

## PUBLICATIONS (total 111)

1. Eisen- and Cobaltkomplexe mit Schwefelliganden: Darstellung und Kristallstrukturen von  $[\text{Me}_4\text{N}][\text{FeCl}\{\text{S}_2\text{P}(\text{OMe})_2\}_2]$ ,  $[\text{Me}_4\text{N}][\text{CoCl}\{\text{S}_2\text{P}(\text{OMe})_2\}_2]$ ,  $[\text{Et}_4\text{N}][\text{FeCl}\{\text{S}_2\text{P}(p\text{-C}_6\text{H}_4\text{Me})_2\}_2]$ ,  $[\text{Et}_4\text{N}]_2[\text{FeCl}\{\text{S}_2\text{PS}(\text{OMe})\}_2]$ ,  $[\text{Fe}\{\text{S}_2\text{P}(\text{OMe})_2\}_3]$ .  
Kristin Kirschbaum, Uta Bönnighausen, Ewald Gesing, Klaus Greiwe, Ulrich Kuhlmann, Henry Strasdeit, Bernt Krebs, Gerald Henkel  
*Z. Naturforsch.* **1990**, 45b, 245.
2. Eisen- and Cobaltkomplexe mit Schwefelliganden: Darstellung und Kristallstrukturen von  $[\text{Fe}\{\text{S}_2\text{P}(p\text{-C}_6\text{H}_4\text{Me})_2\}_2(\text{MeOH})_2] \cdot 2\text{MeOH}$ ,  $[\text{Fe}\{\text{S}_2\text{P}(p\text{-C}_6\text{H}_4\text{Me})_2\}_2(\text{THF})_2]$ ,  $[\text{Fe}\{\text{S}_2\text{P}(p\text{-C}_6\text{H}_4\text{Me})_2\}_2(\text{THT})_2] \cdot \text{oTHT}$ ,  $[\text{Fe}\{\text{S}_2\text{P}(p\text{-C}_6\text{H}_4\text{Me})_2\}_2(\text{DMF})_2] \cdot 2\text{DMF}$ ,  $\text{Co}\{\text{S}_2\text{P}(p\text{-C}_6\text{H}_4\text{Me})_2\}_2(\text{DMF})_2 \cdot 2\text{DMF}$ .  
Kristin Kirschbaum, Klaus Greiwe, Kay Müller, Henry Strasdeit, Bernt Krebs, Gerald Henkel  
*Z. Naturforsch.* **1990**, 45b, 497.
3. Structure of Trichloro( $\mu$ 5-methylcyclo-pentadienyl)titanium(IV).  
Kristin Kirschbaum, Dean M. Giolando  
*Acta Cryst.* **1991**, C47, 2216.
4. An Efficient One-pot Synthesis of 1,2-Benzenedithiol from Benzenethiol.  
Dean M. Giolando, Kristin Kirschbaum  
*Synthesis* **1992**, 5, 451.
5. Structure of Dichloro-azido( $\mu$ 5-methylcyclopentadienyl)- titanium(IV) Dimer.  
Kristin Kirschbaum, Dean M. Giolando  
*Acta Cryst.* **1992**, C48, 1837.
6. Amido Complexes of (Cyclopentadienyl)dichlorotitanium(IV): Ti-N multiple bond character.  
Dean M. Giolando, Lisa Graves, Kristin Kirschbaum, Urs Bolle  
*Inorg. Chem.* **1992**, 31, 3887.
7. Synthese, Struktur und Bindungseigenschaften von Chalkogeno- und Halogenoverbindungen schwerer Hauptgruppenelemente mit  $s^2$ -Konfiguration.  
Bernt Krebs, Frank-Peter Ahlers, Stefan Bonmann, Andreas Brommelhaus, Horst Greiwing, Berthold Kersting, Kristin Kirschbaum, Thomas Lindner, Markus Nienhaus, Norbert Taubken  
in: *Unkonventionelle Wechselwirkungen in der Chemie metallischer Elemente*, VCH Weinheim, **1992**.
8. Z-Perchlorostilbene.  
James E. Gano, Ewa Skrzypczak-Jankun, Kristin Kirschbaum, Dieter Lenoir, Rudolph Frank  
*Acta Cryst.* **1993**, C49, 1985.

