

Dr. Carsten Milsmann

West Virginia University

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A. Experience

West Virginia University, Morgantown, WV, USA

Associate Professor of Chemistry, C. Eugene Bennett Department of Chemistry 2020 – present

Assistant Professor of Chemistry, C. Eugene Bennett Department of Chemistry 2014 – 2020

Princeton University, Princeton, NJ, USA

Postdoctoral Research Associate 2010 – 2014

Advisor: Prof. Dr. Paul J. Chirik

Cornell University, Ithaca, NY, USA

2010

Postdoctoral Research Associate

Advisor: Prof. Dr. Paul J. Chirik

Max Planck Institute for Bioinorganic Chemistry, Mülheim an der Ruhr, Germany

2009 – 2010

Postdoctoral Research Associate

Advisor: Prof. Dr. Karl Wieghardt

B. Education

Max Planck Institute for Bioinorganic Chemistry, Mülheim an der Ruhr, Germany / Ruhr University Bochum, Bochum, Germany

2006 – 2009

Dr. rer. nat., *summa cum laude* (equivalent to Ph.D. in Chemistry) May 2009

Advisor: Prof. Dr. Karl Wieghardt

Dissertation (in English): *Spectroscopic and Density Functional Theoretical Investigation of the Electronic Structure of Octahedral Dithiolene Complexes (Cr, Fe, Co, and Ru).*

Philipps University Marburg, Germany

2000 – 2005

Diploma in Chemistry (“Diplom-Chemiker”) October 2005

Advisor: Prof. Dr. Martin Bröring

Thesis (in German): *Pd-katalysierte Amidierung – eine effiziente Strategie zum Aufbau sterisch abgeschirmter Corrolliganden.* [Translation: *Pd-Catalyzed Amidation – An Efficient Strategy for the Synthesis of Sterically Encumbered Corrole Ligands*]

University of Sydney, Australia

2003 - 2004

Semester abroad (undergraduate)

Advisor: Prof. Dr. Peter A. Lay

Research topic: *X-ray Absorption Spectroscopic and Electrochemical Studies of Vanadium and Chromium Catecholate Complexes.*

C. National Service – non military option (“Zivildienst”)

Verein für ambulante soziale therapeutische Beratungs und Behandlungsdienste mit integrativen Gruppen für Kinder mit und ohne Behinderung e.V. 1999 - 2000
[Translation: *Association for Ambulant Social Therapeutic Counseling and Care Services with Integrated Groups for Children with and without Disabilities*]

D. Selected Honors and Awards

West Virginia University

National Science Foundation CAREER Award 2018
Thieme Chemistry Journals Award 2017
Don and Linda Brodie Award for Innovation 2016

Princeton University

Feodor Lynen Research Fellowship for Postdoctoral Researchers 2011-2012
Alexander von Humboldt Foundation

Max Planck Institute for Bioinorganic Chemistry

Ernst Haage Prize in Chemistry 2010
Presented by the Ernst Haage-Foundation to honor young scientists for outstanding achievements in the field of chemistry.
Ph.D. fellowship of the Max Planck Society 2006 – 2009

Philipps University Marburg

Undergraduate Fellowship of the *Studienstiftung des deutschen Volkes* 2000 – 2005
[Translation: *German Academic Scholarship Foundation*]

