VITA

DATE: January 24, 2015

NAME: Thomas M. Gilbert RANK: Associate Professor

DEPARTMENT: Chemistry and Biochemistry DATE OF BIRTH: December 26, 1959

EDUCATION:

B. S. in Chemistry, 1980, Purdue University, West Lafayette, Indiana
Ph. D., 1985, University of California, Berkeley, California

RESEARCH INTERESTS:

Computational studies of (1) the structures and reactions of main-group "frustrated Lewis pair" complexes; (2) ring strain energies and their application to physical chemistry and catalysis; (3) organic transformations catalyzed by Lewis acids; (4) the structures and cyclization reactions of main-group compounds that represent single-source precursors to materials; (5) the structures, photophysics and photochemistry of filter compounds present in human eyes related to cataract formation; (6) structures, bonding attributes, and energetics of gas phase reactions of hypervalent compounds; and (7) tests of models and basis sets, especially the behavior of density functional approaches when applied to large compounds.

PROFESSIONAL EXPERIENCE:

Graduate Research, University of California, Berkeley, 1981–85
Postdoctoral Fellow, Inorganic Division (INC-4), Los Alamos National Laboratory, NM, 1985–87
Postdoctoral Fellow, University of Pittsburgh, PA, 1987–89
Assistant Professor, Chemistry and Biochemistry, Northern Illinois University, 1989–95
Associate Professor, Chemistry and Biochemistry, Northern Illinois University, 1995–present
Visiting Professor, Department of Chemistry, University of Calgary, Calgary, Alberta, Canada, 1998–99
Visiting Fellow, Theoretical Division (T-14), Los Alamos National Laboratory, NM, 2002
Visiting Fellow, Ames Laboratory and Department of Chemistry, Iowa State University, Ames, IA, 2006
Visiting Professor, Department of Chemistry, Santa Clara University, Santa Clara, CA, 2007 & 2008

MEMBERSHIP IN PROFESSIONAL ORGANIZATIONS:

American Chemical Society, Division of Computers in Chemistry
American Chemical Society, Division of Inorganic Chemistry, Organometallic Subdivision
American Chemical Society, Division of Physical Chemistry

PUBLICATIONS (refereed):

1) "Preparation and Reactions of Tetrahydrido(pentamethylcyclopentadienyl)iridium: A Novel Iridium (V) Polyhydride", T. M. Gilbert and R. G. Bergman, *Organometallics* **1983**, *2*, 1458–1460.

2) "Oxidative Addition of Soluble Iridium and Rhodium Complexes to Carbon–Hydrogen Bonds in Alkanes", A. H. Janowicz, C. A. Kovac, R. A. Periana–Pillai, J. M. Buchanan, T. M. Gilbert, and R. G. Bergman, in *Organometallic Compounds: Synthesis, Structure and Theory*, B. L. Shapiro, Ed. Texas A & M University Press: College Station, Texas, 1983; 420–452.

3) "1,1,1,2,2,2,3,3,3–Nonacarbonyl–μ_3–cyclopropylmethylidyne–triangulo–tricobalt , (μ_3–c–C_3H_5–C)Co_3–$(CO)_9$", P. F. Seidler, S. T. McKenna, M.A. Kulzick, and T. M. Gilbert, *Acta Crystallographica, Section C: Crystal Structure Communications* **1985**, *41*, 352–355.

4) "Synthesis of Trimethylphosphine–Substituted (Pentamethylcyclopentadienyl)iridium Hydride Complexes; Protonation and Deprotonation of $(C_5(CH_3)_5)Ir(P(CH_3)_3)H_2$", T. M. Gilbert and R. G. Bergman, *J. Am. Chem. Soc*. **1985**, *107*, 3502–3507.

5) "(Pentamethylcyclopentadienyl)iridium Polyhydride Complexes: Synthesis of Intermediates in the Mechanism of Formation of $(C_5(CH_3)_5)IrH_4$, and the Preparation of Several Iridium(V) Compounds", T. M. Gilbert, F. J. Hollander, and R. G. Bergman, *J. Am. Chem. Soc*. **1985**, *107*, 3508–3516.

