song, Y.; Medforth, C. J.; Shelnett, J. A., *J. Am. Chem. Soc.* **128**, 9284-9285 (2006).
173. “Selective detection of divalent and trivalent metal ions with functionalized lipid membranes” Pincus, J. L.; Jin, C.; Huang, W.; Jacobs, H. K.; Gopalan, A. S.; Song, Y.; Shelnett, J. A.; Sasaki, D. Y., *J. Mater. Chem.* **15**, 2938-2945 (2005).
174. “Foamlike Nanostructures Created from Dendritic Platinum Sheets on Liposomes” Song, Y.; Steen, W. A.; Peña, D.; Jiang, Y.-B.; Medforth, C. J.; Huo, Q.; Pincus, J. L.; Qiu, Y.; Sasaki, D. Y.; Miller, J. E.; Shelnett, J. A. *Chem. Mater.* **18**, 2335-2346 (2006).
175. “Platinum Nanodendrites” Song, Y.; Jiang, Y.-B.; Wang, H.; Pena, D. A.; Qiu, Y.; Miller, J. E.; Shelnett, J. A., *Nanotechnology* **17**, 1300-1308 (2006).
176. “Chelataes: Distort to select?” Al-Karadaghi, S.; Franco, R.; Hansson, M.; Shelnett, J. A.; Isaya, G.; Ferreira, G. C.; *TiBS* **31**, 135-142 (2006).
177. “Porphyrin nanofiber bundles from interfacial ionic self-assembly and their photocatalytic self-metallization” Wang, Z.; Ho, K. J.; Medforth, C. J.; Shelnett, J. A., *Adv. Mater.* **18**, 2557-2560 (2006).
178. “Self-Assembly and Self-Metallization of Porphyrin Nanosheets” Wang, Z.; Li, Z.; Medforth, C. J.; Shelnett, J. A., *J. Am. Chem. Soc.* **129**, 2440-2441 (2007).
179. “Synthesis of Platinum Nanowire Networks Using a SoftTemplate” Song, Y.; Garcia, R. M.; Dorin, R. M.; Wang, H.; Qiu, Y.; Coker, E. N.; Miller, J. E.; Shelnett, J. A., *Nano Lett.* **7**, 3650-3655 (2007)
180. “Synthesis of Monodisperse Nanospheres of Porphyrin-based Coordination Polymers and their Use as Nanoscale Light-harvesting Components” Wang, Z.; Lybarger, L. E.; Medforth, C. J.; Miller, J. E.; Shelnett, J. A., *Nanotechnology* **19**, 395604 (2008).
181. “Light-driven Synthesis of Hollow Platinum Nanospheres” Garcia, R. M.; Song, Y.; Dorin, R. M.; Wang, H.; Li, P.; Qiu, Y.; van Swol, F.; Shelnett, J. A., *Chem. Commun.* 2535-3537 (2008).
182. “Calcium-dependent Heme Structure in the Reduced Forms of the Bacterial Cytochrome c Peroxidase from *Paracoccus pantotrophus*” Pauleta, S. R.; Lu, Y.; Goodhew, C. F.; Moura, I.; Pettigrew, G. W.; Shelnett, J. A., *Biochemistry* **47**, 5841-5850 (2008).
183. “Synthesis of Platinum Nanowheels Using a Bicellar Template” Song, Y.; Dorin, R. M.; Garcia, R. M.; Jiang, Y.-B.; Wang, H.; Li, P.; Qiu, Y.; van Swol, F.; Miller, J. E.; Shelnett, J. A., *J. Am. Chem. Soc.* **130** 12602-12603 (2008).
184. “Silica–Metal Core–Shells and Metal Shells Synthesized by Porphyrin-Assisted Photocatalysis” Wang, H.; Song, Y.; Wang, Z.; Medforth, C. J.; Miller, J. E.; Evans, L.; Li P.; Shelnett, J. A., *Chem. Mater.* **20**, 7434–7439 (2008).
185. “Evolution of Dendritic Platinum Nanosheets into Ripening-Resistant Holey Sheets” Song, Y.; Hickner, M. A.; Challa, S. R.; Dorin, R. M.; Garcia, R. M.; Wang, H.; Jiang, Y.-B.; Li, P.; Qiu, Y.; van Swol, F.; Medforth, C. J.; Miller, J. E.; Nwoga, T.; Kawahara, K.; Li, W.; Shelnett, J. A., *Nano Lett.* **2009**, 9, 1534-1539.
186. “Internal Structure of Porphyrin Nanotubes Revealed by Resonance Raman Spectroscopy” Franco, R.; Jacobsen, J.; Wang, H.; Wang, Z.; Istvan, K.; Schore, N. E.; Medforth, C. J.; Shelnett, J. A., *Phys. Chem. Chem. Phys.* submitted (2009).
187. “An Analysis of the Conformational Flexibility and Dynamic Properties of Highly Nonplanar Porphyrins” Muzzi, C. M.; Medforth, C. J.; Nurco, D. J.; Clement, T.; Khoury, R. J.; Smith, K. M.; Cancilla, M.; Voss, L.; Lebrilla, C.; Ma, J.-G.; Shelnett, J. A., *J. Am. Chem. Soc.* submitted (2009).
188. “Structural Contributions to Porphyrin Basicity and Protonation Behavior” Medforth, C. J.;

