

## Publications Youngstown State University Department of Chemistry, 1999-2009

### 2009:

1. Mercury(II) acetate/thiocyanate coordination polymers with n-donor ligands, spectroscopic, thermal and structural studies. Mahmoudi, Ghodrat; Morsali, Ali; Zeller, Matthias, *Inorg. Chim. Acta* **2009**, 362(1), 217-225.
2. trans-Dimethanolbis(1,1,1-trifluoro-5,5-dimethylhexane-2,4-dionato)zinc(II), Gerald O. Hunter, Matthias Zeller and Brian D. Leskiw, *Acta Cryst. E* **2009**, E65, m24.
3. A New Two-dimensional Thallium(I) Coordination Polymer With 4-hydroxybenzylidene-4-aminobenzoate: Thermal, Structural, Solution and Solvatochromic Studies. Kamran Akhbari, Kamal Alizadeh, Ali Morsali, Matthias Zeller, *Inorganica Chimica Acta*, 362(8), 2589-2594.
4. Shape-Selective Sorption and Fluorescence Sensing of Aromatics in a Flexible Network of Tetrakis[(4-methylthiophenyl)ethynyl]silane and AgBF<sub>4</sub>, Guo Huang, Chen Yang, Zhengtao Xu, Haohan Wu, Jing Li, Matthias Zeller, Allen D. Hunter, Stephen Sin-Yin Chui and Chi-Ming Che, *Chem. Mat.* **2009**, 21(3), 541-546.
5. Copper (II) oligomeric derivatives for deposition of copper thin films, Muhammad Shahid, Asif Ali Tahir, Mazhar Hamid, Muhammad Mazhar, Matthias Zeller, Kieran C. Molloy, and Allen D. Hunter, *Eur. J. Inorg. Chem.* **2009**, 1043-1050.
6. Reversible Low Temperature Phase Change and Twinning in Lithium Acetyl Acetate, Calvin A. Austin, Brian D. Leskiw and Matthias Zeller, *Phase Transitions* **2009**, 82(3) 211-220.
7. Facile Synthesis of (Phosphine)- and (N-heterocyclic Carbene)Gold(I) and Silver(I) Azide Complexes, Partyka, David V.; Robilotto, Thomas J.; Updegraff, James B., III; Zeller, Matthias; Hunter, Allen D.; Gray, Thomas G., *Organometallics* **2009**, 28(3), 795-801.
8. Structural Investigations of Novel Indoloacridines, Makuteswaran Sridharan, Karnam Jayarampillai Rajendra Prasad, Aimable Ngendahimana and Matthias Zeller, *J. Chem Cryst.* **2009**, 39(4), 270-278.
9. "Systematic comparison of second-order polarization propagator approximation (SOPPA) and equation-of-motion coupled cluster singles and doubles (EOM-CCSD) spin-spin coupling

- constants for molecules with C, N, and O double and triple bonds, and selected F-substituted derivatives” J. E. Del Bene, I. Alkorta, and J. Elguero. *J. Chem. Theory Comput.* **2009**, 5, 208.
10. “Prebiotic Selection of the A-U Base Pair?” J. R. Quinn, S. C. Zimmerman, J. E. Del Bene, and I. Shavitt. ACS Books (in press).
  11. “Substituent Effects on B-N Bonding and Coupling Constants in Five-Membered, Rings  $N_3B_2H_4X$  and  $N_2B_3H_4X$ , for X = H, F, and Li” J. E. Del Bene, O. M6, and M. Ya6ez, *Croatica Chemica Acta* **2009**, (in press).
  12. “What factors determine whether a proton-bound homodimer has a symmetric or an asymmetric hydrogen bond?” B. Chan, J. E. Del Bene, and L. Radom, *Mol. Phys.* **2009** (in press).
  13. Cancer biomarker AKR1B10 and carbonyl metabolism. Balendiran GK, Martin HJ, El-Hawari Y, Maser E., *Chem Biol Interact.* **2009**, 178(1-3), 134-137.
  14. Flexible Thioether-Ag(I) Interactions for Assembling Large Organic Ligands into Crystalline Networks. Huang, Guo; Tsang, Chun-Kwan; Xu, Zhengtao; Li, Kunhao; Zeller, Matthias; Hunter, Allen D.; Chui, Stephen Sin-Yin; Che, Chi-Ming. *Crystal Growth & Design* **2009**, 9(3), 1444-1451.
  15. cis-[Aqua/methanol(0.45/1.55)](1,1,1-trifluoro-5,5-dimethylhexane-2,4-dionato)nickel(II)-cis-[aqua/methanol(1.49/0.51)](1,1,1-trifluoro-5,5-dimethylhexane-2,4-dionato)nickel(II) (1/1). G. O. Hunter, M. Zeller & B. D. Leskiw, *Acta Cryst.* **2009**, E65, m221-m222.
  16. [Bis(diphenylphosphino)methane-2P,P']dichloridopalladium(II). M. Shahid, Imtiaz-ud-Din, M. Mazhar, M. Zeller & A. D. Hunte. *Acta Cryst.* **2009**, E65, m158-m159.
  17. Synthesis, Structure and Optical Properties of the Platinum(II) Complexes of Indaphyrin and Thiaindaphyrin, Kim S. F. Lau, Shengxian Zhao, Claudia Ryppa, Steffen Jokusch, Nicholas N. Turro, Matthias Zeller, Martin Gouterman, Gamal E. Khalil, and Christian Br6ckner, *Inorg. Chem.* **2009**, 48(9), 4067-4074.
  18. Facile Synthesis of (Phosphine)- and (N-heterocyclic Carbene)Gold(I) and Silver(I) Azide Complexes Partyka, David V.; Robilotto, Thomas J.; Updegraff, James B., III; Zeller, Matthias; Hunter, Allen D.; Gray, Thomas G., *Organometallics* **2009**, 28(3), 795-801.

19. Synthesis, characterization and thermal behavior of two 4d-4f coordination polymers based on N and O donor ligands, Lian, Qing-Yang; Huang, Chun-De; Zeng, Rong-Hua; Qiu, Yong-Cai; Mou, Ji-Xia; Deng, Hong; Zeller, Matthias, *Z. Anorg. Allg. Chem.* **2009**, 635(2), 393-398.
20. Tetrakis[(3-hydroxypropyl)dimethylammonium] tetra- $\mu$ -acetato- $\kappa^8$ O'O'-bis[chloridocuprate(II)](Cu-Cu) dichloride, Shahid, Muhammad; Mazhar, Muhammad; Zeller, Matthias; Hunter, Allen D., *Acta Cryst. E* **2009**, 65(3), m345-m346.
21. Networks of Hexagonal Hierarchy from a Self-Similar Tritopic Molecule, Yan-Quiong Sun, Chen Yang, Zhengtao Xu, Matthias Zeller, Allen D. Hunter, *Crystal Growth & Design* **2009**, 9(4), 1663-1665.
22. Probing the Steric Limits of Carbon-Gold Bond Formation: (Dialkylbiarylphosphine)gold(I) Aryls, Davod V. Partyka, James B. Updegraff III, Matthias Zeller, Allen D. Hunter, and Thomas G. Gray, *Organometallics* **2009**, 28(6), 1666-1674.
23. An aza-cyclophane stacked in racemic columnar assemblies: Whole molecular disorder in a 2D solid solution, Matthias Zeller, Marlon R Lutz Jr., Daniel P. Becker, *Acta Cryst. B* **2009**, B65(2), 223-229, S223/1-S223/10.
24. 9-Chloro-1-methyl-7-phenyl-5,6-dihydro-13H-indolo[3,2-c]acridine, Makuteswaran Sridharan, Karnam J. Rajendra Prasad and Matthias Zeller, *Acta Cryst. E* **2009**, E65, o1064.
25. MTO/H<sub>2</sub>O<sub>2</sub>/Pyrazole-Mediated N-Oxidation of *meso*-Tetraarylporphyrins and -chlorins, and S-Oxidation of a *meso*-Tetraaryldithiaporphyrin and -chlorin, Subhadeep Banerjee, Matthias Zeller and Christian Brückner, *J. Org. Chem.*, Articles ASAP, Publication Date (Web): May 7, **2009**.
26. Building thiol and metal-thiolate functions into coordination nets: Clues from a simple molecule, Jun He, Chen Yang, Zhengtao Xu, Matthias Zeller, Allen D. Hunter, Jianhua Lin, *J. Solid State Chem.*, In Press, Accepted Manuscript, Available online 4 May **2009**.
27. Structural characterization of sulfoildenafilil, an analog of sildenafilil, Samuel R. Gratz, Matthias Zeller, Daryl W. Mincey, Cheryl L. Flurer, *J. Pharmac. and Biomed. Anal.*, In Press, Corrected Proof, Available online 10 April **2009**.
28. Ru(II)-DMSO complexes containing aromatic and heterocyclic acid hydrazides: Structure, electrochemistry and biological activity, Viswanathan Mahalingam, Nataraj Chitrapriya, Matthias

Zeller, Karuppanan Natarajan, *Polyhedron*, In Press, Corrected Proof, Available online 31 March 2009.

29. Whole Molecule Disorder in a Solid Solution of Two Indoloacridines, Makuteswaran Sridharan, Karnam Jayarampillai Rajendra Prasad, Amanda E. Kotheimer, Timothy R. Wagner and Matthias Zeller, *J. Chem. Cryst.* **2009**, accepted manuscript, in press.
30. Oxazolochlorins. 2. Intramolecular Cannizzaro Reaction of *meso*-Tetraphenylsecochlorin Bisaldehyde, Joshua Akhigbe, Claudia Ryppa, Matthias Zeller, and Christian Brückner, *J. Org. Chem.* **2009**, accepted manuscript, in press.

**2008:**

1. Pyranosyl N-glycosyl amines: emerging targets with diverse biological potential, (Review article) P. Norris, *Current Topics in Medicinal Chemistry* **2008**, 8, 101-113.
2. 6-Rings, 1 other element, (Book chapter) P. Norris, in *Comprehensive Heterocyclic Chemistry*, A. R. Katritzky (Ed.), Elsevier, **2008**.
3. 1-Oxa-2,4-diazines and 1-thia-2,4-diazines, (Book chapter) P. Norris, in *Comprehensive Heterocyclic Chemistry*, A. R. Katritzky (Ed.), Elsevier, **2008**.
4. Carbohydrate mimetics as potential antiinfective treatments for *Staphylococcus aureus*, D. L. Fagan, M. Royal, M. L. Vicarel, and P. Norris, *FASEB J.* **2008**, 22:859.20.
5. Del Bene, Janet E.; Alkorta, Ibon; Elguero, Jose. Systematic Comparison of Second-Order Polarization Propagator Approximation (SOPPA) and Equation-of-Motion Coupled Cluster Singles and Doubles (EOM-CCSD) Spin-Spin Coupling Constants for Molecules with C, N, and O Double and Triple Bonds and Selected F-Substituted Derivatives. *Journal of Chemical Theory and Computation* **2008**, 5(1), 208-216.
6. Wepukhulu, Wickliffe O.; Smiley, Vanessa L.; Vemulapalli, Bhargavi; Smiley, Jeffrey A.; Phillips, Linda M.; Lee, Jeehiun K. A substantial oxygen isotope effect at O2 in the OMP decarboxylase reaction: Mechanistic implications. *Organic & Biomolecular Chemistry* **2008**, 6(24), 4533-4541.

7. Del Bene, Janet E.; Provasi, Patricio F.; Alkorta, Ibon; Elguero, Jose. Resolving an apparent discrepancy between theory and experiment: spin-spin coupling constants for FCCF. *Magnetic Resonance in Chemistry* **2008**, *46*(11), 1003-1006.
8. Del Bene, Janet E.; Elguero, Jose.  $^{19}\text{F}$ - $^{19}\text{F}$  and  $^{19}\text{F}$ - $^1\text{H}$  spin-spin coupling constants in cyclic FH polymers  $(\text{FH})_n$ ,  $n=2-6$ . *Solid State Nuclear Magnetic Resonance* **2008**, *34*(1-2), 86-92.
9. Del Bene, Janet E.; Elguero, Jose. Spin-spin coupling constants for water polymers and hydronium ion complexes with water. *Molecular Physics* **2008**, *106*(12-13), 1461-1471.
10. Chandler, Julie M.; Treece, Erin R.; Trenary, Heather R.; Brenneman, Jessica L.; Flickner, Tressa J.; Frommelt, Jonathan L.; Oo, Zaw M.; Patterson, Megan M.; Rundle, William T.; Valle, Olga V.; Kim, Thomas D.; Walker, Gary R.; Cooper, Chester R., Jr. Protein profiling of the dimorphic, pathogenic fungus, *Penicillium marneffeii*. *Proteome Science* **2008**, *6*, No pp. given.
11. Del Bene, Janet E.; Alkorta, Ibon; Elguero, Jose. Spin-Spin Coupling across Intermolecular F-Cl $\cdots$ N Halogen Bonds. *Journal of Physical Chemistry A* **2008**, *112*(34), 7925-7929.
12. Del Bene, Janet E.; Alkorta, Ibon; Elguero, Jose. Ab Initio EOM-CCSD Spin-Spin Coupling Constants for Hydrogen-Bonded Formamide Complexes: Bridging Complexes with  $\text{NH}_3$ ,  $(\text{NH}_3)_2$ ,  $\text{H}_2\text{O}$ ,  $(\text{H}_2\text{O})_2$ , FH, and  $(\text{FH})_2$ . *Journal of Physical Chemistry A* **2008**, *112*(28), 6338-6343.
13. The hydrogen bond, A.D. Buckingham, J.E. Del Bene and S.A.C. McDowell, *Chemical Physics Letters* **2008**, *463*(1-3), 1-10
14. "Spin-spin Coupling across Intramolecular N-H $\cdots$ N Hydrogen Bonds in Models For Proton Sponges: An Ab Initio Investigation" J. E. Del Bene, I. Alkorta, and J. Elguero. *Magn. Reson. Chem.* **2008**, *46*(5), 457-463.
15. A Systematic Comparison of Second-Order Polarization Propagator Approximation (SOPPA) and Equation-of-Motion Coupled Cluster Singles and Doubles (EOM-CCSD) Spin-Spin Coupling Constants for Selected Singly Bonded Molecules, and the Hydrides  $\text{NH}_3$ ,  $\text{H}_2\text{O}$ , and HF and Their Protonated and Deprotonated Ions and Hydrogen-Bonded Complexes, Del Bene, Janet E.; Alkorta, Ibon; Elguero, Jose., *J. Chem. Theor. Comput.* **2008**, *4*(6), 967-973.