6) "NMR Spectra of $(C_5(CH_3)_5)IrH_2SiMe_3Li(pmdeta)$ and $(C_5(CH_3)_5)IrH_3Li(pmdeta)$: The First Direct Observation of Resolved ^7Li–^1H Coupling", T. M. Gilbert and R. G. Bergman, *J. Am. Chem. Soc*. **1985**, *107*, 6391–6393.

7) "Mono(cyclooctatetraenyl) Actinide Complexes. 1. Preparation of the Diamides $(C_8H_8)An[N(SiMe_3)_2]_2$ (An = Th, U), and the Structure of $(C_8H_8)Th[N(SiMe_3)_2]_2$", T. M. Gilbert, R. R. Ryan, and A. P. Sattelberger, *Organometallics* **1988**, *7*, 2514–2518.

8) "Synthesis of Mixed–Ring Organoactinide Complexes: $[(C_8H_8)(C_5Me_5)ThCl]_2$ and its Derivatives", T. M. Gilbert, R. R. Ryan, and A. P. Sattelberger, *Organometallics* **1989**, *8*, 857–859.

9) "Tetrahydrido(η^5–pentamethylcyclopentadienyl)iridium", T. M. Gilbert and R. G. Bergman, *Inorg. Syn.* **1990**, *27*, 19–23.

10) "Nonlinear Optical and Excited–State Properties of Conjugated One–Dimensional $[:N{\equiv}M(OR)_3]_n$ Polymers", T. P. Pollagi, T. C. Stoner, R. F. Dallinger, T. M. Gilbert, and M. D. Hopkins, *J. Am. Chem. Soc*. **1991**, *113*, 703–704.

11) "Spectroscopic Properties of Conjugated Metal–Carbon Multiple Bonds: Synthesis and Absorption Spectra of the "Dialkylidynes" $(RO)_3W{\equiv}C–C{\equiv}W(OR)_3$ (OR = $OCMe_3$, $OCMe_2CF_3$, $OCMe_2Et$)", T. M. Gilbert, and R. D. Rogers, *J. Organomet. Chem.* **1991**, *421*, C1–C5.

12) "Synthesis and Electronic Properties of Triply Bonded Hexa(fluoroalkoxide)dimolybdenum Complexes. Structure of $Mo_2[OCMe(CF_3)_2]_6$ and Investigation of the Nature of the Frontier Orbitals in Triply Bonded M_2X_6 Compounds", T. M. Gilbert, A. M. Landes, and R. D. Rogers, *Inorg. Chem.* **1992**, *31*, 3438–3444.

13) "Nature of the Frontier Orbitals of Tungsten Benzylidyne Complexes", J. Manna, T. M. Gilbert, R. F. Dallinger, S. J. Geib, and M. D. Hopkins, *J. Am. Chem. Soc*. **1992**, *114*, 5870–5872.

14) "Structure of $(\mu–C)_2W_2[OC(CH_3)_3]_6$: A Dimetallabutadiyne", T. M. Gilbert and R. D. Rogers, *Acta Crystallographica* **1993**, *C49*, 677–680.

15) "Crystal Structures of $(\eta^6–C_7H_8)M(CO)_3$ (M = Cr, W). Comparisons Among a Homologous Series of Cycloheptatriene Complexes and Experimental Evidence for a Boat Conformation of the Coordinated Ring", F. J. Hadley, T. M. Gilbert and R. D. Rogers, *J. Organomet. Chem.* **1993**, *455*, 107–113.

16) "Organotransition Metal Compounds for Photonics: Syntheses and Structures of E–(Nitrostilbene)–Chromium Tricarbonyl Complexes", T. M. Gilbert, F. J. Hadley, C. B. Bauer, and R. D. Rogers, *Organometallics* **1994**, *13*, 2024–2034.

17) "Structures of Z–(nitrostilbene)chromium tricarbonyl complexes: the effect of metal coordination on the nonplanarity of the stilbene system", T. M. Gilbert and R. D. Rogers, *J. Chem. Cryst.* **1994**, *24*, 315–320.

18) "Structures of a Series of $[4\text{–}R\text{–}C_6H_4\text{–}CH(OR')_2]Cr(CO)_3$ Complexes: Evidence Against a Favored Carbonyl Orientation in (*Para*–disubstituted Arene)chromium Tricarbonyl Compounds", T. M. Gilbert, A. H. Bond, and R. D. Rogers, *J. Organomet. Chem.* **1994**, *479*, 73–86.