9. Synthesis, Crystal Structure and Electrochemistry of Bis(N,N-dimethylammonium) Tris(1,2-benzenedithiolato)titanate(IV).  
Martin Könemann, Wolfram Stürer, Kristin Kirschbaum, Dean M. Giolando  
*Polyhedron* **1994**, *13*, 1415.
10. Co-crystallized Bis( $\mu$ -*tert*-butylphosphido-1:2 $\kappa^2$ P)bis(di-*tert*-butylgallium) and Tetra-*tert*-butylcyclotetra-phosphane.  
Kristin Kirschbaum, Dean M. Giolando  
*Acta Cryst.* **1994**, *C50*, 1244.
11. Synthesis, Properties and Crystal Structures of Benzene-1,2-dithiolato Complexes of Antimony-(III) and -(V)  
Joachim Wegener, Dean M. Giolando, Kristin Kirschbaum  
*J. Chem. Soc. Dalton Trans.* **1994**, 1213.
12. Homoleptic Thiolate Complexes: Di- and Tri-nuclear Complexes of Ti(IV) with Unexpected Metal-sulfur Cores, [NMe<sub>2</sub>H<sub>2</sub>][Ti<sub>2</sub>(SMe)<sub>9</sub>] and [Ti<sub>3</sub>(SMe)<sub>12</sub>].  
Wolfram Stuer, Kristin Kirschbaum, D. M. Giolando  
*Angew. Chem.* **1994**, *33*, 1981.
13. Reactions of Dimeric Palladium(I) Complexes with Sulfur-Substituted Acetylenes: 1,2-Heteroatomic Shift Reactions versus Adduct Formation. X-ray Crystal Structures of [Pd<sub>2</sub>Cl<sub>2</sub>( $\mu$ -dppm)<sub>2</sub>( $\mu$ -CH<sub>3</sub>SCCSCH<sub>3</sub>)].CH<sub>2</sub>Cl<sub>2</sub>, [Pd<sub>2</sub>Cl<sub>2</sub>( $\mu$ -dppm)<sub>2</sub>( $\mu$ -CH<sub>3</sub>SCCSCH<sub>3</sub>)], and [Pd<sub>2</sub>Cl<sub>2</sub>( $\mu$ -dppm)<sub>2</sub>( $\mu$ -?-C=C(CH<sub>3</sub>)(SCH<sub>3</sub>))].  
J. A. Davies, K. Kirschbaum, C. Kluwe  
*Organometallics* **1994**, *13*, 3664.
14. Synthesis, Properties and Crystal Structures of Benzene-1,2-dithiolato Complexes of Thallium-(I) and -(III).  
Boris E. Bosch, Martin Eisenhauer, Berthold Kersting, Kristin Kirschbaum, Bernt Krebs, and Dean M. Giolando  
*Inorg. Chem.* **1996**, *35*, 6599.
15. (E)-2,2,5,5-Tetramethyl-3,4-bis[4-(tribromometyl)phenyl]hex-3-ene.  
James A. Gano, Kristin Kirschbaum, Padmanabhan Sekher  
*Acta Cryst.* **1996**, *C52*, 2334.
16. The Reaction of [Pd<sub>2</sub>Cl<sub>2</sub>( $\mu$ -PP)<sub>2</sub>] (PP = dppm, dppm) with Et<sub>2</sub>NCCNEt<sub>2</sub> in Methylen Chloride Solution: X-ray Crystal Structure of [Pd<sub>2</sub>Cl<sub>2</sub>( $\mu$ -CH<sub>2</sub>) ( $\mu$ -dppm)<sub>2</sub>] and Hexakis(diethylamino)benzene, C<sub>6</sub>(NEt<sub>2</sub>)<sub>6</sub>.  
Sean Klopfenstein, Constanze Kluwe, Kristin Kirschbaum, Julian A. Davies  
*Canad. J. Chem.* **1996**, *74*, 2331-2339.
17. Lambda/2 contamination in CCD area detector data.  
Kristin Kirschbaum, Anthony Martin, A. Alan Pinkerton

*J. Appl. Cryst.* **1997**, *30*, 514-516.