16. Single Source Heterobimetallic Precursors for the Deposition of Cu-Ti Mixed Metal Oxide Thin Films, Asif Ali Tahir, Mazhar Hamid, Muhammad Mazhar, Matthias Zeller, Allen D. Hunter, Muhammad Nadeem, Muhammad Javed Akhtar, *Dalton Trans.* **2008**, 1224-1232.
17. Dialkylbiarylphosphine Complexes of Gold(I) Halides. Gold-Aryl  $\pi$ -Interactions in the Solid State. Partyka, David V.; Robilotto, Thomas J.; Zeller, Matthias; Hunter, Allen D.; Gray, Thomas G., *Organometallics* **2008**, 27(1), 28-32.
18. Triethynylphosphine oxide. Kallamadi, Ramnath; Jackson, John A.; Zeller, Matthias, *Acta Cryst E* **2007**, E63(12), o4563.
19. Crystal Structure of 2,8,14,20-tert-Butylpyrogallol[4]arene, Dueno, Eric E.; Hunter, Allen D.; Zeller, Matthias; Ray, Thomas A.; Salvatore, Ralph N.; Zambrano, Cesar H. *J. Chem. Cryst.* **2008**, 38(3), 181-187.
20. A new two-dimensional AgI coordination polymer with Ag...C interactions: Thermal, fluorescence, structural and solution studies. Akhbari, Kamran; Morsali, Ali; Rafiei, Shahnaz; Zeller, Matthias. *J. Organometal. Chem.* **2008**, 693(2), 257-262.
21. Bis(diphenylphosphino)methane Induces Unusual Cyclometalation of Thiophene and Phenyl Rings (R) at the C2 Carbon of Thiosemicarbazones {R-C<sub>2</sub>(H) = N<sub>3</sub>-N<sub>2</sub>H-C(=S)-N<sub>1</sub>H<sub>2</sub>} in Ruthenium(II) Complexes. Lobana, Tarlok S.; Bawa, Gagandeep; Castineiras, A.; Butcher, Ray J.; Zeller, M.. *Organometallics* **2008**, 27(2), 175-180.
22. Novel homochiral holodirected three-dimensional lead(II) coordination polymer, [Pb<sub>2</sub>( $\mu$ -bpa)<sub>3</sub>( $\mu$ -NO<sub>3</sub>)<sub>2</sub>(NO<sub>3</sub>)<sub>2</sub>]<sub>n</sub>: Spectroscopic, thermal, fluorescence and structural studies, Alireza Aslani, Ali Morsali and Matthias Zeller, *Solid State Sciences*, **2008**, 10(7), 854-858.
23. Synthesis, crystal structure and biological activities of dehydroacetic acid complexes of Ru(II) and Ru(III) containing PPh<sub>3</sub>/AsPh<sub>3</sub>, N. Chitrapriya, V. Mahalingam, M. Zeller, R. Jayabalan, K. Swaminathan and K. Natarajan, *Polyhedron* **2008**, 27(3), 939-946.
24. Coordination behaviour of ferrocenylthiosemicarbazone in a novel hetero trinuclear nickel(II) complex: Synthesis, spectral, electrochemistry and X- ray crystallography, R. Prabhakaran, R. Huang, S.V. Renukadevi, R. Karvembu, M. Zeller and K. Natarajan, *Inorg. Chim. Acta* **2008**, 361(8), 2547-2552.

25. Mercury(II) bromide/iodide coordination polymers by self-assembly of a long flexible Schiff base ligand, Ghodrath Mahmoudi, Ali Morsali and Matthias Zeller, *Solid State Sciences* **2008**, 10(3), 283-290.
26. Nano-structures of Two New Lead(II) coordination polymers; New Precursors For Preparation of PbS Nano-structures, Alireza Aslani, Ali Morsali and Matthias Zeller, *Solid State Sciences* **2008**, 10(11), 1591-1597.
27. A Three-dimensional AgI Coordination Polymer Constructed via  $\eta^2$  Ag-C Bonds: Thermal, Fluorescence, Structural and Solution Studies, Robabeh Bashiri, Kamran Akhbari, Ali Morsali and Matthias Zeller, *J. Organomet. Chem.* **2008**, 693(10), 1903-1911.
28. Novel Ru(II) oximate Complexes with Silent oxygen atom: Synthesis, Chemistry and Biological activities, Nataraj Chitrapriya, Viswanathan Mahalingam, Landry C Channels, Matthias Zeller, Frank R. Fronczek and Karuppanan Natarajan, *Inorg. Chim. Acta* **2008**, 361(9-10), 2841-2850.
29. Reversible shrinkage and expansion of a blue photofluorescent cadmium coordination polymer and in situ tetrazole ligand synthesis. Deng, Hong; Qiu, Yong-Cai; Li, Ying-Hua; Liu, Zhi-Hui; Zeng, Rong-Hua; Zeller, Matthias; Batten, Stuart R. *Chem. Commun.* **2008**, 2239-2241.
30. Synthesis, characterization and crystal structures of cyclometalated Ru(II) carbonyl complexes formed by hydrazones. Chitrapriya, Nataraj; Mahalingam, Viswanathan; Zeller, Matthias; Natarajan, Karuppanan. *Polyhedron* **2008**, 27(6), 1573-1580.
31. CuCN Pillars Induce Face-to-Face  $\pi$ -Overlap of Anthracene-Based Thioether Molecules within a Hybrid Coordination Network. Sun, Yan-Qiong; Tsang, Chun-Kwan; Xu, Zhengtao; Huang, Guo; He, Jun; Zhou, Xiao-Ping; Zeller, Matthias; Hunter, Allen D. *Crystal Growth & Design* **2008**, 8(5), 1468-1470.
32. The influence of substituents at C2 carbon atom of thiosemicarbazones {R(H)C2=N3-N2(H)-C1(=S)-N1H2} on their dentacy in PtII/PdII complexes: synthesis, spectroscopy, and crystal structures, Lobana, Tarlok S.; Bawa, Gagandeep; Hundal, Geeta; Zeller, M., *Z. Anorg. Allgem. Chem.* **2008**, 634(5), 931-937.
33. Construction of an Unusual Three-dimensional Transition-Metal Lanthanide Ln/Cu(Br/Cl) Coordination Polymer with Isonicotinate as the Single Ligand, Hong Deng, Zhihui Liu, Yongcai Qiu, YingHua Li, Matthias Zeller, *Inorg. Chem. Commun.* **2008**, 11(9), 978-981.

34. The influence of the substituents at N<sup>1</sup> nitrogen on geometry of nickel(II) complexes with heterocyclic thiosemicarbazones, Tarlok S. Lobana, Poonam Kumari, Matthias Zeller, Ray J. Butcher, *Inorg. Chem. Commun.* **2008**, 11(9), 972-974.
35. Rhodium(II)-catalyzed decomposition of 3-O-(2-diazo-2-phenylacetyl)-1,2;5,6-di-O-isopropylidene- $\alpha$ -D-allofuranose: diastereoselective ether formation, Iulia A. Sacui, Matthias Zeller, Peter Norris, *Carbohydrate Research* **2008**, 343(10-11), 1819-1823.
36. Synthesis of New Copper Cyanide complexes via the Transformation of Organonitrile to Inorganic Cyanide, Deng, Hong; Qiu, Yongcai; Daiguebonne, Carole; Kerbellec, Nicolas; Guillou, Olivier; Zeller, Matthias; Batten, Stuart R. *Inorg. Chem.* **2008**, 47(13), 5866-5872.
37. Dinuclear copper(II) complexes with bis-thiocarbohydrazone ligands, Diana Dragancea, Anthony W. Addison, Matthias Zeller, Laurence K. Thompson, Dushyanthi Hoole, Mihail D. Revenco & Allen D. Hunter, *Eur. J. Inorg. Chem.* **2008**, 16, 2530-2536.
38. 7,8,9,10-Tetrahydro-2-methylcyclohepta[b]indol-6(5H)-one. Sridharan, Makuteswaran; Prasad, Karnam J. Rajendra; Ngendahimana, Aimable; Zeller, Matthias. *Acta Cryst. E* **2008**, E64(7), o1207.
39. Spectroscopic, thermal and structural studies of a new mercury(II) one-dimensional coordination polymer, [Hg(3-bpo)<sub>2</sub>(SCN)<sub>2</sub>], 3-bpo = 2,5-bis(3-pyridyl)-1,3,4-oxadiazole. Fard-Jahromi, Mohammad Jafar Soltanian; Morsali, Ali; Zeller, Matthias. *J. Coord. Chem.* **2008**, 61(14), 2227-2233.
40. Reversible Anion Exchange and Sensing in Large Porous Materials Built from 4,4'-Bipyridine via  $\pi$ - $\pi$  and H-Bonding Interactions. Qiu, Yongcai; Liu, Zhihui; Li, Yinghua; Deng, Hong; Zeng, Ronghua; Zeller, Matthias. *Inorg. Chem.* **2008**, 47(12), 5122-5128.
41. A three-dimensional AgI coordination polymer constructed via  $\eta^2$  Ag-C bonds: Thermal, fluorescence, structural and solution studies. Bashiri, Robabeh; Akhbari, Kamran; Morsali, Ali; Zeller, Matthias. *J. Organometal. Chem.* **2008**, 693(10), 1903-1911.
42. Beckmann rearrangement of cyclotrimeratrylene (CTV) oxime: tandem Beckmann-electrophilic aromatic addition, Marlon R. Lutz Jr., Matthias Zeller, Daniel P. Becker, *Tetrahedron Let.* **2008**, 49(34), 5003-5005.

43. Coordination Networks from a Bifunctional Molecule Containing Carboxyl and Thioether Groups. Zhou, Xiao-Ping; Xu, Zhengtao; Zeller, Matthias; Hunter, Allen D.; Chui, Stephen Sin-Yin; Che, Chi-Ming. *Inorg. Chem.* **2008**, *47*(17), 7459-7461.
44. Construction of isostructural Ln–Ag (Ln = Eu; Tb; Dy) nano-channel heterometallic coordination frameworks based on pyrazine-2-carboxylate and oxalate ligands, Hong Deng, Ying-Hua Li, Yong-Cai Qiu, Zhi-Hui Liu, Matthias Zeller, *Inorg. Chem. Commun.* **2008**, *11*(10), 1151-1154.
45. Dynamic crystal-to-crystal conversion of a 3D-3D coordination polymer by de- and re-hydration. Aslani, Alireza; Morsali, Ali; Zeller, Matthias, *Dalton Trans.* **2008**, *38*, 5173-5177.
46. Pyridine Adducts of Nickel(II) Xanthates as Single-Source Precursors for the Aerosol-Assisted Chemical Vapor Deposition of Nickel Sulfide. Alam, Naveed; Hill, Michael S.; Kociok-Kohn, Gabriele; Zeller, Matthias; Mazhar, Muhammad; Molloy, Kieran C., *Chemistry of Materials* **2008**, *20*(19), 6157-6162.
47. A porphyrin complex of Gold(I): (phosphine)gold(I) azides as cation precursors. Partyka, David V.; Robilotto, Thomas J.; Zeller, Matthias; Hunter, Allen D.; Gray, Thomas G., *Proceedings of the National Academy of Sciences of the United States of America*, Early Edition **2008**, (Sept 9 2008), 1-5.
48. A porphyrin complex of Gold(I): (phosphine)gold(I) azides as cation precursors. Partyka, David V.; Robilotto, Thomas J.; Zeller, Matthias; Hunter, Allen D.; Gray, Thomas G., *Proceedings of the National Academy of Sciences of the United States of America*, **2008**, *105*(38), 14293-14297.
49. Di- $\mu$ -bromido-bis[bromido(di-2-pyridylmethanediol- $\kappa^2N,N'$ )copper(II)] dihydrate, B. L. Westcott, K. M. Kopp-Vaughn, L. M. Daniels and M. Zeller, *Acta Cryst. E* **2008**, *E64*, m1122-m1123.
50. *catena*-Poly[[ $\mu$ -bromido-( $\mu$ -hydroxydi-2-pyridylmethanolato- $\kappa^4N,O:N'$ )dicopper(II)(Cu-Cu)]-di- $\mu$ -bromido], M. Zeller, B. L. Westcott, K. M. Kopp-Vaughn and A. D. Hunter, *Acta Cryst. E* **2008**, *E64*, m1121.
51. Syntheses of pyrazolo-, isoxazolo-, pyrido- and pyrimido-carbazoles from 2-(3',4'-dimethoxybenzylidene)-2,3,4,9-tetrahydrocarbazol-1-ones. Makuteswaran Sridharan, Lucas K. Beagle, Matthias Zeller and Karnam Jayarampillai Rajendra Prasada, *J. Chem. Res.* **2008**, 572-577.

52. 2,2-Dimethyl-2,3-dihydropyrano[2,3-a]carbazol-4(1H)-one, Makuteswaran Sridharan, Karnam J. Rajendra Prasad, Aimable, Ngendahimana and Matthias Zeller, *Acta Cryst. E* **2008**, E64, o2155.
53. 2,2,9-Trimethyl-2,3-dihydropyrano[2,3-a]carbazol-4-(1H)-one, Makuteswaran Sridharan, Karnam J. Rajendra Prasad and Matthias Zeller, *Acta Cryst. E* **2008**, E64, o2156.
54. 2,2,10-Trimethyl-2,3-dihydropyrano[2,3-a]carbazol-4(1H)-one Makuteswaran Sridharan, Karnam J. Rajendra Prasad, Aimable, Ngendahimana and Matthias Zeller, *Acta Cryst. E* **2008**, E64, o2157.
55. Construction of three-dimensional Ln-Ag (Ln=Eu; Tm) coordination polymers based on isonicotinate and oxalate ligands. Mou, Ji-Xia; Zeng, Rong-Hua; Qiu, Yong-Cai; Zhang, Wei-Guang; Deng, Hong; Zeller, Matthias. *Inorg. Chem. Commun.* **2008**, 11(11), 1347-1351.
56. Synthesis, structures and luminescent properties of 4d-4f heterometallic coordination frameworks based on lanthanide oxalate substructures with nicotinate bridging ligands. Liu, Zhi-Hui; Qiu, Yong-Cai; Li, Ying-Hua; Deng, Hong; Zeller, Matthias. *Polyhedron* **2008**, 27(17), 3493-3499.
57. Three-dimensional hemidirected mixed-ligand lead(II) coordination polymer,  $[\text{Pb}_2(\text{bpa})_2(\text{SCN})_3(\text{NO}_3)]_n$  (bpa = 1,2-di(4-pyridyl)ethane). Abedini, Jafar; Morsali, Ali; Zeller, Matthias; *Z. Anorg. Allg. Chem.* **2008**, 634(14), 2659-2662.
58. "Structures, bonding, and one-bond B-N and B-H spin-spin coupling constants for a series of neutral and anionic five-membered rings containing BN bonds" M. Yáñez, O. Mó, I. Alkorta, and J. E. Del Bene. *J. Chem. Theory Comput.* **2008**, 4, 1869.
59. Spectroscopic, Thermal and Structural Studies of a New Mercury(II) Complex of 4'-(4-Pyridyl)-2,2':6',2''-terpyridine (Pyterpy) Ligand,  $[\text{Hg}(\text{Hpyterpy})(\text{SCN})_2]_2(\text{MeSO}_4)_2$  G. Mahmoudi, A. Morsali, and M. Zeller, *J. Iran. Chem. Soc.* **2008**, 5(4), 574-578.
60. "Changing Science Teachers' Beliefs." Cripe, M. K.; Lovelace-Cameron, S. *Academic Exchange Quarterly*, **2008**, (2), #4032-81.
61. "Mechanical and Chemical Modification of Wood Materials – Compressed Wood and Oxidized Charcoal." Vasily I. Patyakin, Uzum. U. Sugaipov, Alexei R. Birman, Sergei M. Bazarov, Yuri N. Pilshikov, Andrei A. Spitsyn and Howard D. Mettee, *BioResources*, 3(3), **2008**. pp731-744.