19) "Syntheses and Structures of Bis(tricarbonylchromium)–substituted α, ω–Diphenylhexatriene Complexes", T. M. Gilbert, F. J. Hadley, M. D. Simmons, C. B. Bauer, and R. D. Rogers, *J. Organomet. Chem.* **1996**, *510*, 83–92.

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21) "Raman Spectra of $M_2(OR)_6$ and M_2R_6 (M = Mo, W) Compounds: Assignment of the M≡M Stretching Frequency in M_2X_6 Dimers", J. C. Littrell, C. E. Talley, R. F. Dallinger, and T. M. Gilbert, *Inorg. Chem.* **1997**, *36*, 760–761.

22) "*Ab initio* prediction of ring strain enthalpies of cyclic amine–boranes", Thomas M. Gilbert, *Tetrahedron Lett.* **1998**, *39*, 9147–9150.

23) "*Ab initio* Studies of Pericyclic Reactions of Aminoboranes. [2+2] Dimerization and [4+2] Diels–Alder Reactions of H_2BNH_2, Me_2BNMe_2 and $(F_3C)_2BNMe_2$", Thomas M. Gilbert, *Organometallics* **1998**, *17*, 5513–5520

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33) “Effect of Substituents on the Strength of Hypervalent Phosphorus–Halogen Bonds“, Catherine E. Check, Kim C. Lobring, Pamela R. Keating, Thomas M. Gilbert, and Lee S. Sunderlin, *J. Phys. Chem. A* **2003**, *107*, 8961–8967.

34) "Comparison of M–S, M–O, and M–(η^2–SO) Structures and Bond Dissociation Energies in d^6 $(CO)_5M(SO_2)^{pq}$ Complexes using Density Functional Theory", Heather J. Retzer and Thomas M. Gilbert, *Inorg. Chem.* **2003**, *42*, 7207–7218.

35) "Computational Studies of the Origin of Regiospecificity in the [4+2] Diels–Alder Reaction between $R_2B{=}NR_2'$ Compounds and Substituted *cis*–Butadienes ", Thomas M. Gilbert, *Organometallics* **2003**, *22*, 3748–3752.

36) "Density Functional Theory Study of the d^{10} Series $(H_3P)_3M(\eta^1–SO_2)$ and $(Ph_xMe_{3–x}P)_3M(\eta^1–SO_2)$ (M = Ni, Pd, Pt; x = 0–3): SO_2 Pyramidality and M–S Bond Dissociation Energies", Daniel J. Brust and Thomas M. Gilbert, *Inorg. Chem.*, **2004**, *43*, 1116–1121.

37) "Pericyclic Reactions between Aminoboranes $R_2B{=}NR_2'$ and Alkenes: [4+2] vs [2+2] Transition States", Kirk M. Bissett and Thomas M. Gilbert, *Organometallics*, **2004**, *23*, 850–854.

38) “Experimental and Computational Studies of the Metal–Metal Stretching Vibration in $X_3M{\equiv}MX_3$ Compounds (X = Alkoxide, Alkyl, Amide)", Thomas M. Gilbert, John C. Littrell, Chad E. Talley, Michael A. Vance, Richard F. Dallinger, and Robin D. Rogers, *Inorg. Chem.*, **2004**, *44*, 1762–1769.

39) "Molecular and Electronic Structure of Platinum Bis(*N*–arylamino)phosphenium Complexes including [Pt(phosphine)(phosphenium)(*N*–heterocyclic carbene)]", Ned J. Hardman, Michael B. Abrams, Melanie A. Pribisko, Thomas M. Gilbert, Richard L. Martin, Gregory J. Kubas, and R. Tom Baker, *Angew. Chem., Int. Ed. Engl.*, **2004**, *43*, 1955–1958.

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41) "Pericyclic Reactions between Iminoboranes RB≡NR' and Alkynes: [4+2] vs [2+2] Transition States", K. M. Bissett and T. M. Gilbert, *Organometallics* **2004**, *23*, 5048–5053.