E. Publications

At West Virginia University

52. Long-Lived Photoluminescence of Molecular Group 14 Compounds through Thermally Activated Delayed Fluorescence. Gowda, A. S.; Lee, T. S.; Rosko, M. C.; Petersen, J. L.; Castellano, F. N.*; **Milsmann, C.***; *Inorg. Chem.* **2022**, available online, DOI: 0.1021/acs.inorgchem.2c00182.
51. Synthesis and Characterization of Pyridine Dipyrrolide Uranyl Complexes. Hakey, B. M.; Leary, D. C.; Lopez, L. M.; Valerio, L. R.; Brennessel, W. W.; **Milsmann, C.***; Matson, E. M.*; *Inorg. Chem.* **2022**, *61*, 6182.
50. High Magnetic Anisotropy of a Square-Planar Iron-Carbene Complex. Hakey, B. M.; Leary, D. C.; Xiong, J.; Harris, C. F.; Darmon, J. M.; Petersen, J. L.; Berry, J. F.*; Guo, Y.*; **Milsmann, C.***; *Inorg. Chem.* **2021**, *60*, 18575. Selected as a *Featured Article* by the ACS Editorial Staff.
49. Effects of 2,6-Dichlorophenyl Substituents on the Coordination Chemistry of Pyridine Dipyrrolide Iron Complexes. Hakey, B. M.; Leary, D. C.; Rodriguez, J. G.; Martinez, J. C.; Vaughan, N. B.; Darmon, J. M.; Akhmedov, N. G.; Petersen, J. L.; Dolinar, B. S.; **Milsmann, C.***; *Z. Anorg. Allg. Chem.* **2021**, *647*, 1503. Invited contribution to the *Special Issue: Pincer Ligands*.
48. Low power threshold photochemical upconversion using a zirconium(IV) LMCT photosensitizer. Yang, M.; Sheykhi, S.; Zhang, Y.; **Milsmann, C.**; Castellano, F. N.; *Chem. Sci.* **2021**, *12*, 9069.
47. Effects of Ligand Substitution on the Optical and Electrochemical Properties of (Pyridinedipyrrolide)zirconium Photosensitizers. Zhang, Y.; Leary, D. C.; Belldina, A. M.; Petersen, J. L.; **Milsmann, C.***; *Inorg. Chem.* **2020**, *59*, 14716. Invited contribution to the *Forum on Light-Controlled Reactivity of Metal Complexes*.
46. Photochemical Synthesis of a Zirconium Cyclobutadienyl Complex. Do, P. M. N.; Akhmedov, N. G., Petersen, J. L.; Dolinar, B. S.; **Milsmann, C.***; *Chem. Commun.* **2020**, *56*, 5397.
45. Delayed Fluorescence from Ligand-to-Metal Charge Transfer Excited States. Zhang, Y.; Lee, T. S.; Favale, J. M.; Petersen, J. L.; Scholes, G. D.; Castellano, F. N.; **Milsmann, C.***; *Nat. Chem.* **2020**, *12*, 345.
44. Reactivity of Pyridine Dipyrrolide Iron(II) Complexes with Organic Azides: C-H Amination and Iron Tetrazene Formation. Hakey, B. M.; Darmon, J. M.; Akhmedov, N. G.; Petersen, J. L.; **Milsmann, C.***; *Inorg. Chem.* **2019**, *58*, 11028.
43. Synthesis and Electronic Structure of Neutral Square-Planar High-Spin Iron(II) Complexes Supported by a Dianionic Pincer Ligand. Hakey, B. M.; Darmon, J. M.; Zhang, Y.; Petersen, J. L.; **Milsmann, C.***; *Inorg. Chem.* **2019**, *58*, 1252.
42. Photoluminescence of Seven-Coordinate Zirconium and Hafnium Complexes with 2,2'-Pyridylpyrrolide Ligands. Zhang, Y.; Akhmedov, N. G.; Petersen, J. L.; **Milsmann, C.***; *Chem. Eur. J.* **2019**, *25*, 3042.

41. Photochemical C-C Bond Formation in Luminescent Zirconium Complexes with CNN Pincer Ligands. Zhang, Y.; Petersen, J. L.; **Milsmann, C.***; *Organometallics* **2018**, *37*, 4488. Invited contribution to the *Special Issue: Organometallic Complexes of Electropositive Elements for Selective Synthesis*.
40. A Zirconium Photosensitizer with a Long-Lived Excited State: Mechanistic Insight into Photo-Induced Single Electron Transfer. Zhang, Y.; Lee, T. S.; Petersen, J. L.; **Milsmann, C.***; *J. Am. Chem. Soc.* **2018**, *140*, 5934.
39. Synthesis of a Cyclophane Bearing Two Benzo[a]anthracene Units Connected at 5 and 7 Positions with two Naphth-1,4- diyl Groups. Thakellapalli, H.; Farajidizaji, B.; Li, S.; Heller, J. C.; Zhang, Y.; Akhmedov, N. G.; **Milsmann, C.**; Petersen, J. L.; Wang, K. K.*; *J. Org. Chem.* **2018**, *83*, 2455.
38. Redox Chemistry of Bis(pyrrolyl)pyridine Chromium and Molybdenum Complexes: An Experimental and Density Functional Theoretical Study. Gowda, A. S.; Petersen, J. L.; **Milsmann, C.***; *Inorg. Chem.* **2018**, *57*, 1919.
37. Synthesis and Structure of a Functionalized [9]Cycloparaphenylene Bearing Three Indeno[2,1-a]fluorene-11,12-dione-2,9-diyl Units. Li, S.; Aljhdli, M.; Thakellapalli, H.; Farajidizaji, B.; Zhang, Y.; Akhmedov, N. G.; **Milsmann, C.**; Popp, B. V.; Wang, K. K.*; *Org. Lett.* **2017**, *19*, 4078.
36. A Luminescent Zirconium(IV) Complex as a Molecular Photosensitizer for Visible Light Photoredox Catalysis. Zhang, Y.; Petersen, J. L.; **Milsmann, C.***; *J. Am. Chem. Soc.* **2016**, *138*, 13115.