- Somma, M. S.; Shyr, D. C.; Nurco, D. J.; Goodrow, M.; Smith, K. M.; Haddad, R. E.; Qiu, Y.; Shelnett, J. A., *J. Am. Chem. Soc.* submitted (2009).
189. "Self-Assembled Porphyrin Nanostructures" Medforth, C. J.; Wang, Z.; Martin, K. E.; Song, Y.; Jacobsen, J. L.; Shelnett, J. A., *Chem. Commun.* DOI:10.1039/B914432C (2009).
190. "Donor-Acceptor Biomorphs from the Ionic Self-assembly of Porphyrins" Martin, K. E.; Wang, Z.; Garcia, R. M.; Song, Y.; Jacobsen, J. L.; Schore, N. E.; Busani, T.; Swartzentruber, B. S.; Medforth, C. J.; Shelnett, *Angew. Chem., Int. Ed.*, submitted (2009).

### **In Preparation:**

191. "Steric Bulkiness of the Pyrrole Substituents Influences the Out-of-Plane Deformations of Porphyrins: Nickel(II) Octa(isopropyl)porphyrin and its *meso*-Nitro Derivative" Shelnett, J. A.; Haddad, R.; Lu, Y.; Quirke, J. M. E., *J. Am. Chem. Soc.* in preparation (2009).
192. "Stochastic Treatment of the Interaction of Light with a Molecule Interacting with a Reservoir at Constant Temperature" Shelnett, J. A., *J. Chem. Phys.*, in preparation (2009).

### **PATENTS**

1. "Method for Improving Product Yields in Anionic Metalloporphyrin-based Artificial Photosynthesis System" U.S. Patent No. 4,568,435 (Feb. 4, 1986), J. A. Shelnett.
2. "Process for Light-Driven Hydrocarbon Oxidation at Ambient Temperatures" U.S. Patent No. 4,917,784 (April 1990), J. A. Shelnett.
3. "Boronated Porphyrins and Methods for their Use" U.S. Patent No. 5,877,165 (March 2, 1999), M. Miura, J. A. Shelnett, D. Slatkin.
4. "Nickel Porphyrins for Memory Optical Applications" U.S. Patent No. 6,117,369 (Sept. 12, 2000) Shelnett, J. A., Jia, S.-L., Medforth, C. J., Holten, D., Nelson, N. Y., Smith, K. M.
5. "Reductive Precipitation of Metals Photosensitized By Tin and Antimony Porphyrins" U.S. Patent No. 6,627,048 B1 (Sept. 30, 2003), Shelnett, J. A.; Gong, W. L.; Abdelouas, A.; Lutze, W.
6. "Heteroporphyrin Nanotubes and Composites" U.S. Patent No. 7,132,163 (Nov. 7, 2006), Wang, Z.; Medforth, C. J.; Shelnett, J. A.
7. "Heteroporphyrin Nanotubes and Composites" U.S. Patent No. 7,223,474 (May 29, 2007), Wang, Z.; Medforth, C. J.; Shelnett, J. A.
8. "Water-splitting using Photocatalytic Porphyrin-nanotube Composite Device" U.S. Patent No. 7,338,590 B1 (Mar 4, 2008), Shelnett, J. A.; Miller, J. E.; Wang, Z.; Medforth, C. J.
9. "Dendritic Metal Nanostructures" U.S. Patent No. 7,374,599 B1 (May 20, 2008), Song, Y.; Pereira, E.; Medforth, C. J.; Shelnett, J. A.

**+10 patent applications pending.**

### **BOOKS**

1. "Fundamental of Vibronic Spectroscopy" Shelnett, J. A., (2009) Chapter 1-5 on Web at <http://jasheln.unm.edu> .