62. Pyridine Adducts of Nickel(II) Xanthates as Single-Source Precursors for the Aerosol-Assisted Chemical Vapor Deposition of Nickel Sulfide, Naveed Alam, Michael S. Hill, Gabriele Kociok-Kohn, Matthias Zeller, Muhammad Mazhar, and Kieran C. Molloy, *Chem. Mater.* **2008**, 20 (19), 6157-6162.

**2007:**

1. Carbohydrate mimetics for *Staphylococcus aureus* capsule, D. L. Fagan, M.L. Vicarel, A.-B. Alhassan, and P. Norris, *FASEB J.* **2007**, 21:712.1.
2. Carbonyl(5-carboxypyridine-2-carboxylato- $\kappa^2N,O^2$ )chlorobis(triphenylphosphine- $\kappa P$ )ruthenium(II) 0.345-hydrate benzene sesquisolvate Duraiswamy Sukanya, Karuppanan Natarajan, Brian Dobosh and Matthias Zeller, *Acta Cryst. E* **2007**, E63, m-135-m137.
3. Carbon-Gold Bond Formation through [3 + 2] Cycloaddition Reactions of Gold(I) Azides and Terminal Alkynes, David V. Partyka, James B. Updegraff, Matthias Zeller, Allen D. Hunter, and Thomas G. Gray, *Organometallics* **2007**, 26(1), 183-186.
4. Dimethylthioarsinic anhydride: A Standard for Arsenic Speciation. Michael Fricke, Matthias Zeller, William Cullen, Mark Witkowski and John Creed, *Analytica Chimica Acta* **2007**, 583, 78-83.
5. Bis( $\mu$ -acetylacetonato- $\kappa^2O:O'$ )bis[(acetylacetonato- $\kappa^2O:O'$ )-aquanickel(II)] hemihydrate, Asif A. Tahir, Mazhar Hamid, Matthias Zeller, Muhammad Mazhar and Allen D. Hunter, *Acta Cryst. E* **2007**, E63, m272-m274.
6. Attacking Boron Nucleophiles: NMR Properties of 5-Members Diazaborole Rings, J. E. Del Bene, J. Elguero, I. Alkorta, M. Yañez and O. Mó, *J. Phys. Chem. A* **2007**, 111(3), 418-421.
7.  $[Tl_2(\mu-Htdp)_2(\mu-H_2O)]_n$  ( $H_2tdp = 4,4'$ -thiodiphenol): A One-Dimensional Thallium(I) Coordination Polymer with a large Tetranuclear Metallacycle; Thermal, Emission and Structural Studies, Kamran Akhbari, Ali Morsali, Allen D. Hunter and Matthias Zeller, *Inorganic Chemistry Communications* **2007**, 10, 178-182.

8. Bis(dimethylphosphorylmethylene)durene, Allen D. Hunter and Matthias Zeller, *Acta Cryst. E* **2007**, *E63*, o802-o803.
9. Chloro[2-(N,N-dimethylamino)ethanol- $\kappa$ N]-[2-(N,N-dimethylamino)ethanolato- $\kappa^2$ N,O]-palladium(II) Mazhar Hamid, Asif Ali Tahir, Muhammad Mazhar, Matthias Zeller and Allen D. Hunter, *Acta Cryst. E* **2007**, *E63*, m728-m730.
10. Chloro[2-(N,N-dimethylamino)ethanol- $\kappa$ N][2-(N,N-dimethylamino)ethanolato- $\kappa^2$ N,O]palladium(II), Hamid, Mazhar; Tahir, Asif Ali; Mazhar, Muhammad; Zeller, Matthias; Hunter, Allen D., *Acta Cryst. E* **2007**, *E63*(3), m728-m730.
11.  $[\text{Th}_2(\text{m-Htdp})_2(\text{m-H}_2\text{O})]_n$  (H<sub>2</sub>tdp = 4,4'-thiodiphenol) - A one-dimensional thallium(I) coordination polymer with a large tetranuclear metallacycle: Thermal, emission and structural studies, Akhbari, Kamran; Morsali, Ali; Hunter, Allen D.; Zeller, Matthias. *Inorganic Chemistry Communications* **2007**, *10*(2), 178-182.
12. Spin-spin coupling constants for iminoboranes RBNH, HBNR, and RBNR, and comparisons with corresponding isoelectronic acetylenes RCCH and RCCR, for R = H, CH<sub>3</sub>, NH<sub>2</sub>, OH, F, J. E. Del Bene, J. Elguero, I. Alkorta, M. Yañez and O. Mó. *J. Chem. Theor. & Comp.* **2007**, *3*(2), 549-556.
13. Does the A-T or G-C Base-Pair Possess Enhanced Stability? Quantifying the Effects of CH...O Interactions and Secondary Interactions on Base-Pair Stability Using a Phenomenological Analysis and Ab Initio Calculations, J. R. Quinn, S. C. Zimmerman, J. E. Del Bene, and I. Shavitt, *J. Am. Chem. Soc.* **2007**, *129*(4), 934-941.
14. Crystal structure of 1-(2,3:5,6-Di-O-isopropylidene- $\beta$ -D-mannofuranosyl)-1H-[1,2,3]triazol-4,5-dicarboxylic acid diethyl ester, Seibel, Harry; Miner, Penny L.; Norris, Peter; Wagner, Timothy R., *J. Chem. Cryst.* **2007**, *37*(3), 157-163.
15. Variation of One-Bond X-Y Coupling Constants  $^1J(\text{X-Y})$  and the Components of  $^1J(\text{X-Y})$  with Rotation about the X-Y Axis for Molecules H<sub>m</sub>X-YH<sub>n</sub>, with X = N, O, P, S: The Importance of Nonbonding Electrons, J. E. Del Bene and J. Elguero, *J. Phys. Chem. A* **2007**, *111*, 2517.
16. N-(3-Phenylpropyl)guanidinium bromide. Stanford, Daniel J.; Fernandez, Richard A.; Zeller, Matthias; Hunter, Allen D. *Acta Cryst. E* **2007**, *E63*(4), o1934-o1936.

17. A Nickel(II) di- $\mu_2$ -Phenolato Bridged Dinuclear Complex: Weak Antiferromagnetic Interactions in Nickel(II) Dimers, Michael J. Prushan, Diana M. Tomezsko, Sam Lofland, Matthias Zeller and Allen D. Hunter, *Inorg. Chim. Acta* **2007**, 360(7), 2245-2254.
18. Heterobimetallic Molecular Cages for the Deposition of Cu/Ti and Cu/Zn Mixed-Metal Oxides. Hamid, Mazhar; Tahir, Asif A.; Mazhar, Muhammad; Zeller, Matthias; Hunter, Allen D, *Inorganic Chemistry* **2007**, 46(10), 4120-4127.
19. Ring opening of pyridines: the pseudo-cis and pseudo-trans isomers of tetra-n-butylammonium 4-nitro-5-oxo-2-pentenitrilate, Matthias Zeller, Virginia B. Pett and LeRoy W. Haynes, *Acta Cryst. C* **2007**, C63, o343-o346.
20. Multiple Bismuth(III)-Thioether Secondary Interactions Integrate Metalloporphyrin Ligands into Functional Networks. Li, Kunhao; Huang, Guo; Xu, Zhengtao; Zhang, Mingliang; Zeller, Matthias; Hunter, Allen D.; Chui, Stephen Sin-Yin; Che, Chi-Ming; Wong, Wai-Yeung. *Inorg. Chem.* **2007**, 46, 4844-4849.
21. 3,4,5-Trimethyl-1,2,4-triazole trihydrate. Beitelman, Adam D.; Sieracki, Nathan A.; Zeller, Matthias; Ferrence, Gregory M, *Acta Cryst. E* **2007**, E63(5), o2739-o2741.
22. Probing P-H<sup>+</sup>-P Hydrogen Bonds: Structures, Binding Energies, and Spin-Spin Coupling Constants, J. E. Del Bene, J. Elguero, I. Alkorta, *J. Phys. Chem. A* **2007**, 111(17), 3416-3422.
23. Hydrothermal synthesis and structure of an open framework Co<sub>0.7</sub>Zn<sub>1.3</sub>(PO<sub>4</sub>)<sub>2</sub>(NH<sub>3</sub>-CH<sub>2</sub>CH<sub>2</sub>NH<sub>3</sub>) and Co<sub>6.2</sub>(OH)<sub>4</sub>(PO<sub>4</sub>)<sub>4</sub>Zn<sub>1.80</sub>, a new adamite type phase, Aderemi Oki, Matthias Zeller, Yaneth Coranza, Jose Luevano and Allen D. Hunter, *Inorg. Chim. Acta* **2007**, 360(9), 2917-2922.
24. Synthesis, Characterization and Reactivity of a Trinuclear Copper(II) Thiocyanurate Complex: A Spin-Frustrated Molecular Propeller, Michael J. Prushan, Natalie K. Privette, Matthias Zeller, Allen D. Hunter, Sam Lofland and Stephen D. Preite, *Inorg. Chem. Commun.* **2007**, 10(6), 631-635.
25. Crystal structure of a butyllithium · 1,2-dipiperidinoethane dimer complex, Michael A. Nichols, Rachel M. Sobinsky, Allen D. Hunter, and Matthias Zeller, *J. Chem. Cryst.* **2007**, 37(6), 433-438.

26. Novel Coordination Mode of Chloride Ion in Holo- and Hemidirected One-dimensional PbII Coordination Polymer, Nader Noshiranzadeh, Ali Ramazani, Ali Morsali, Allen D. Hunter and Matthias Zeller, *Inorg. Chem. Commun.* **2007**, *10*, 738-742.
27.  $[\text{Hg}(\mu\text{-}4,4'\text{-bipy})(\mu\text{-AcO})(\text{AcO})]_n \times n/2\text{H}_2\text{O}$ , one-dimensional double-chain coordination polymer, syntheses, characterization, thermal, fluorescence, porous and structural studies, Ghodrath Mahmoudi, Ali Morsali, Allen D. Hunter, Matthias Zeller, *Inorg. Chim. Acta* **2007**, *360*, 3196–3202.
28. Gold(I) Pyrenyls: Excited-State Consequences of Carbon-Gold Bond Formation, David V. Partyka, Arthur E. Esswein, James B. Updegraff, Matthias Zeller, Allen D. Hunter, and Thomas G. Gray, *Organometallics* **2007**, *26*(14), 3279-3282.
29. p-Ferrocenylaniline, Danielle M. Bequeath, Matthias Zeller, William J. Karnofel, Courtney L. Hoch and Larry S. Curtin, *Acta Cryst. E* **2007**, *E63*, m1866–m1867.
30. Lobana, Tarlok S.; Khanna, Sonia; Butcher, Ray J.; Hunter, A. D.; Zeller, M., Methyl Substituent at C2 Carbon of Acetophenone Thiosemicarbazone Induces Unusual Heterobridging in the  $[(\text{Ph}_3\text{P})\text{Cu}(\mu\text{-I})_2(\mu\text{-S-Haptsc})\text{Cu}(\text{PPh}_3)]$  Dimer. *Inorg. Chem.* **2007**, *46*(15), 5826-5828.
31. 4'-(4-Pyridyl)-2,2':6',2''-terpyridine as ligand in the lead(II) complexes,  $[\text{Pb}(\text{pyterpy})(\text{MeOH})_2] \cdot \text{MeOH}$  and  $[\text{Pb}(\text{pyterpy})(\mu\text{-AcO})]_2(\text{ClO}_4)_2$  Nader Noshiranzadeh, Ali Ramazani, Ali Morsali, Allen D. Hunter, Matthias Zeller, *Inorg. Chim. Acta* **2007**, *360*, 3603–3609.
32. Unique Ag–C bonds, thermal, fluorescence, structural and solution studies of two-dimensional silver(I) coordination polymer, Kamran Akhbari, Ali Morsali, Matthias Zeller, *J. Organomet. Chem.* **2007**, *692*, 3788–3795.
33. Unusual substituent effects on the bonding of iminoboranes. Mo, Otilia; Yanez, Manuel; Martin Pendas, Angel; Del Bene, Janet E.; Alkorta, Ibon; Elguero, Jose. *Physical Chemistry Chemical Physics* **2007**, *9*(30), 3970-3977.
34. Can Changes in One-bond Spin-spin Coupling Constants in Acids Be Related to Gas-Phase Proton Affinities of Bases? Del Bene, Janet E.; Elguero, Jose. *Journal of Physical Chemistry A* **2007**, *111*(28), 6443-6448.