Prior to West Virginia University

35. N-N Bond Cleavage of 1,2-Diarylhydrazines and N-H Bond Formation via H-Atom Transfer in Vanadium Complexes Supported by a Redox-Active Ligand. **Milsmann, C.**; Semproni, S. P.; Chirik, P. J.; *J. Am. Chem. Soc.* **2014**, *136*, 12099.
34. Four-Coordinate Cobalt Pincer Complexes: Electronic Structure Studies and Ligand Modification by Homolytic and Heterolytic Pathways. Semproni, S. P.; **Milsmann, C.**; Chirik, P. J.; *J. Am. Chem. Soc.* **2014**, *136*, 9211.
33. Synthesis, Electronic Structure and Reactivity of Bis(imino)pyridine Iron Carbene Complexes: Evidence for a Carbene Radical. Russell, S. K.; Hoyt, J. M.; Bart, S. C.; **Milsmann, C.**; Stieber, S. C. E.; Semproni, S. P.; DeBeer, S.; Chirik, P. J.; *Chem. Sci.* **2014**, *5*, 1168.
32. Catalytic Hydrogenation Activity and Electronic Structure Determination of Bis(arylimidazol-2-ylidene)pyridine Cobalt Alkyl and Hydride Complexes. Yu, R., Darmon, J. M.; **Milsmann, C.**; Margulieux, G.; Stieber, S. C. E.; DeBeer, S.; Chirik, P. J.; *J. Am. Chem. Soc.* **2013**, *135*, 13168.
31. Reversible Carbon-Carbon Bond Formation Induced by Oxidation and Reduction at a Redox-Active Cobalt Complex. Atienza, C. C. H.; **Milsmann, C.**; Semproni, S. P.; Turner, Z. R.; Chirik, P. J.; *Inorg. Chem.* **2013**, *52*, 5403.
30. Redox-Induced N₂ Hapticity Switching in Zirconocene Dinitrogen Complexes. Semproni, S. P.; Knobloch, D. J.; **Milsmann, C.**; Chirik, P. J.; *Angew. Chem. Int. Ed.* **2013**, *52*, 5372.