42) “The Effect of Substituents on the Strength of A–Cl^- (A = Si, Ge, and Sn) Bonds in Hypervalent Systems: ACl_5^-, ACl_4F^-, and $A(CH_3)_3Cl_2^-$“, Changtong Hao, Jennifer D. Kaspar, Catherine E. Check, Kim C. Lobring, Thomas M. Gilbert, and Lee S. Sunderlin, *J. Phys. Chem. A*, **2005**, *109*, 2026–2034.

43) “Progressive Systematic Underestimation of Reaction Energies by the B3LYP model as the Number of C–C Bonds Increases: Why Organic Chemists Should Use Multiple DFT Models for Calculations involving Poly–carbon Hydrocarbons“, Catherine E. Check and Thomas M. Gilbert, *J. Org. Chem.* **2005**, *70*, 9828–9834.

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46) “Computational Studies of [2+2] and [4+2] Pericyclic Reactions between Phosphinoboranes and Alkenes. Steric and Electronic Effects in Identifying a Reactive Phosphinoborane that Should Avoid Dimerization”, Thomas M. Gilbert and Steven M. Bachrach, *Organometallics* **2007**, *26*, 2672–2678.

47) “Superacid promoted reactions of N–acyliminium salts and evidence for the involvement of superelectrophiles”, Yiliang Zhang, Daniel J. DeSchepper, Thomas M. Gilbert, Kiran Kumar S. Sai, and Douglas A. Klumpp, *Chem. Commun.* **2007**, 4032–4034.

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50) “Synthesis and Characterization of Platinum(II)- and Platinum(IV)- Pyrophosphato Complexes” Robert J. Mishur, Chong Zheng, Thomas M. Gilbert, and Rathindra N. Bose, *Inorg. Chem.* **2008**, *47*, 7972–7982.

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53) “Donor-Acceptor Dissociation Energies of Group 13-15 Donor-Acceptor Complexes Containing Fluorinated Substituents: Approximate Lewis Acidities of $(F_3C)_3M$ vs $(F_5C_6)_3M$ and the Effects of Phosphine Steric Bulk.”, Austin L. Gille and Thomas M. Gilbert, *J. Chem. Theory and Comp.* **2008** *3*, 1681–1689.

54) “N-Heterocyclic Superelectrophiles and Evidence for Single Electron Transfer Chemistry.” Kiran Kumar Solingapuram Sai, Matthew J. Tokarz, Andrew P. Malunchuk, Chong Zheng, Thomas M. Gilbert, and Douglas A. Klumpp, *J. Am. Chem. Soc.* **2008**, *130*, 14388-14389.

55) “Computational Studies of Pericyclic Reactions between Aminoalanes and Ethyne, Ethene, and Dienes. A Reactive Aminoalane that Should Prefer [2+2] and [4+2] Cyclizations to Dimerization“, John M. Bailey, Catherine E. Check, and Thomas M. Gilbert, *Organometallics* **2009**, *28*, 787–794.

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65) “Computational Studies of Complexation of Nitrous Oxide by Borane-Phosphine Frustrated Lewis Pairs”, Thomas M. Gilbert, *Dalton Trans.*, **2012**, *41*, 9046–9055.

66) “Optimized Structures and Ring Strain Energies of Isoelectronic Homo- and Heterosiliranes *c*-$AX_2SiR_2SiR_2^q$ (A/q = Al/–1, Si/0, P/+1): Unexpected Effects of Charge and Size”, Christina L. Allard, Philippe Gauthier, Austin L. Gille, Gerald E. Thomas, and Thomas M. Gilbert, *Organometallics*, **2013**, *32*, 2558–2566.

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68) “Stoichiometric Reduction of CO_2 to CO Using AlX_3-Based Frustrated Lewis Pairs: A Combined Theoretical and Experimental Mechanistic Investigation”, Gabriel Ménard, Thomas M. Gilbert, Jillian A. Hatnean, Anne Kraft, Ingo Krossing, and Douglas W. Stephan, *Organometallics*, **2013**, *32*, 4416–4422.

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REVIEWS

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2) "Computational Studies of Lewis Acidity and Basicity in Frustrated Lewis Pairs (FLPs)", Thomas M Gilbert, *Topics Curr. Chem.* **2013**, 332, 267–289

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