35. Solvent effects on one-bond B-Li coupling constants in boryllithium compounds. Del Bene, Janet E.; Elguero, Jose. *Magnetic Resonance in Chemistry* **2007**, *45*(6), 484-487.
36. Complexes with N-H+P Hydrogen Bonds: Structures, Binding Energies, and Spin-Spin Coupling Constants. Del Bene, Janet E.. *Journal of Physical Chemistry A* **2007**, *111*(25), 5509-5514.
37. Hexakis( $\mu$ -3-N,N-diisopropylthiocarbamate)hexasilver(I)(6 Ag-Ag), Yin, Xia; Xie, Mu Biao; Zhang, Wei Guang; Fan, Jun; Zeller, Matthias, *Acta Cryst. E* **2007**, *E63*, m2063-m2064.
38. 2,8,14,20-para-Methoxytetraphenylpyrogallol[4]arene dimethylformamide hexasolvate, Zambrano, Cesar; Thomas, Ray E.; Zeller, Matthias; Salvatore, Ralph N.; Dueno, Eric E., *Acta Cryst. E* **2007**, *E63*, o3452-o3453.
39. 3,4-Di-O-acetyl-2-azidodeoxy-1-O-nitro- $\alpha$ -L-fucose, McCutcheon, David C.; Norris, Peter; Zeller, Matthias, *Acta Cryst. E* **2007**, *E63*, o3484.
40. Preparation and Reactivity of 4,4'-diaminostilbene-2,2'-disulphonate, Rader, Natalie C.; Nees, Heather A.; Szalay, Paul S.; Zeller, Matthias; Hunter, Allen D., *J. Chem. Cryst.* **2007**, *37*(9), 609-614.
41. Metal complexes of pyrimidine derived ligands – Syntheses, characterization and X-ray crystal structures of Ni(II), Co(III) and Fe(III) complexes of Schiff base ligands derived from S-methyl/S-benzyl dithiocarbamate and 2-S-methylmercapto-6-methylpyrimidine-4-carbaldehyde, Somnath Roy, Tarak Nath Mandal, Anil Kumar Barik, Sachindranath Pal, Samik Gupta, Arijit Hazra, Ray J. Butcher, Allen D. Hunter, Matthias Zeller, Susanta Kumar Kar, *Polyhedron* **2007**, *26*, 2603–2611.
42. Synthesis and crystal structure of a neutral open framework cobalt(II) phosphate  $\text{Co}_6(\text{PO}_4)_4 \cdot 7\text{H}_2\text{O}$  with a channel structure, Aderemi Oki; Matthias Zeller; Aurelia Reynolds; Xiangdong Qiu; Allen D. Hunter, *J. Coord. Chem.* **2007**, *60*(9), 995-1004.
43. 2,3,8,12,13-Pentamethoxy-5H-dibenzo[*c,n*]acridin-7(6H)-one toluene solvate Marlon R. Lutz Jr, Matthias Zeller and Daniel P. Becker, *Acta Cryst.* **2007**, *E63*, o3857–o3858.
44. Luminescent, three-coordinate azadipyromethene complexes of d(10) copper, silver, and gold. Thomas S. Teets, David V. Partyka, Arthur J. Esswein, James B. Updegraff, III, Matthias Zeller, Allen D. Hunter, and Thomas G. Gray, *Inorg. Chem.* **2007**, *46*(16), 6218-6220.

45. Spectroscopy, Thermal and Structural Studies of New ZnII Coordination Polymer,  $[\text{Zn}_3(\mu\text{-bpa})_{4.5}(\text{AcO})_3](\text{ClO}_4)_3 \cdot 4.26\text{H}_2\text{O}$ . Maryam Ghoreishi Amiri, Ali Morsali, Allen D. Hunter and Matthias Zeller. *Solid State Sciences* **2007**, *9*, 1079-1084.
46. Hydrolytic cleavage of Schiff bases by  $[\text{RuCl}_2(\text{DMSO})_4]$ . Duraiswamy Sukanya, Michael R. Evans, Matthias Zeller and Karuppanan Natarajan. *Polyhedron* **2007**, *26*(15), 4314-4320.
47.  $\text{HC}\equiv\text{P}$  and  $\text{H}_3\text{C}-\text{C}\equiv\text{P}$  as Proton Acceptors in Protonated Complexes Containing Two Phosphorus Bases: Structures, Binding Energies, and Spin-Spin Coupling Constants. Alkorta, Ibon; Elguero, Jose; Del Bene, Janet E, *J. Phys. Chem.* **2007**, *111*(39), 9924-9930.
48. Zinc(II) nitrite coordination polymers based on rigid and flexible organic nitrogen donor ligands, Maryam Ghoreishi Amiri, Ghodrat Mahmoudi, Ali Morsali, Allen D. Hunter and Matthias Zeller, *Cryst. Eng. Comm.* **2007**, *9*, 686-697.
49. Mercury(II) coordination polymers generated from 1,4-bis(2 or 3 or 4-pyridyl)-2,3-diaza-1,3-butadiene ligands, Ghodrat Mahmoudi, Ali Morsali, Allen D. Hunter and Matthias Zeller, *Cryst. Eng. Comm.* **2007**, *9*, 704-714.
50. Probing the proton-transfer coordinate of complexes with F-H... P hydrogen bonds using one- and two-bond spin-spin coupling constants. Del Bene, Janet E.; Elguero, Jose, *Magnetic Resonance in Chemistry* **2007**, *45*(9), 714-719.
51. Proton-Bound Homodimers: How Are the Binding Energies Related to Proton Affinities? Chan, Bun; Del Bene, Janet E.; Radom, Leo, *J. Am. Chem. Soc.* **2007**, *129*(40), 12197-12199.
52. 2,2,8-Trimethyl-2,3-dihydropyrano[2,3-a]carbazol-4(1H)-one, Makuteswaran Sridharan, Karnam J. Rajendra Prasad and Matthias Zeller, *Acta Cryst.* **2007**, *E63*, o4344.
53. trans-Dimethanolbis(1,1,1-trifluoro-5,5-dimethylhexane-2,4-dionato)cobalt(II), Jordan O. Lerach, Matthias Zeller and Brian D. Leskiw, *Acta Cryst.* **2007**, *E63*, m2639.
54. Centripetal molecules as multifunctional building blocks for coordination networks. Sun, Yan-Qiong; He, Jun; Xu, Zhengtao; Huang, Guo; Zhou, Xiao-Ping; Zeller, Matthias; Hunter, Allen D., *Chem. Comm.* **2007**, *45*, 4779-4781.

55. Crystal Structures of Hexameric and Dimeric Complexes of Lithioisobutyrophenone, Nichols, Michael A.; Leposa, Christina M.; Hunter, Allen D.; Zeller, Matthias, *J. Chem. Cryst.* **2007**, 37(12), 825-829.
56. 3D Ln–Ag (Ln = Nd; Eu) coordination polymers based on N- and O-donor ligands: Synthesis, crystal structures and luminescence, Yongcai Qiu, Hanguo Liu, Yun Ling, Hong Deng, Ronghua Zeng, Guoyong Zhou and Matthias Zeller, *Inorg. Chem. Commun.* **2007**, 10, 1399-1403.
57. Triethynylphosphine oxide. Kallamadi, Ramnath; Jackson, John A.; Zeller, Matthias, *Acta Cryst E* **2007**, 63(12), o4563.
58. [5,10,15,20-Tetrakis(2,6-dimethoxyphenyl)porphyrinato]nickel(II)-toluene-dichloromethane (3/2/4): a mixed solvate. Conrad, Diane; DeCoskey, Jennifer; Yeisley, Christopher; Zeller, Matthias; Hunter, Allen D.; Zovinka, Edward P. *Acta Cryst E* **2007**, 63(11), m2824, Sm2824/1-Sm2824/17.
59. Methyl Substituent at C2 Carbon of Acetophenone Thiosemicarbazone Induces Unusual Heterobridging in the [(Ph<sub>3</sub>P)Cu(m-I)<sub>2</sub>(m-S-Haptsc)Cu(PPh<sub>3</sub>)] Dimer. Lobana, Tarlok S.; Khanna, Sonia; Butcher, Ray J.; Hunter, A. D.; Zeller, M. *Inorg. Chem.* **2007**, 46(15), 5826-5828.
60. Assembly of Large Aromatic Selenoether Ligands into Cubic and Non-interpenetrated (10,3)-a Nets, Huang, Guo; Xu, Hanhui; Zhou, Xiao-Ping; Xu, Zhengtao; Li, Kunhao; Zeller, Matthias; Hunter, Allen D., *Crystal Growth & Design* **2007**, 7(12), 2542-2547.

## 2006:

1. Origin of the bathochromically shifted optical spectra of meso-tetrathien-2'- and 3'-ylporphyrins as compared to meso-tetraphenylporphyrin. Christian Brückner, Paul C. D. Foss, James O. Sullivan, Ryan Pelto, Matthias Zeller, Robert R. Birge, Guy Crundwell, *Phys. Chem. Chem. Phys.* **2006**, 8, 2402-2412.
2. Application of Bis(diphenylphosphino)ethane (DPPE) in Staudinger-type N-Glycopyranosyl Amide Synthesis. David P. Temelkoff, Craig R. Smith, Daniel A. Kibler, Shawn McKee, Sara J. Duncan, Matthias Zeller, Mo Hunsen, Peter Norris, *Carbohydrate Research* **2006**, 341(10), 1645-1656.

3. (4a*SR*,7*RS*,9a*RS*)-7-*tert*-Butyl-9a-methyl-5,5-dioxo-1,2,4a,9a-tetrahydro-8-oxa-5 $\lambda$ <sup>6</sup>-thiabenzocycloheptan-9-one, Matthias Zeller, Allen D. Hunter, Paul Sampson and Nataliya Chumachenko, *Acta Cryst. E* **2006**, E62, o367-o367.
4. (4a*SR*,7*SR*,9a*SR*)-7-*tert*-Butyl-9a-methyl-5,5-dioxo-1,2,4a,9a-tetrahydro-8-oxa-5 $\lambda$ <sup>6</sup>-thiabenzocycloheptan-9-one, Matthias Zeller, Allen D. Hunter, Paul Sampson and Nataliya Chumachenko, *Acta Cryst. E* **2006**, E62, o368-o369.
5. (4a*SR*,7*SR*,9a*SR*)-7-*tert*-Butyl-5,5-dioxo-1,2,4a,9a-tetrahydro-8-oxa-5 $\lambda$ <sup>6</sup>-thiabenzocycloheptan-9-one, Matthias Zeller, Allen D. Hunter, Paul Sampson and Nataliya Chumachenko, *Acta Cryst. E* **2006**, E62, o370-o371.
6. The Synthesis, Spectroscopic, Electrochemical and X-ray Diffraction Characterization of Novel Bridged Ferrocene Precursors for Use in Self-Assembled Monolayers. Carolyn A. Pugh, Michael W. Lufaso, Matthias Zeller, Timothy R. Wagner and Larry S. Curtin, *J. Organometal. Chem.* **2006**, 691, 680-686.
7. [2-(*N,N*-Dimethylamino)ethanol- $\kappa^2$ N,O]bis(2,4-pentanedionato- $\kappa^2$ O,O')manganese(II). Muhammad, Sultan; Mazhar, Muhammad; Zeller, Matthias; Hunter, Allen D. *Acta Cryst E* **2006**, 62(2), m224-m226.
8. 1-[(*E*)-Butadienylsulfonyl]-3,3-dimethylbut-2-yl methacrylate. Matthias Zeller, Allen D. Hunter, Paul Sampson and Nataliya Chumachenko, *Acta Cryst. E* **2006**, E62, o1369-o1370.
9. (3*RS*,4*RS*,4a*SR*,7*SR*,9a*RS*)-7-*tert*-Butyl-9a-methyl-5,5-dioxo-3,4-epoxy-1,2,3,4,4a,9a-hexahydro-8-oxa-5 $\lambda$ <sup>6</sup>-thiabenzocycloheptan-9-one, Matthias Zeller, Allen D. Hunter, Paul Sampson and Nataliya Chumachenko, *Acta Cryst. E* **2006**, E62, o1411-o1413.
10. Bis[2-(dimethylamino)ethanol- $\kappa^2$ N,O]-(2,4-pentanedionato- $\kappa^2$ O,O')nickel(II) acetate, Sultan Muhammad, Muhammad Mazhar, Matthias Zeller and Allen D. Hunter, *Acta Cryst. E* **2006**, E62, m824-m826.
11. 4-Acetamidobenzenesulfonyl azide, Monica L. Vicarel, Peter Norris, Matthias Zeller, *Acta Cryst. E* **2006**, E62, o1751-o1753.

12. Crystal structures of the methylene chloride disolvates of tetrakis(3,5-imethoxyphenyl)porphyrin and its isotopic copper(II) and nickel(II) complexes,  $C_{52}H_{46}N_4O_8 \times 2CH_2Cl_2$ ,  $Cu(C_{52}H_{44}N_4O_8) \times 2CH_2Cl_2$ ,  $Ni(C_{52}H_{44}N_4O_8) \times 2CH_2Cl_2$ . Matthias Zeller, Steven J. Dimuzio, Kyle Bee, Joseph Clemente, Jason Frederick, Anthony Fucci, Lia Gordon, Ashley Harper, Anthony Kasmar, Christopher Kasmar, Sarah Polomsky, Anita Simmons, David Smallsreed, Tomithia Underwood and Allen D. Hunter, *Z. Krist. NCS* **2006**, 221, 15-19.
13. N-Glycoside neoglycotrimers from 2,3,4,6-tetra-O-acetyl- $\beta$ -D-glucofuranosyl azide. David P. Temelkoff, Matthias Zeller and Peter Norris, *Carbohydrate Research* **2006**, 341, 1081-1090.
14. Del Bene, Janet E.; Elguero, Jose. Systematic ab Initio Study of  $^{15}N$ - $^{15}N$  and  $^{15}N$ - $^1H$  Spin-Spin Coupling Constants Across N-H $^+$ -N Hydrogen Bonds: Predicting N-N and N-H Coupling Constants and Relating Them to Hydrogen Bond Type. *Journal of Physical Chemistry A* **2006**, 110(23), 7496-7502.
15. Del Bene, Janet E. Anharmonicities, isotopes, and IR and NMR properties of hydrogen-bonded complexes. *Isotope Effects in Chemistry and Biology* **2006**, 153-174.
16. Kim, Myung Hwa; Leskiw, Brian D.; Shen, Lei; Suits, Arthur G. Velocity map imaging mass spectrometry. *International Journal of Mass Spectrometry* **2006**, 252(1), 73-78.
17. Dioxobis(pentane-2,4-dionato)(tetrahydrofuran)uranium(VI) Asif A. Tahir, Mazhar Hamid, Muhammad Mazhar, Matthias Zeller and Allen D. Hunter, *Acta Cryst. E* **2006**, E62, m1780-m1781.
18. 2,8,14,20-Tetraphenylpyrogallol[4]arene dimethylformamide octasolvate, Kass, Jordan Paul; Zambrano, Cesar H.; Zeller, Matthias; Hunter, Allen D.; Dueno, Eric Efrain, *Acta Cryst E* **2006**, E62(8), o3179-o3180.
19. Bis(acetate-O)bis(N,N-dimethylaminoethanol- $\kappa$ 2N,O)Cobalt(II), Asif A. Tahir, Mazhar Hamid, Muhammad Mazhar, Matthias Zeller, Allen D. Hunter, *Acta Cryst. E* **2006**, m1974-m1976.
20. Synthesis, crystal structures and multinuclear NMR spectroscopy of copper(I) complexes with benzophenone thiosemicarbazone, Tarlok S. Lobana, Sonia Khanna, Ray J. Butcher, A.D. Hunter, M. Zeller, *Polyhedron* **2006**, 25, 2755-2763.