29. Oxidation and Reduction of Bis(imino)pyridine Iron Dinitrogen Complexes: Evidence for Formation of a Chelate Trianion. Tondreau, A. M.; Stieber, S. C. E.; **Milsmann, C.**; Lobkovsky, E.; Weyhermüller, T.; Chirik, P. J.; *Inorg. Chem.* **2013**, *52*, 635.
28. Spin Crossover in a 3,5-Bis(2-pyridyl)-1,2,4-triazolate-Bridged Dinuclear Iron(II) Complex $[\{\text{Fe}(\text{NCBH}_3)(\text{py})\}_2(\mu\text{-L}^1)_2]$ – Powder versus Single Crystal Study. Schneider, C. J.; Cashion, J. D.; Chilton, N. F.; Etrillard, C.; Fuentealba, M.; Howard, J. A. K.; Létard, J.-F.; **Milsmann, C.**; Moubaraki, B.; Sparkes, H. A.; Batten, S. R.; Murray, K. S.; *Eur. J. Inorg. Chem.* **2013**, 850.
27. Synthesis, Electronic Structure and Alkene Hydrosilylation Activity of Terpyridine and Bis(imino)pyridine Iron Dialkyl Complexes. Tondreau, A. M.; Atienza, C. C. H.; Darmon, J. M.; **Milsmann, C.**; Hoyt, H. M.; Weller, K. J.; Nye, S. A.; Lewis, K. M.; Boyer, J.; Delis, J. G. P.; Lobkovsky, E.; Chirik, P. J.; *Organometallics* **2012**, *31*, 4886.
26. Azo N=N Bond Cleavage with a Redox-Active Vanadium Compound Involving Metal-Ligand Cooperativity. **Milsmann, C.**; Turner, Z. R.; Semproni, S. P.; Chirik, P. J.; *Angew. Chem. Int. Ed.* **2012**, *51*, 5386.
25. Side-on Dinitrogen Complexes of Titanocenes with Disubstituted Cyclopentadienyl Ligands: Synthesis, Structure and Spectroscopic Characterization. Semproni, S. P.; **Milsmann, C.**; Chirik, P. J.; *Organometallics* **2012**, *31*, 3672.
24. Structure and Reactivity of a Hafnocene μ -Nitride Prepared From Dinitrogen Cleavage. Semproni, S. P.; **Milsmann, C.**; Chirik, P. J.; *Angew. Chem. Int. Ed.* **2012**, *51*, 5213.
23. Bis(imino)pyridine Iron Dinitrogen Compounds Revisited: Differences in Electronic Structure Between Four- and Five-Coordinate Derivatives. Stieber, S. C. E.; **Milsmann, C.**; Hoyt, J. M.; Turner, Z. R.; Finkelstein, K. D.; Wieghardt, K.; DeBeer, S.; Chirik, P. J.; *Inorg. Chem.* **2012**, *51*, 3770.
22. Synthesis and Electronic Structure Determination of *N*-Alkyl-Substituted Bis(imino)pyridine Iron Imides Exhibiting Spin Crossover Behavior. Bowman, A. C.; **Milsmann, C.**; Bill, E.; Turner, Z. R.; Lobkovsky, E.; DeBeer, S.; Wieghardt, K.; Chirik, P. J.; *J. Am. Chem. Soc.* **2011**, *133*, 17353.
21. Synthesis, Electronic Structure and Ethylene Polymerization Activity of Bis(imino)pyridine Cobalt Alkyl Cations. Atienza, C. C. H.; **Milsmann, C.**; Lobkovsky, E.; Chirik, P. J.; *Angew. Chem. Int. Ed.* **2011**, *50*, 8143.
20. Oxidation and Reduction of Bis(imino)pyridine Dicarboxyl Complexes. Tondreau, A. M.; **Milsmann, C.**; Lobkovsky, E.; Chirik, P. J.; *Inorg. Chem.* **2011**, *50*, 9888.
19. Spin States and Redox Changes in Iron bis-terdentate Nitroxide {NNO} Chelates. Murray, K.; Gass, I.; Gartshore, C.; Lupton, D.; Moubaraki, B.; Nafady, A.; Bond, A.; Boas, J.; Cashion, J.; **Milsmann, C.**; Wieghardt, K.; *Inorg. Chem.* **2011**, *50*, 3052.
18. Synthesis, Electronic Structure and Catalytic Activity of Reduced Bis(aldimino)pyridine Iron Compounds: Experimental Evidence for Ligand Participation. Russell, S. K.; **Milsmann, C.**; Lobkovsky, E.; Weyhermüller, T.; Chirik, P. J.; *Inorg. Chem.* **2011**, *50*, 3159.
17. Synthesis and Electronic Structure of Cationic, Neutral and Anionic Bis(imino)pyridine Iron Alkyl Complexes: Evaluation of Redox Activity in Single Component Ethylene Polymerization Catalysts.

Tondreau, A. M.; **Milsmann, C.**; Patrick, A. D.; Hoyt, H. M.; Lobkovsky, E.; Wieghardt, K.; Chirik, P. J.; *J. Am. Chem. Soc.* **2010**, *132*, 15046.

16. Reduced N-Alkyl Substituted Bis(imino)pyridine Cobalt Complexes: Molecular and Electronic Structures for Compounds Varying by Three Oxidation States. Bowman, A. C.; **Milsmann, C.**; Bill, E.; Lobkovsky, E.; Weyhermüller, T.; Wieghardt, K.; Chirik, P. J.; *Inorg. Chem.* **2010**, *49*, 6110.

15. Stabilization of High-Valent Fe^{IV}S₆-Cores by Dithiocarbamate(1-) and 1,2-Dithiolate(2-) Ligands in Octahedral [Fe^{IV}(Et₂dtc)_{3-n}(mnt)_n]⁽ⁿ⁻¹⁾⁻ Complexes (n = 0, 1, 2, 3). A Spectroscopic and Density Functional Theory Computational Study. **Milsmann, C.**; Sproules, S.; Bill, E.; Weyhermüller, T.; DeBeer George, S.; Wieghardt, K.; *Chem. Eur. J.* **2010**, *16*, 3628.

14. Synthesis, Molecular and Electronic Structures of Reduced Bis(imino)pyridine Cobalt Dinitrogen Complexes: Ligand versus Metal Reduction. Bowman, A. C.; **Milsmann, C.**; Hojilla Atienza, C. C.; Lobkovsky, E.; Wieghardt, K.; Chirik, P. J.; *J. Am. Chem. Soc.* **2010**, *132*, 1676.

13. Reversible P₄ Activation with Nickel(I) and a Hapto-3-Coordinated Tetrphosphorus Ligand between Two Ni(I) Centers. Yao, S.; Xiong, Y.; **Milsmann, C.**; Bill, E.; Pfirrmann, S.; Limberg, C.; Driess, M.; *Chem. Eur. J.* **2010**, *16*, 436.