21. The structure of protonated HCP: A classical or non-classical ion? Del Bene, Janet E.; Alkorta, Ibon; Elguero, Jose, *Chemical Physics Letters* **2006**, 429(1-3), 23-26.
22. Del Bene, Janet E.; Elguero, Jose. Substitution and protonation effects on spin-spin coupling constants in prototypical aromatic rings: C<sub>6</sub>H<sub>6</sub>, C<sub>5</sub>H<sub>5</sub>N and C<sub>5</sub>H<sub>5</sub>P. *Magnetic Resonance in Chemistry* **2006**, 44(8), 784-789.
23. Del Bene, Janet E.; Elguero, Jose; Alkorta, Ibon; Yanez, Manuel; Mo, Otilia. An ab Initio Study of <sup>15</sup>N-<sup>11</sup>B Spin-Spin Coupling Constants for Borazine and Selected Derivatives. *Journal of Physical Chemistry A* **2006**, 110(32), 9959-9966.
24. Synthesis, crystal structures and multinuclear NMR spectroscopy of copper(I) complexes with benzophenone thiosemicarbazone, Tarlok S. Lobana, Sonia Khanna, Ray J. Butcher, A.D. Hunter, M. Zeller, *Polyhedron* **2006**, 25, 2755-2763.
25. Crystal and molecular structure of the β-anomer of 6,7-dideoxy-1,2;3,4;9,10-tris-O-(1-methylethylidene)-D-erythro-α-D-galacto-undecopyranosid-8-ulose, Travis D. Weaver, Matthias Zeller, Peter Norris, *J. Chem. Cryst.* **2006**, 36(1), 647-654
26. 2,3,7,8-Tetrakis(5-chlorothien-2-yl)pyrazino[2,3-g]quinoxaline-para-xylene (3/2). Bellizzi, Mary; Crundwell, Guy; Zeller, Matthias; Hunter, Allen D.; McBurney, Brian. *Acta Cryst. E* **2006**, E62(11), o5249-o5251.
27. Del Bene Janet E; Elguero Jose Ab initio study of hydrogen bonding and proton transfer in 3:1 FH:NH<sub>3</sub> and FH:collidine complexes: structures and one- and two-bond coupling constants across hydrogen bonds. *The journal of physical chemistry. A, Molecules, spectroscopy, kinetics, environment & general theory* **2006**, 110(3), 1128-33.
28. Jimeno, Maria-Luisa; Alkorta, Ibon; Elguero, Jose; Del Bene, Janet E.. Computed coupling constants in X(CH<sub>3</sub>)<sub>n</sub>H<sub>(4-n)</sub> moieties where X = <sup>13</sup>C and <sup>15</sup>N+, and n = 0-4: comparisons with experimental data. *Magnetic Resonance in Chemistry* **2006**, 44(7), 698-707.
29. Del Bene, Janet E.; Elguero, Jose. Karplus-Type Equations for <sup>1</sup>J(X-Y) in Molecules HmX-YHn: (X, Y = N, O, P, S). *Journal of Physical Chemistry A* **2006**, 110(46), 12543-12545.

30. Del Bene, Janet E.; Elguero, Jose. Predicting and understanding the signs of one- and two-bond spin-spin coupling constant across X-H-Y hydrogen bonds. *Computational Chemistry (Singapore, Singapore)* **2006**, *10*, 229-264.
31. Ezer, Muhsin; Elwood, Seth A.; Jones, Bradley T.; Simeonsson, Josef B. Evaluation of a tungsten coil atomization-laser-induced fluorescence detection approach for trace elemental analysis. *Analytica Chimica Acta* **2006**, *571*(1), 136-141.
32. Relativistic Protons: Carbon-Gold Bond Formation by Transmetallation Reactions of Boronic Acids, David V. Partyka, Matthias Zeller, Allen D. Hunter, and Thomas G. Gray, *Angew. Chem. Int. Ed. Engl.* **2006**, *45*(48), 8188-8191.
33. Synthesis of Isostructural Cage Complexes of Copper with Cobalt and Nickel for Deposition of Mixed Ceramic Oxide Materials. Mazhar Hamid, Asif A. Tahir, Muhammad Mazhar, Matthias Zeller, Kieran C. Molloy, Allen D. Hunter, *Inorg. Chem.* **2006**, *45*(26), 10457-10466.
34. "Computed Coupling Constants in X(CH<sub>3</sub>)<sub>n</sub>H<sub>(4-n)</sub> Moieties where X = <sup>13</sup>C and <sup>15</sup>N<sup>+</sup>, and n = 0 – 4: Comparisons with Experimental Data" M.-L. Jimeno, I. Alkorta, J. Elguero, and J. E. Del Bene, *Magn. Reson. Chem.* **2006**, *44*, 698.

**2005:**

1. Chromatographic Separation and Identification of Products from the Reaction of Dimethylarsinic Acid with Hydrogen Sulfide. Fricke, Michael W.; Zeller, Matthias; Sun, Hongsui; Lai, Vivian W.-M.; Cullen, William R.; Shoemaker, Jody A.; Witkowski, Mark R.; Creed, John T. *Chemical Research in Toxicology* **2005**, 18(12), 1821-1829.
2. Alkorta, Ibon; Elguero, Jose; Del Bene, Janet E.. A theoretical investigation of N-H...OP hydrogen bonds through  $^{15}\text{N}$ - $^{31}\text{P}$  and  $^1\text{H}$ - $^{31}\text{P}$  coupling constants. *Chemical Physics Letters* (2005), 412(1-3), 97-100.
3. Alkorta, Ibon; Elguero, Jose; Mo, Otilia; Yanez, Manuel; Del Bene, Janet E.. Are resonance-assisted hydrogen bonds 'resonance assisted'? A theoretical NMR study. *Chemical Physics Letters* (2005), 411(4-6), 411-415.
4. Mo, Otilia; Yanez, Manuel; Del Bene, Janet E.; Alkorta, Ibon; Elguero, Jose. Cooperativity and proton transfer in hydrogen-bonded triads. *ChemPhysChem* (2005), 6(7), 1411-1418.
5. Chan, Bun; Del Bene, Janet E.; Elguero, Jose; Radom, Leo. On the Relationship between the Preferred Site of Hydrogen Bonding and Protonation. *Journal of Physical Chemistry A* (2005), 109(24), 5509-5517.
6. Krungkrai, Sudaratana R.; DelFraino, Brian J.; Smiley, Jeffrey A.; Prapunwattana, Phisit; Mitamura, Toshihide; Horii, Toshihiro; Krungkrai, Jerapan. A novel enzyme complex of orotate phosphoribosyltransferase and orotidine 5'-monophosphate decarboxylase in human malaria parasite *Plasmodium falciparum*: Physical Association, Kinetics, and Inhibition Characterization. *Biochemistry* (2005), 44(5), 1643-1652.
7. Hutchinson, Kelly M.; Bretz, Stacey Lowery; Mettee, Howard D.; Smiley, Jeffrey A.. A guided inquiry experiment for the measurement of activation energies in the biophysical chemistry laboratory. Decarboxylation of pyrrole-2-carboxylate. *Biochemistry and Molecular Biology Education* (2005), 33(2), 123-127.
8. Van Droogenbroeck, J.; Van Alsenoy, C.; Aucott, S. M.; Wheatley, M.; Woollins, J. D.; Hunter, A. D.; Blockhuys, F.: "Structure, Bonding and Reactivity of the Organometallic 1,3,2,4-Dithiadiazole Complex,  $\text{CpCoS}_2\text{N}_2$ ," *Organometallics*, 2005, 24, 1004-1011.

9. Pratap, P.; Hunter, A. D.; West, A.: "Remote Instrumentation," Proceedings of the NSF/AAAS Conference - "Invention and Impact: Building Excellence in Undergraduate Science, Technology, Engineering and Mathematics (STEM) Education", 2005, 99-104.
10. "The Influence of *Harmonia axyridis* on Wine Composition and Aging," Pickering, G. J., Lin, Y., Reynolds, A, Soleas, G, Riesen, R., Brindle, I. *J. Food Sci.* 2005, *70*(2), 128-135.
11. "The influence of *Harmonia axyridis* on wine composition and aging," Pickering, Gary J.; Lin, Yong; Reynolds, Andrew; Soleas, George; Riesen, Roland; Brindle, Ian *Journal of Food Science* 2005, *70*(2), S128-S135.
12. Chromatographic Separation and Identification of Products of the Reaction of DMA and H<sub>2</sub>S. Michael W. Fricke, Matthias Zeller, Hongsui Sun, Vivian W.-M. Lai, William R. Cullen, Jody Shoemaker, Mark R. Witkowski, John T. Creed, *Tox. & Appl. Pharm.* 2005, in press.
13. Semiconductive Coordination Networks from Bismuth(III) Bromide and 1,2-Bis(methylthio)phenylacetylene-Based Ligands. Li, Kunhao; Xu, Hanhui; Xu, Zhengtao; Zeller, Matthias; Hunter, Allen D., *Inorg. Chem.* 2005, ACS ASAP online & in press.
14. Glagovich, Neil M.; Reed, Elizabeth M.; Crundwell, Guy; Updegraff, James B., III; Zeller, Matthias; Hunter, Allen D.. N,N'-Bis(9H-fluoren-9-ylidene)benzene-1,2-diamine. *Acta Crystallographica, Section E: Structure Reports Online* (2005), E61(5), o1251-o1253.
15. McBurney, Brian; Crundwell, Guy; Updegraff, James B., III; Zeller, Matthias; Hunter, Allen D.. 5-Nitrothiophene-2-carbaldehyde. *Acta Crystallographica, Section E: Structure Reports Online* (2005), E61(5), o1221-o1222.
16. Stacy, Vanessa; Crundwell, Guy; Updegraff, James B., III; Zeller, Matthias; Hunter, Allen D.. 2,3-Bis(5-bromo-2-thienyl)-6,7-dichloroquinoxaline. *Acta Crystallographica, Section E: Structure Reports Online* (2005), E61(4), o904-o905.
17. Bis(acetylacetonato- $\kappa^2O,O'$ )(*N,N*-dimethylaminoethanol- $\kappa^2N,O$ )zinc(II). Mazhar Hamid, Muhammad Mazhar, Asif Ali, Matthias Zeller and Allen D. Hunter, *Acta Cryst. E* 2005, *E61*, m1539-m1541.
18. □-Acyloxysulfonyl Tethers for Intramolecular Diels-Alder Cycloaddition Reactions. Nataliya Chumachenko, Paul Sampson, Allen D. Hunter, Matthias Zeller. *Organic Letters* 2005, *7*(15),

3203-3206.

19. Bis(benzylsulfanyl)maleonitrile. Stanley Backiel, Besnik Bajrami, Allen D. Hunter, Matthias Zeller, M. J. Gerald Lesley, *Acta Cryst. E* 2005, *E61*(9), 2817-2819.
20. Inhibition of Carboxylesterases by Benzil (Diphenylethane-1,2-dione) and Heterocyclic Analogues is Dependent upon the Aromaticity of the Ring and the Flexibility of the Dione Moiety. Hyatt, Janice L.; Stacy, Vanessa; Wadkins, Randy M.; Yoon, Kyoung Jin P.; Wierdl, Monika; Edwards, Carol C.; Zeller, Matthias; Hunter, Allen D.; Danks, Mary K.; Crundwell, Guy; Potter, Philip M. *Journal of Medicinal Chemistry* 2005, *48*(17), 5543-5550.
21. Crystal and molecular structure of [5,10,15,20-tetrakisphenyl-2-ethoxy-3-oxa-chlorinato] Ag(II). Matthias Zeller, Allen D. Hunter, Jason R. McCarthy, Steven H. Capetta, Christian Brückner, *J. Chem. Cryst.* 2005, *35*(12), 935-942.
22. Redetermination of bis(2,4-pentanedionato)palladium(II). Hamid, Mazhar; Zeller, Matthias; Hunter, Allen D.; Mazhar, Muhammad; Tahir, Asif Ali, *Acta Cryst. E* 2005, *E61*(11), m2181-m2183.
23. The Incorporation of Single Crystal X-ray Diffraction into the Undergraduate Chemistry Curriculum Using Internet Facilitated Remote Diffractometer Control. Paul S. Szalay, Allen D. Hunter, Matthias Zeller. *J. Chem. Ed.* 2005, *82*(10), 1555-1557.
24. Humphries, J. A.; Ashe, A. M. H.; Smiley, J. A.; Johnston, C. G. Microbial community structure and trichloroethylene degradation in groundwater. *Canadian Journal of Microbiology* (2005), *51*(6), 433-439.
25. Alhassan, Abdul Basit; Norris, Peter; Zeller, Matthias. 1,2,3,4-Tetra-O-acetyl- $\alpha$ -L-fucopyranose. *Acta Crystallographica, Section E: Structure Reports Online* (2005), *E61*(11), o3668-o3669.
26. Del Bene, Janet E.; Elguero, Jose. Characterizing Hydrogen Bonding and Proton Transfer in 2:1 FH:NH<sub>3</sub> and FH:Collidine Complexes through One- and Two-Bond Spin-Spin Coupling Constants across Hydrogen Bonds. *Journal of Physical Chemistry A* (2005), *109*(47), 10759-10769.
27. Del DelBene, Janet E.; Elguero, Jose. Ab Initio Study of Complexes with Two Cations as N-H Donors to F<sup>-</sup>: Structures and Spin-Spin Coupling Constants across N-H-F Hydrogen Bonds.

Journal of Physical Chemistry A (2005), 109(47), 10753-10758.