12. Electronic Structures of [Ru^{II}(cyclam)(Et₂dtc)]⁺, [Ru(cyclam)(tdt)]⁺, and [Ru(cyclam)(tdt)]²⁺. An X-Ray Absorption Spectroscopic and Computational Study (tdt = toluene-3,4-dithiolate; Et₂dtc = *N,N*-diethyldithiocarbamate(1-)). **Milsmann, C.**; Bill, E.; Weyhermüller, T.; DeBeer George, S.; Wieghardt, K.; *Inorg. Chem.* **2009**, *48*, 9754.

11. Octahedral Monodithiolene Complexes of Iron: Characterization of *S,S'*-Coordinated Dithiolate(1-) π Radical Monoanions. A Spectroscopic and Density Functional Theoretical Investigation. **Milsmann, C.**; Patra, G. K.; Bill, E.; Weyhermüller, T.; DeBeer George, S.; Wieghardt, K.; *Inorg. Chem.* **2009**, *48*, 7430.

10. Octahedral Monodithiolene Complexes of Cobalt(III) and Chromium(III). Spectroscopic and Density Functional Theoretical Characterization of *S,S'*-Coordinated Benzene-1,2-dithiolate(1-) π Radicals. **Milsmann, C.**; Bothe, E.; Bill, E.; Weyhermüller, T.; Wieghardt, K.; *Inorg. Chem.* **2009**, *48*, 6211.

9. Facile Dissociation of [(LNi^{II})₂E₂] Dichalcogenides (E = Se, Te): Evidence for [LNi^{II}E₂] Superselenides and Supertellurides in Solution. Yao, S.; Xiong, Y.; Zhang, X.; **Milsmann, C.**; Schwarz, H.; Driess, M.; *Angew. Chem.* **2009**, *121*, 4621.

8. Reduction Chemistry of Aryl- and Alkyl-Substituted Bis(imino)pyridine Iron Dihalide Compounds: Molecular and Electronic Structures of [(PDI)₂Fe]. Wile, B. M.; Trovitch, R. J.; Bart, S. C.; Tondreau, A. M.; Lobkovsky, E.; **Milsmann, C.**; Bill, E.; Wieghardt, K.; Chirik, P. J.; *Inorg. Chem.* **2009**, *48*, 4190.

7. The Striking Stabilization of Ni⁰(η⁶-Arene) Complexes by an Ylide-Like Silylene Ligand. Meltzer, A.; Präsaug, C.; **Milsmann, C.**; Driess, M.; *Angew. Chem. Int. Ed.* **2009**, *48*, 3170.

6. Bis-picket-fence corroles. Bröring, M.; **Milsmann, C.**; Ruck, S.; Köhler, S.; *J. Organomet. Chem.* **2009**, *694*, 1011.

5. Investigating different strategies towards the preparation of chiral and achiral bis-picket fence corroles. Bröring, M.; Funk, M.; **Milsmann, C.**; *J. Porph. Phthalocyanines* **2009**, *13*, 107.

4. A "side-on" superoxonickel complex [LNi(O₂)] with a square-planar tetracoordinate nickel(II) center and its conversion into [LNi(μ-OH)₂NiL]. Yao, S.; Bill, E.; **Milsmann, C.**; Wieghardt, K.; Driess, M.; *Angew. Chem. Int. Ed.* **2008**, *47*, 7110.
3. From a Paramagnetic, Mononuclear Supersulfidonickel(II) Complex to a Diamagnetic Dimer with a Four-Sulfur Two-Electron Bond. Yao, S.; **Milsmann, C.**; Bill, E.; Wieghardt, K.; Driess, M.; *J. Am. Chem. Soc.* **2008**, *130*, 13536.
2. One- and Two-Electron Reduced 1,2-Diketone Ligands in [Zn^{II}(L^{*})₂(Et₂O)], [Co^{II}(L^{*})₂(Et₂O)], and Na₂(Et₂O)₄[Co^{II}(L^{Red})₂]. Spikes, G. H.; **Milsmann, C.**; Bill, E.; Weyhermüller, T.; Wieghardt, K.; *Inorg. Chem.* **2008**, *47*, 11745.
1. Charge Distribution in Chromium and Vanadium Catecholato Complexes: X-Ray Absorption Spectroscopic and Computational Study. **Milsmann, C.**; Levina, A.; Harris, H. H.; Foran, G. J.; Turner, P.; Lay, P. A.; *Inorg. Chem.* **2006**, *45*, 4743.