28. Grove, Nathaniel; Bretz, Stacey Lowery. Sherlock Holmes and the case of the raven and the ambassador's wife: An inquiry-based murder mystery. *Journal of Chemical Education* (2005), 82(10), 1532-1533.
29. Zeller, Matthias; Wilcox, Robert J.; Snyder, Floyd G., III; Seibel, Harry A., II; Takas, Nathan J.; Hunter, Allen D. Hydrogen bonding in aromatic formamides. *Journal of Chemical Crystallography* (2005), 35(9), 723-729.
30. Perrine, Cynthia L.; Zeller, Matthias; Woolcock, John; Hunter, Allen D. Crystal structure of ferrocenyl amine. *Journal of Chemical Crystallography* (2005), 35(9), 717-721.
31. Zeller, Matthias; Chema, Andrew R.; Szalay, Paul S.; Hunter, Allen D. Reactivity of 1,2,4,5-tetracarboxylatebenzene with cobalt(II). *Journal of Chemical Crystallography* (2005), 35(6), 433-441.
32. Bequeath, Danielle M.; Porter, Richard L.; Lufaso, Michael W.; Wagner, Timothy R.; Kusnic, Rachel L.; Zeller, Matthias; Curtin, Larry S. 1,12-Diferrocenyldodecane at 100 K. *Acta Crystallographica, Section E: Structure Reports Online* (2005), E61(6), m1070-m1072.
33. Smiley, Jeffrey A.; Kundracik, Melisa; Landfried, Daniel A.; Barnes, Vincent R.; Axhemi, Armend A. Genes of the thymidine salvage pathway: Thymine-7-hydroxylase from a *Rhodotorula glutinis* cDNA library and iso-orotate decarboxylase from *Neurospora crassa*. *Biochimica et Biophysica Acta, General Subjects* (2005), 1723(1-3), 256-264.
34. Miner, Penny L.; Wagner, Timothy R.; Norris, Peter. Cu(I)-catalyzed formation of D-mannofuranosyl 1,4-disubstituted 1,2,3-triazolecarbohydrids. *Heterocycles* (2005), 65(5), 1035-1049.
35. Howard, Karen L.; Mike, James H.; Riesen, Roland. Validation of a solid-phase microextraction method for headspace analysis of wine aroma components. *American Journal of Enology and Viticulture* (2005), 56(1), 37-45.
36. Smith, Craig R.; Norris, Peter; Zeller, Matthias. Methyl 2,3,4-tri-O-acetyl-1-azido-1-deoxy- $\alpha$ -D-glucopyranuronate at 100 K. *Acta Crystallographica, Section E: Structure Reports Online* (2005), E61(3), o736-o737.

37. Norris, Peter; Zeller, Matthias. 2,3,4-Tri-O-acetyl- $\beta$ -L-fucopyranosyl azide. *Acta Crystallographica, Section E: Structure Reports Online* (2005), E61(3), o729-o730.
38. Maust, Mathew T.; Norris, Peter; Zeller, Matthias. Methyl 4-O-benzyl-6-deoxy-2,3-O-isopropylidene- $\beta$ -L-talopyranoside. *Acta Crystallographica, Section E: Structure Reports Online* (2005), E61(3), o643-o644.
39. Del Bene, Janet E.; Elguero, Jose; Alkorta, Ibon; Mo, Otilia; Yanez, Manuel. Ab Initio Study of the Influence of Trimer Formation on One- and Two-Bond Spin-Spin Coupling Constants Across an X-H-Y Hydrogen Bond: AH:XH:YH<sub>3</sub> Complexes for A, X = <sup>19</sup>F, <sup>35</sup>Cl and Y = <sup>15</sup>N, <sup>31</sup>P. *Journal of Physical Chemistry A* (2005), 109(10), 2350-2355.
40. Jack, Danielle R.; Zeller, Matthias; Wagner, Timothy R. Doubled-cubic Ca<sub>2</sub>NF. *Acta Crystallographica, Section C: Crystal Structure Communications* (2005), C61(1), i6-i8.
41. Zeller, Matthias; Hunter, Allen D. Tricarbonyl( $\eta^6$ -N,N-dimethylaniline)chromium(0). *Acta Crystallographica, Section E: Structure Reports Online* (2005), E61(1), m23-m24.
42. 2,5-Bis(2,2-diphenylethenyl)thiophene. Matthias Zeller, Allen D. Hunter, Roel Hoefnagels, Herman Geise and Frank Blockhuys *Acta Cryst. E* **2005**, E61, 61(12), 4183-4184.
43. Del Bene, Janet E.; Elguero, Jose. Two-bond spin-spin coupling constants (<sup>2</sup>hJ<sub>X-Y</sub>) across X-H-Y hydrogen bonds: some fundamental questions. *Advances in Quantum Chemistry* **2005**, 50, 23-35.

**2004:**

1. Wagner, N. L.; Murphy, K. L.; Haworth, D. T.; Bennett, D. W.; Hunter, A. D.; Zeller, M.; Takas, N.; DiMuzio, S. J.: "Para-Substituted Aryl-Isocyanides," *Inorganic Syntheses*, 2004, 34, 24-29.
2. Alkorta, Ibon; Elguero, Jose; Mo, Otilia; Yanez, Manuel; Del Bene, Janet E.. Do coupling constants and chemical shifts provide evidence for the existence of resonance-assisted hydrogen bonds? *Molecular Physics* (2004), 102(23-24), 2563-2574.
3. The Influence of the Side Chain Length on -OCH<sub>3</sub>  $\pi$ -Interactions Determining the Crystal Packing of Four Substituted 1,4-Bis( $\pi$ -styryl)benzenes. Christophe M. L. Vande Velde, Li-Juan Chen, Jan K. Baeke, Maarten Moens, Pieter Dieltiens, Herman J. Geise, Matthias Zeller, Allen D. Hunter, and Frank Blockhuys, *Crystal Growth & Design* 2004, 4(4), 823-830 .
4. *p*-Anisolecarbonitrile. M. J. G. Lesley, M. R. Pineau, A. D. Hunter and M. Zeller, *Acta Cryst. E* 2004, E60, o1937-o1938 .
5. Synthesis and Characterization of ReO<sub>4</sub> -Containing Microporous and Open Framework Structures. Luo, Junhua; Alexander, Ben; Wagner, Timothy R.; Maggard, Paul A. *Inorg. Chem.* 2004, 43(18), 5537-5542 .
6. 1,1'-Dibromoferrocene. Hnetinka, Chrissy A., Hunter, Allen D., Zeller, Matthias, Lesley, M. J. Gerald, *Acta Cryst. E* 2004, E60, m1806-m1807 .
7. Kanaras, C.; Westcott, B. L.; Crundwell, G.; Updegraff, J. B., III; Zeller, M.; Hunter, A. D.; Sommerer, S. O. Crystal structures of (di-2-pyridyl ketone)zinc dibromide and diiodide, Zn(C<sub>11</sub>H<sub>8</sub>N<sub>2</sub>O)<sub>2</sub>X<sub>2</sub> (X = Br, I). *Zeitschrift fuer Kristallographie - New Crystal Structures* (2004), 219(4), 393-394. CODEN: ZKNSFT ISSN:1433-7266.
8. McBurney, Brian; Foss, Paul C. D.; Reed, Elizabeth M.; Shine, Timothy D.; Glagovich, Neil M.; Westcott, Barry L.; Crundwell, Guy; Zeller, Matthias; Hunter, Allen D.. 1-Ethoxy-4-nitrobenzene. *Acta Crystallographica, Section E: Structure Reports Online* (2004), E60(12), o2179-o2180. CODEN: ACSEBH ISSN:1600-5368.
9. Glagovich, Neil M.; Foss, Paul C. D.; Michalewski, Oliver; Reed, Elizabeth M.; Strathearn, Katherine E.; Weiner, Yan F.; Crundwell, Guy; Updegraff, James B., III; Zeller, Matthias; Hunter,

- Allen D.. Redetermination of 9-nitroanthracene at 100 K. *Acta Crystallographica, Section E: Structure Reports Online* (2004), E60(11), o2125-o2126. CODEN: ACSEBH ISSN:1600-5368.
10. Glagovich, Neil M.; Reed, Elizabeth M.; Crundwell, Guy; Updegraff, James B., III; Zeller, Matthias; Hunter, Allen D.. N-(9H-Fluoren-9-ylidene)-N-(2-methoxyphenyl)amine. *Acta Crystallographica, Section E: Structure Reports Online* (2004), E60(11), o2000-o2001. CODEN: ACSEBH ISSN:1600-5368.
  11. Foss, Paul C. D.; Crundwell, Guy; Updegraff, James B., III; Zeller, Matthias; Hunter, Allen D.. 2,3-Dithien-2-ylquinoxalin-1-ium perchlorate. *Acta Crystallographica, Section E: Structure Reports Online* (2004), E60(8), o1281-o1282.
  12. Bellizzi, M.; Foss, P. C. D.; Pelto, R.; Crundwell, G.; Brueckner, C.; Updegraff, J. B., III; Zeller, M.; Hunter, A. D.. Crystal structure of 5,10,15,20-tetrakis(5'-methylthien-2'-yl)porphyrin, C<sub>40</sub>H<sub>30</sub>N<sub>4</sub>S<sub>4</sub>. *Zeitschrift fuer Kristallographie - New Crystal Structures* (2004), 219(2), 129-131.
  13. Glagovich, Neil M.; Reed, Elizabeth M.; Crundwell, Guy; Updegraff, James B., III; Zeller, Matthias; Hunter, Allen D.. N-9H-Fluoren-9-ylidene-3,4-dimethylaniline. *Acta Crystallographica, Section E: Structure Reports Online* (2004), E60(7), o1269-o1270.
  14. Westcott, Barry L.; Crundwell, Guy; Burkholder, Thomas R.; Michelsen, Laura A.; Gardner, Caroline B.; Gruhn, Nadine E.; Hunter, Allen D.; Miner, Penny; Zeller, Matthias. The molecular and electronic structure of N,N'-ethylenebis(acetylacetyldeiminato)oxovanadium(IV) and the electronic structure of its thio analogue. *Journal of Electron Spectroscopy and Related Phenomena* (2004), 135(1), 1-5.
  15. Crundwell, Guy; Linehan, Justin; Updegraff, James B., III; Zeller, Matthias; Hunter, Allen D.. 2,3-Bis(5-bromothien-2-yl)quinoxaline. *Acta Crystallographica, Section E: Structure Reports Online* (2004), E60(4), o656-o657.
  16. Glagovich, Neil; Reed, Elizabeth; Crundwell, Guy; Updegraff, James B., III; Zeller, Matthias; Hunter, Allen D.. N-(9H-Fluoren-9-ylidene)-N-(4-methoxyphenyl)amine. *Acta Crystallographica, Section E: Structure Reports Online* (2004), E60(4), o623-o625.
  17. Akula, Rakesh A.; Temelkoff, David P.; Artis, Nicole D.; Norris, Peter. Rapid access to glucopyranosyl-1,2,3-triazoles via Cu(I)-catalyzed reactions in water. *Heterocycles* (2004), 63(12), 2719-2725.

18. Zeller, M.; Hunter, A. D. Crystal structure of molybdenum and tungsten trans-bis(dinitrogen)bis{bis(di(p-ethylphenyl)phosphino)ethane} toluene solvate,  $M(C_{34}H_{40}P_2)_2(N_2)_2 \cdot C_7H_8$  (M = Mo, W). *Zeitschrift fuer Kristallographie - New Crystal Structures* (2004), 219(3), 249-254.
19. Del Bene, Janet E.; Elguero, Jose. Predicted Signs of One-Bond Spin-Spin Coupling Constants ( $1hJH-Y$ ) across X-H-Y Hydrogen Bonds for Complexes with Y =  $^{15}N$ ,  $^{17}O$ , and  $^{19}F$ . *Journal of Physical Chemistry A* (2004), 108(52), 11762-11767.
20. Temelkoff, David P.; Norris, Peter; Zeller, Matthias. Prop-2-ynyl 1,2,3,4-tetra-O-acetyl- $\beta$ -D-glucopyranuronate. *Acta Crystallographica, Section E: Structure Reports Online* (2004), E60(12), o2273-o2274.
21. Del Bene, Janet E. Characterizing two-bond NMR  $^{13}C$ - $^{15}N$ ,  $^{15}N$ - $^{15}N$ , and  $^{19}F$ - $^{15}N$  spin-spin coupling constants across hydrogen bonds using ab initio EOM-CCSD calculations. *Calculation of NMR and EPR Parameters* (2004), 353-370.
22. Del Bene, Janet E.; Elguero, Jose. One-Bond Spin-Spin Coupling Constants of X- $^1H$  Proton Donors in Complexes with X-H-Y Hydrogen Bonds, for X =  $^{13}C$ ,  $^{15}N$ ,  $^{17}O$ , and  $^{19}F$ : Predictions, Comparisons, and Relationships among  $1JX-H$ ,  $1KX-H$ , and X-H Distances. *Journal of the American Chemical Society* (2004), 126(47), 15624-15631.
23. Weaver, Travis D.; Norris, Peter; Zeller, Matthias. 6-Deoxy-1,2:3,4-di-O-isopropylidene- $\beta$ -D-galacto-heptodialdo-1,5-pyranose diphenyl dithioacetal. *Acta Crystallographica, Section E: Structure Reports Online* (2004), E60(11), o2113-o2114.
24. Temelkoff, David P.; Norris, Peter; Zeller, Matthias. 2,3,4,6-Tetra-O-acetyl- $\beta$ -D-glucopyranosyl azide. *Acta Crystallographica, Section E: Structure Reports Online* (2004), E60(11), o1975-o1976.
25. Zeller, Matthias; DiMuzio, Steven J.; Hunter, Allen D. Dibromobis(methyldiphenylphosphine)nickel(II). *Acta Crystallographica, Section E: Structure Reports Online* (2004), E60(11), m1595-m1596.
26. Smiley, Jeffrey A. Survey of enzymological data on ODCase. *Topics in Current Chemistry* (2004), 238(Orotidine Monophosphate Decarboxylase), 63-78.

27. Seibel, H.; Wagner, T. R. Preparation and crystal structure of Ba<sub>2</sub>NF. *Journal of Solid State Chemistry* (2004), 177(8), 2772-2776.
28. Del Bene, Janet E. Two-Bond Spin-Spin Coupling across a Hydrogen Bond: X-Y Coupling in the Presence and Absence of the Proton. *Journal of Physical Chemistry A* (2004), 108(33), 6820-6822.
29. Root, Yuriko Y.; Bailor, Maximillian S.; Norris, Peter. Synthesis of Glucopyranosyl Amides Using Polymer-Supported Reagents. *Synthetic Communications* (2004), 34(13), 2499-2506.
30. Zeller, Matthias; Hunter, Allen D. p-Nitrophenyl isocyanide. *Acta Crystallographica, Section C: Crystal Structure Communications* (2004), C60(6), o415-o417. CODEN: ACSCEE ISSN:0108-2701.
31. Zeller, Matthias; Hunter, Allen D.; Sampson, Paul; Chumachenko, Nataliya. (4aSR,9aSR)-9a-Methyl-5,5-dioxo-1,2,4a,6,7,9a-hexahydro-8-oxa-5 $\square$ 6-thiabenzo-1,4-cyclohepten-9-one. *Acta Crystallographica, Section E: Structure Reports Online* (2004), E60(5), o731-o732.
32. Zeller, Matthias; Hunter, Allen D.; Sampson, Paul; Chumachenko, Nataliya. (4aSR,7RS,9aSR)-7,9a-Dimethyl-5,5-dioxo-1,2,4a,6,7,9a-hexahydro-8-oxa-5 $\square$ 6-thia-1,4-benzocyclohepten-9-one. *Acta Crystallographica, Section E: Structure Reports Online* (2004), E60(5), o729-o730.
33. Zeller, Matthias; Hunter, Allen D.; Sampson, Paul; Chumachenko, Nataliya. (4aSR,7RS,9aRS)-9a-Bromo-7-methyl-5,5-dioxo-1,2,4a,6,7,9a-hexahydro-8-oxa-5 $\square$ 6-thia-1,4-benzocyclohepten-9-one. *Acta Crystallographica, Section E: Structure Reports Online* (2004), E60(5), o727-o728.
34. Zeller, Matthias; Hunter, Allen D.; Sampson, Paul; Chumachenko, Nataliya. (4aSR,7SR,9aRS)-9a-Bromo-7-methyl-5,5-dioxo-1,2,4a,6,7,9a-hexahydro-8-oxa-5 $\square$ 6-thia-1,4-benzocyclohepten-9-one. *Acta Crystallographica, Section E: Structure Reports Online* (2004), E60(5), o724-o726.
35. Zeller, Matthias; Hunter, Allen D.; Perrine, Cynthia L.; Payton, John. Tricarbonyl( $\square$ 6-trifluoromethylbenzene)chromium(0). *Acta Crystallographica, Section E: Structure Reports Online* (2004), E60(5), m668-m669.
36. Zeller, Matthias; Hunter, Allen D.; Perrine, Cynthia L.; Payton, John. Tricarbonyl( $\square$ 6-fluorobenzene)chromium. *Acta Crystallographica, Section E: Structure Reports Online* (2004), E60(5), m650-m651.

37. Koknat, Friedrich W.; Marko, David J.; Hay, Daniel N. T.; Messerle, Louis. Cluster and polynuclear compounds. Tetradecachlorohexatantalum octahydrate, Ta<sub>6</sub>Cl<sub>14</sub>·8H<sub>2</sub>O. *Inorganic Syntheses* (2004), 34 187-191.
38. Del Bene, Janet E.; Elguero, Jose. Predicted signs of reduced two-bond spin-spin coupling constants (<sup>2</sup>hKX-Y) across X-H-Y hydrogen bonds. *Magnetic Resonance in Chemistry* (2004), 42(5), 421-423.
39. Del Bene Janet E; Elguero Jose; Alkorta Ibon; Yanez Manuel; Mo Otilia <sup>19</sup>F-<sup>19</sup>F spin-spin coupling constant surfaces for (HF)<sub>2</sub> clusters: the orientation and distance dependence of the sign and magnitude of J(F-F). *Journal of chemical physics* (2004), 120(7), 3237-43.
40. Zeller, Matthias; Hunter, Allen D.; Takas, Nathan J. Tricarbonyl(1,3-dimethoxybenzene)chromium. *Acta Crystallographica, Section E: Structure Reports Online* (2004), E60(4), m434-m435.
41. Zeller, Matthias; Hunter, Allen D.; Meta, Chris. Tricarbonyl(1,3-dimethylbenzene)chromium. *Acta Crystallographica, Section E: Structure Reports Online* (2004), E60(4), m432-m433.
42. Del Bene, Janet E.; Elguero, Jose; Alkorta, Ibon. Computed Spin-Spin Coupling Constants (<sup>1</sup>JX-Y) in Molecules HmX-YHn for X and Y = <sup>13</sup>C, <sup>15</sup>N, and <sup>31</sup>P: Comparisons with Experiment and Insights into the Signs of <sup>1</sup>JX-Y. *Journal of Physical Chemistry A* (2004), 108(16), 3662-3667.
43. Musslimani, Tarek H.; Mettee, Howard. AM1 and PM3 semi-empirical study of the Diels-Alder reaction between N-, P-, O- and S-substituted aromatic heterocyclic five-membered rings with acrolein. *THEOCHEM* (2004), 672(1-3), 35-43.
44. Zeller, Matthias. A half-cleaved zirconacyclopentadiene. *Inorganic Chemistry Communications* (2004), 7(2), 245-248.
45. "Two-bond NMR Spin-Spin Coupling Constants across Hydrogen Bonds" J. E. Del Bene, in *The Electronic Encyclopedia of Computational Chemistry*. P. V. R. Schleyer, N. L. Allinger, T. Clark, J. Gasteiger, H. F. Schaefer, III, and P. R. Schreiner, eds. John Wiley & Sons, Chichester, UK, **2004**
46. Del Bene Janet E; Elguero Jose Predicted signs of reduced two-bond spin-spin coupling constants

(2hKX-Y) across X-H-Y hydrogen bonds. Magnetic resonance in chemistry : MRC (2004), 42(5), 421-3.

**2003:**

1. "2,3-Anhydrosugars in Glycoside Bond Synthesis. Highly Stereoselective Syntheses of Oligosaccharides Containing alpha-and beta-Arabinofuranosyl Linkages", R.R. Gadikota, C.S. Callam, T. Wagner, B. Del Fraino, and T.L. Lowary, *Journal of the American Chemical Society*, 125(14), 4155-4165 (2003).
2. Del Bene, Janet E.; Perera, S. Ajith; Bartlett, Rodney J.; Yanez, Manuel; Mo, Otilia; Elguero, Jose; Alkorta, Ibon. Two-Bond 15N-19F Spin-Spin Coupling Constants ( $2h_{JN-F}$ ) across N-H...F Hydrogen Bonds. *Journal of Physical Chemistry A* (2003), 107(17), 3126-3131.
3. Del Bene, Janet E.; Perera, S. Ajith; Bartlett, Rodney J.; Yanez, Manuel; Mo, Otilia; Elguero, Jose; Alkorta, Ibon. Two-Bond 19F-15N Spin-Spin Coupling Constants ( $2h_{JF-N}$ ) across F-H...N Hydrogen Bonds. *Journal of Physical Chemistry A* (2003), 107(17), 3121-3125.
4. Del Bene, Janet E.; Runge, Keith; Bartlett, Rodney J. A quantum chemical mechanism for the water-initiated decomposition of silica. *Computational Materials Science* (2003), 27(1-2), 102-108.
5. Franz, A. H.; Samoshin, V. V.; Myers, C.; Hunter, A. D.; Gross, P. H.: "C-H - Deprotonation mediated by a remote syn-axial acetoxy group - an unprecedented double bond formation upon cyanation of the dimer from L-Fucal," *Carbohydrate Research*, 2003, 338, 851-854.
6. Crundwell, Guy; Westcott, Barry L.; Coffey, Roderick; Zeller, Matthias; Hunter, Allen D.. Crystal structures of two different cobalt(III) complexes with di-2-pyridyl ketone grown from methanol-bis(methoxy-bis(2-pyridyl)methanolato-O,N,N')cobalt(III) nitrate trihydrate and (hydroxy-bis(2-pyridyl)methanolato-O,N,N')(methoxy-bis(2-pyridyl)methanolato-O,N,N')cobalt(III) nitrate trihydrate. *Inorganica Chimica Acta* (2003), 355 432-437.
7. Stacy, Vanessa L.; Crundwell, Guy; Updegraff, James B., III; Zeller, Matthias; Hunter, Allen D.. 4-Bromothiophene-2-carboxaldehyde. *Acta Crystallographica, Section E: Structure Reports Online* (2003), E59(11), o1812-o1813.
8. Del Bene, Janet E.; Alkorta, Ibon; Elguero, Jose. Computed EOM-CCSD 19F-19F spin-spin coupling constants in small organic molecules. *Zeitschrift fuer Physikalische Chemie (Muenchen, Germany)* (2003), 217(12), 1565-1575.

9. Del Bene, Janet E.; Elguero, Jose. What determines the sign of the Fermi-contact contribution to the NMR spin-spin coupling constant? *Chemical Physics Letters* (2003), 382(1,2), 100-105.
10. McCartney, Jason L.; Meta, Christopher T.; Cicchillo, Robert M.; Bernardina, Matthew D.; Wagner, Timothy R.; Norris, Peter. Addition of lithiated C-nucleophiles to 2,3-O-isopropylidene-D-erythronolactone: stereoselective formation of a furanose C-disaccharide. *Journal of Organic Chemistry* (2003), 68(26), 10152-10155.
11. Zeller, Matthias; Lazich, Evelyn; Wagner, Timothy R.; Hunter, Allen D. 1,2-Bis(ditolylphosphino)ethane. *Acta Crystallographica, Section E: Structure Reports Online* (2003), E59(11), o1721-o1722.
12. Hunter, Allen D.; Zeller, Matthias; McSparrin, Les. Bis[1,2-bis(p-ethylbenzene)phosphino]benzene. *Acta Crystallographica, Section E: Structure Reports Online* (2003), E59(11), o1719-o1720.
13. Zeller, Matthias; Hunter, Allen D.; Perrine, Cynthia L. p-Diisocyanotetramethylbenzene. *Acta Crystallographica, Section E: Structure Reports Online* (2003), E59(11), o1655-o1656.
14. Zeller, Matthias; Hunter, Allen D. 1,4-Diisociano-2,5-dimethylbenzene. *Acta Crystallographica, Section E: Structure Reports Online* (2003), E59(11), o1653-o1654.
15. Zeller, Matthias; Hunter, Allen D. Tricarbonyl( $\eta$ -6-1,3,5-trimethoxybenzene)chromium(0). *Acta Crystallographica, Section E: Structure Reports Online* (2003), E59(11), m1078-m1079.
16. Zeller, Matthias; Hunter, Allen D.; Regula, Jody L.; Szalay, Paul S. Tricarbonyl( $\eta$ -6-4-fluoroaniline)chromium. *Acta Crystallographica, Section E: Structure Reports Online* (2003), E59(11), m975-m976.
17. Zeller, Matthias; Lazich, Evelyn; Hunter, Allen D. Dicarbonyl( $\eta$ -5-cyclopentadienyl)iodoiron(II). *Acta Crystallographica, Section E: Structure Reports Online* (2003), E59(10), m914-m915.
18. Wagner, Timothy R.; Gadikota, Rajendrakumar Reddy; Callam, Christopher S.; Lowary, Todd L. 1-(2',3'-Anhydro-5'-O-benzoyl- $\beta$ -D-lyxofuransoyl)-5-fluorouracil. *Acta Crystallographica, Section E: Structure Reports Online* (2003), E59(7), o1063-o1065.
19. "1-(2',3'-anhydro-5'-O-benzoyl-beta-D-lyxofuranoyl)-5-fluoro-uracil", T.R. Wagner, R.R.

- Gadikota, C.S. Callam, and T.L. Lowary, *Acta Cryst.*, E59, 1-3 (2003).
20. Sheville, Justin; Berndt, Daniel; Wagner, Timothy; Norris, Peter. Crystal structure of 1,2:5,6-di-O-isopropylidene-3-O-(phenylacetyl)- $\alpha$ -D-glucofuranose. *Journal of Chemical Crystallography* (2003), 33(5/6), 409-412.
  21. Smiley, Jeffrey A.; DelFraino, Brian J.; Simpson, Beth A. Hydrogen isotope tracing in the reaction of orotidine-5'-monophosphate decarboxylase. *Archives of Biochemistry and Biophysics* (2003), 412(2), 267-271.

**2002:**

1. Woltz, James; Westcott, Barry L.; Crundwell, Guy; Zeller, Matthias; Hunter, Allen D.; Sommerer, Shaun O. Bis(di-2-pyridylmethanediolato- $\square$ 2N,N')iron(III) nitrate dihydrate. *Acta Crystallographica, Section E: Structure Reports Online* (2002), E58(11), m609-m610.
2. Wagner, T. R. Preparation and single-crystal structure analysis of Sr<sub>2</sub>NF. *Journal of Solid State Chemistry* (2002), 169(1), 13-18.
3. Del Bene, Janet E.; Bartlett, Rodney J.; Elguero, Jose. Interpreting 2hJ(F,N), 1hJ(H,N) and 1J(F,H) in the hydrogen-bonded FH-collidine complex. *Magnetic Resonance in Chemistry* (2002), 40(12), 767-771.
4. Del Bene, Janet E.; Perera, S. Ajith; Bartlett, Rodney J.; Yanez, Manuel; Mo, Otilia; Elguero, Jose; Alkorta, Ibon. Two-Bond <sup>13</sup>C-<sup>15</sup>N Spin-Spin Coupling Constants (2hJC-N) Across C-H-N Hydrogen Bonds. *Journal of Physical Chemistry A* (2003), 107(18), 3222-3227.
5. Root, Yuriko Y.; Wagner, Timothy R.; Norris, Peter. Crystal structure of methyl 1,2,3,4-tetra-O-acetyl- $\square$ -D-glucopyranuronate. *Carbohydrate Research* (2002), 337(21-23), 2343-2346.
6. Schildcrout, Steven M. Learning chemistry research outside the laboratory: Novel graduate and undergraduate courses in research methodology. *Journal of Chemical Education* (2002), 79(11), 1340-1343.
7. Bretz, Stacey Lowery. Implementing the professional development standards: An innovative M.S. degree for high school chemistry teachers. *Journal of Chemical Education* (2002), 79(11), 1307-1309.
8. Del Bene Janet E; Perera S Ajith; Bartlett Rodney J; Elguero Jose; Alkorta Ibon; Lopez-Leonardo Carmen; Alajarin Mateo (3h)J((15)N-(31)P) spin-spin coupling constants across N[bond]H...O[bond]P hydrogen bonds. *Journal of the American Chemical Society* (2002), 124(22), 6393-7.
9. Bartlett, Rodney J.; Del Bene, Janet E.; Perera, S. Ajith. Does the magnitude of NMR coupling constants specify bond polarity? *ACS Symposium Series* (2002), 827(Structures and Mechanisms), 150-164.

10. Del Bene, Janet E.; Perera, S. Ajith; Bartlett, Rodney J.; Alkorta, Ibon; Elguero, Jose; Mo, Otilia; Yanez, Manuel. One-Bond (1dJH-H) and Three-Bond (3dJX-M) Spin-Spin Coupling Constants Across X-H...H-M Dihydrogen Bonds. *Journal of Physical Chemistry A* (2002), 106(40), 9331-9337.
11. Alkorta, Ibon; Elguero, Jose; Mo, Otilia; Yanez, Manuel; Del Bene, Janet E.. Ab Initio Study of the Structural, Energetic, Bonding, and IR Spectroscopic Properties of Complexes with Dihydrogen Bonds. *Journal of Physical Chemistry A* (2002), 106(40), 9325-9330.
12. Berndt, Daniel F.; Norris, Peter. Intramolecular carbene and nitrene insertions at C-2 of diacetone-D-glucose. *Tetrahedron Letters* (2002), 43(21), 3961-3962. CODEN: TELEAY ISSN:0040-4039.
13. Del Bene, Janet E.; Jordan, Meredith J. T. To what extent do external fields and vibrational and isotopic effects influence NMR coupling constants across hydrogen bonds? Two-bond Cl-N spin-spin coupling constants (2hJCl-N) in model ClH:NH3 complexes. *Journal of Physical Chemistry A* (2002), 106(21), 5385-5392.
14. Goebel, James R.; Antle, Kathryn A.; Ault, Bruce S.; Del Bene, Janet E.. Matrix Isolation and ab Initio Study of 1:1 Hydrogen-Bonded Complexes of H2O2 with HF, HCl, and HBr. *Journal of Physical Chemistry A* (2002), 106(26), 6406-6414.
15. Smiley, Jeffrey A.. The most proficient enzyme as the central theme in an integrated, research-based biochemistry laboratory course. *Biochemistry and Molecular Biology Education* (2002), 30(1), 45-50

**2001:**

1. Del Bene, Janet E.; Perera, S. Ajith; Bartlett, Rodney J.  $^{15}\text{N}$ ,  $^{15}\text{N}$  spin-spin coupling constants across N-H-N and N-H<sup>+</sup>-N hydrogen bonds: can coupling constants provide reliable estimates of N-N distances in biomolecules? *Magnetic Resonance in Chemistry* (2001), 39(Spec. Issue), S109-S114.
2. Goebel, James R.; Ault, Bruce S.; Del Bene, Janet E.. Matrix Isolation and ab Initio Study of 1:1 Hydrogen-Bonded Complexes of H<sub>2</sub>O<sub>2</sub> with Phosphorus and Sulfur Bases. *Journal of Physical Chemistry A* (2001), 105(50), 11365-11370.
3. Norris, Peter; Fluxe, Andrew. Preparation of a D-glucose-derived alkene: An E2 reaction for the undergraduate organic chemistry laboratory. *Journal of Chemical Education* (2001), 78(12), 1676-1678. CODEN: JCEDA8 ISSN:0021-9584.
4. Del Bene, J. E.; Jordan, M. J. T. What a difference a decade makes: progress in ab initio studies of the hydrogen bond. *THEOCHEM* (2001), 573 11-23.
5. Del Bene, Janet E.; Jordan, Meredith J. T.; Perera, S. Ajith; Bartlett, Rodney J. Vibrational Effects on the F-F Spin-Spin Coupling Constant ( $2hJ_{\text{F-F}}$ ) in FHF<sup>-</sup> and FDF<sup>-</sup>. *Journal of Physical Chemistry A* (2001), 105(37), 8399-8402.
6. Toh, Justin S.-S.; Jordan, Meredith J. T.; Husowitz, Barry C.; Del Bene, Janet E.. Can Proton-Shared or Ion-Pair N-H-N Hydrogen Bonds Be Produced in Uncharged Complexes? A Systematic ab Initio Study of the Structures and Selected NMR and IR Properties of Complexes with N-H-N Hydrogen Bonds. *Journal of Physical Chemistry A* (2001), 105(48), 10906-10914.
7. Bretz, Stacey Lowery. Novak's Theory of education: Human construction and meaningful learning. *Journal of Chemical Education* (2001), 78(8), 1107.
8. Nicklow, R. A.; Wagner, T. R.; Raymond, C. C. Preparation and Single-Crystal Structure Analysis of Ca<sub>2</sub>NF. *Journal of Solid State Chemistry* (2001), 160(1), 134-138.
9. Del Bene, Janet E.; Perera, S. Ajith; Bartlett, Rodney J. What Parameters Determine N-N and O-O Coupling Constants ( $2hJ_{\text{X-X}}$ ) Across X-H<sup>+</sup>-X Hydrogen Bonds? *Journal of Physical Chemistry A* (2001), 105(5), 930-934.

10. Jordan, M. J. T.; Toh, J. S.-S.; Del Bene, J. E.. Vibrational averaging of NMR properties for an N-H-N hydrogen bond. *Chemical Physics Letters* (2001), 346(3,4), 288-292.
11. Goebel, James R.; Ault, Bruce S.; Del Bene, Janet E.. Matrix Isolation and ab Initio Study of 1:1 Hydrogen-Bonded Complexes of H<sub>2</sub>O<sub>2</sub> with NH<sub>3</sub> and N(CH<sub>3</sub>)<sub>3</sub>. *Journal of Physical Chemistry A* (2001), 105(26), 6430-6435.
12. Norris, Peter; Freeze, Scott; Gabriel, Christopher J. Synthesis of a partially protected azidodeoxy sugar: a project suitable for the advanced undergraduate organic chemistry laboratory. *Journal of Chemical Education* (2001), 78(1), 75-76.
13. Chapman, Karena; Crittenden, Deborah; Bevitt, Joseph; Jordan, Meredith J. T.; Del Bene, Janet E.. Relating Environmental Effects and Structures, IR, and NMR Properties of Hydrogen-Bonded Complexes: ClH:Pyridine. *Journal of Physical Chemistry A* (2001), 105(22), 5442-5449.
14. Bevitt, Joseph; Chapman, Karena; Crittenden, Deborah; Jordan, Meredith J. T.; Del Bene, Janet E.. An ab Initio Study of Anharmonicity and Field Effects in Hydrogen-Bonded Complexes of the Deuterated Analogues of HCl and HBr with NH<sub>3</sub> and N(CH<sub>3</sub>)<sub>3</sub>. *Journal of Physical Chemistry A* (2001), 105(13), 3371-3378.
15. Smiley, Jeffrey A.; Hay, Kelly M.; Levison, Bruce S. A Reexamination of the Substrate Utilization of 2-Thioorotidine-5'-monophosphate by Yeast Orotidine-5'-Monophosphate Decarboxylase. *Bioorganic Chemistry* (2001), 29(2), 96-106.
16. "A Novel Dimanganese Complex Linked by an Unusually Strong Hydrogen Bond. X-Ray Structure of the Hydrogen-bonded Complex and Ab Initio Calculations: T. M. Becker, J. A. Krause-Bauer, J. E. Del Bene, and M. Orchin, *J. Organometallic Chem.* **2001**, 629, 165.

**2000:**

1. Adrian, J. C.; Barkin, J. L.; Fox, R. J.; Chick, J. E.; Hunter, A. D.; Nicklow, R. A.: "Chlorotitanium Enolate Addition to Aldimines: A Stereoselective Route to  $\alpha$ -Oxy- $\beta$ -Substituted- $\beta$ -Amino Esters," *Journal of Organic Chemistry*, 2000, 65, 6264-6267.
2. Bennett, M. A.; Ditzel, E. J.; Hunter, A. D.; Khan, K.; Kopp, M. R.; Neumann, H.; Robertson, G. B.; Zeh, H.: "Coordination and Organometallic Complexes of Iron Containing *o*-phenylenebis(dimethylphosphine)(pdmp). Crystal and Molecular Structure of  $[\text{Fe}(\eta^2\text{-C}_2\text{H}_4)(\text{pdmp})_2]$ ," *Dalton*, 2000, 1733-1741.
3. Del Bene, Janet E. Anharmonicity and environmental effects on hydrogen-bonded clusters. NATO ASI Series, Series C: Mathematical and Physical Sciences (2000), 561(Recent Theoretical and Experimental Advances in Hydrogen Bonded Clusters), 309-321.
4. Kim, Thomas D. PCR primer design: an inquiry-based introduction to bioinformatics on the World Wide Web. *Biochemistry and Molecular Biology Education* (2000), 28(5), 274-276.
5. Schildcrout, Steven M. No, the molecular mass of bromobenzene is not 157 amu: an exercise in mass spectrometry and isotopes for early general chemistry. *Journal of Chemical Education* (2000), 77(11), 1433-1434.
6. Del Bene, Janet E.; Bartlett, Rodney J. N-N spin-spin coupling constants [ $2hJ(15\text{N}-15\text{N})$ ] across N-H $\cdots$ N hydrogen bonds in neutral complexes. To what extent does the bonding at the nitrogens influence  $2hJ_{\text{N}-\text{N}}$ ? *Journal of the American Chemical Society* (2000), 122(42), 10480-10481.
7. Cicchillo, R. M.; Norris, P. A convenient synthesis of glycosyl chlorides from sugar hemiacetals using triphosgene as the chlorine source. *Carbohydrate Research* (2000), 328(3), 431-434.
8. Del Bene, Janet E.; Perera, S. Ajith; Bartlett, Rodney J.; Alkorta, Ibon; Elguero, Jose.  $4hJ(31\text{P}-31\text{P})$  coupling constants through N-H $\cdots$ N hydrogen bonds. A comparison of computed ab initio and experimental data. *Journal of Physical Chemistry A* (2000), 104(31), 7165-7166.
9. Del Bene, Janet E.; Jordan, Meredith J. T. Vibrational spectroscopic and NMR properties of hydrogen-bonded complexes. Do they tell us the same thing? *Journal of the American Chemical Society* (2000), 122(19), 4794-4797.

10. Schildcrout, Steven M. Gaseous-ion fragmentation mechanisms in chlorobenzenes by GC/MS and GC/MS/MS: a physical-chemical approach for undergraduates. *Journal of Chemical Education* (2000), 77(4), 501-502.
11. Szczepaniak, K.; Chabrier, P.; Person, W. B.; Del Bene, J. E.. Experimental infrared spectra of matrix isolated complexes of HCl with 4-substituted pyridines. Evaluation of anharmonicity and matrix effects using data from ab initio calculations. *Journal of Molecular Structure* (2000), 520 1-18.
12. Jordan, Meredith J. T.; Del Bene, Janet E.. Unraveling Environmental Effects on Hydrogen-Bonded Complexes: Matrix Effects on the Structures and Proton-Stretching Frequencies of Hydrogen-Halide Complexes with Ammonia and Trimethylamine. *Journal of the American Chemical Society* (2000), 122(9), 2101-2115.
13. Del Bene, Janet E.; Watts, John D. Base properties of H<sub>2</sub>CO in the excited  $3n \pi \pi^*$  state. *International Journal of Quantum Chemistry* (2000), 77(1), 187-191.
14. Del Bene, Janet E.; Perera, S. Ajith; Bartlett, Rodney J. Predicted NMR Coupling Constants Across Hydrogen Bonds: A Fingerprint for Specifying Hydrogen Bond Type? *Journal of the American Chemical Society* (2000), 122(14), 3560-3561.
15. "Matrix Isolation and Ab Initio Study of the Hydrogen-Bonded Complexes between H<sub>2</sub>O<sub>2</sub> and (CH<sub>3</sub>)<sub>2</sub>O", J. Goebel, B. S. Ault, and J. E. Del Bene, *J. Phys. Chem. A.* **2000**, 104, 2033.

**1999:**

1. Norris, P.; Wagner, T. R. Solution and solid-state structure of 2,6-anhydro-1,1-bis(ethylsulfonyl)-1-deoxy-D-talitol. *Carbohydrate Research* (1999), 322(1-2), 147-150.
2. Del Bene, Janet E.; Perera, S. Ajith; Bartlett, Rodney J. Hydrogen Bond Types, Binding Energies, and <sup>1</sup>H NMR Chemical Shifts. *Journal of Physical Chemistry A* (1999), 103(40), 8121-8124.
3. Freeze, Scott; Norris, Peter. Synthesis of carbohydrate-derived 1,2,3-triazoles using 1,3-dipolar cycloaddition on a soluble polymer support. *Heterocycles* (1999), 51(8), 1807-1817.
4. Smiley, Jeffrey A.; Saleh, Lana. Active Site Probes for Yeast OMP Decarboxylase: Inhibition Constants of UMP and Thio-Substituted UMP Analogues and Greatly Reduced Activity toward CMP-6-Carboxylate. *Bioorganic Chemistry* (1999), 27(4), 297-306.
5. Ciszewski, Gregory M.; Jackson, John A. Michaelis-Becker synthesis of bis(2,2,2-trifluoroethyl)phosphono esters. *Organic Preparations and Procedures International* (1999), 31(2), 240-243.
6. Bowman, Russell A.; Stock, Joseph R.; Jackson, John A. Improved synthesis of bis(2,2,2-trifluoroethyl) phosphorochloridate. *Organic Preparations and Procedures International* (1999), 31(2), 230-231.
7. Del Bene, Janet E.; Jordan, Meredith J. T. Vibrational spectroscopy of the hydrogen bond: an ab initio quantum-chemical perspective. *International Reviews in Physical Chemistry* (1999), 18(1), 119-162.
8. Del Bene, Janet E.; Jordan, Meredith J. T. A comparative study of vibrational anharmonicity in the halide anions XHX<sup>-</sup>: X = F, Cl, Br. *Spectrochimica Acta, Part A: Molecular and Biomolecular Spectroscopy* (1999), 55A(3), 719-729.
9. Norris, Peter. Chiral tetrahydrofuran synthesis from D-ribose diphenyl dithioacetal. *Heterocyclic Communications* (1999), 5(2), 113-114.
10. Smiley, Jeffrey A.; Angelot, Julie M.; Cannon, Renita C.; Marshall, Eva M.; Asch, David K. Radioactivity-based and spectrophotometric assays for isoorotate decarboxylase: identification of the thymidine salvage pathway in lower eukaryotes. *Analytical Biochemistry* (1999), 266(1), 85-

11. Miller, Brian G.; Smiley, Jeffrey A.; Short, Steven A.; Wolfenden, Richard. Activity of yeast orotidine-5'-phosphate decarboxylase in the absence of metals. *Journal of Biological Chemistry* (1999), 274(34), 23841-23843.