18. Highly Stereoselective Synthesis of Perhydro-8a-(hydroxymethyl)-phenanthrene-1,2,4,5,7,8-hexol and Derivatives.  
Herve Mosimann, Pierre Vogel, A. Alan Pinkerton, Kristin Kirschbaum  
*J. Org. Chem.* **1997**, *62*, 3002-3007.
19. (E)-2,2,5,5-Tetramethyl-3,4-diphenylhex-3-ene.  
James E. Gano, Constanze Kluwe, Kristin Kirschbaum, A. Alan Pinkerton, Padmanabhan Sekher, Ewa Skrzypczak-Jankun, Girija Subramaniam, Dieter Lenoir  
*Acta Cryst.* **1997**, *C53*, 1723-1725.
20. Diastereoselective Synthesis of *trans*-2-(1-Triphenylmethyl-1*H*-Imidazol-4-yl)cyclopropanecarboxylic acids: Key Intermediates for the Preparation of Potent and Chiral Histamine H3 Receptor Agents.  
M. Amin Khan, Stephen L. Yates, Clark E. Tedford, Kristin Kirschbaum and James G. Phillips  
*Bioorganic & Medicinal Chemistry Letters* **1997**, *7*, 3017-3022.
21. Studies on Lateral Stereocontrol Using the ( $\pi$ -Allyl)molybdenum System.  
Anthony J. Pearson, Irina. B. Neagu, A. Alan Pinkerton, Kristin Kirschbaum, and Michaela J. Hardie  
*Organometallics* **1997**, *16*, 4346-4354.
22. Complexes of Niobium and Tantalum with Chloride, Sulfide and Oxide Ligands: Synthesis and Crystal Structure of the (Tetrachloro)bis(h<sub>2</sub>-disulfido)(m-oxo)(m-h<sub>2</sub>:h<sub>2</sub>-disulfido)bismetallates  $[Cl_2(S_2)Nb(m-O)(m-S_2)Nb(S_2)Cl_2]^{2-}$  and  $[Cl_2(S_2)Ta(m-O)(m-S_2)Ta(S_2)Cl_2]^{2-}$  as their Tetraphenylphosphonium salts.  
Michael Bösing, Olaf Conrad, Birgit Hommerich, Kristin Kirschbaum, Endre Kövari, Bernt Krebs, A. Alan Pinkerton, Werner Steinforth  
*Inorg. Chim. Acta* **1998**, *274*, 251-256.
23. Comparative X-ray Crystallographic Characterization of the Mono- and Bimetallic Complexes of Rhenium(I) Tricarbonyl Chloride with 2,3-bis(2-pyridyl)pyrazine.  
Jon R. Kirchhoff, Kristin Kirschbaum  
*Polyhedron* **1998**, *17*, 4033-4039.
24. 1,4-Di(1,2-di-*tert*-butyl-2-phenylethenyl)benzene and Related Twist-twist Pi Conjugated Stilbene (PPV) Systems.  
James E. Gano, Kristin Kirschbaum, Eddie D. Luzik, Jr., Padmanabhan Sekher  
*Tetrahedron Letters* **1998**, *39*, 6641.
25. An Open Flow Helium Cryostat for X-ray Diffraction Experiments.  
Michaela J. Hardie, Kristin Kirschbaum, Anthony Martin, A. Alan Pinkerton  
*J. Appl. Cryst.* **1998**, *31*, 815-817.

26. Synthesis and characterization of novel dinuclear and cationic cyclobutadiene platinum complexes.  
Michael Gerisch, Kristin Kirschbaum, Clemens Bruhn, Harry Schmidt, Julian A. Davies, Dirk Steinborn  
*J. Organometal. Chem.* **1998**, 570, 129-139.
27. Stereocontrolled Cyclization of Unactivated Alkene Onto Cationic Dienyl Iron Tricarbonyl Systems  
Anthony J. Pearson, Asaf Alimardanov, A. Alan Pinkerton, David M. Fouchard, Kristin Kirschbaum  
*Tetrahedron Letters* **1998**, 39, 5919-5922.
28. Use of an open-flow helium cryostat for macromolecular crystallography  
B. Leif Hanson, Anthony Martin, Joel M. Harp, Damon A. Parrish, Christopher G. Bunick, Kristin Kirschbaum, A. Alan Pinkerton, Gerard J. Bunick  
*J. Appl. Cryst.* **1999**, 32, 814-820.
29. Energetic Materials: the preparation and structural characterization of melaminium dinitramide and melaminium nitrate  
Rasim Tanbug, Kristin Kirschbaum, A. Alan Pinkerton  
*J. Chem. Crystallogr.* **1999**, 29, 45-55.
30. Cooperative Jahn-Teller induced phase transition of TbVO<sub>4</sub>: single crystal structure analyses of the tetragonal high temperature phase and the twinned orthorhombic phase below 33K  
Kristin Kirschbaum, Anthony Martin, Damon Parrish, A. Alan Pinkerton  
*J. Phys. C: Condensed Matter* **1999**, 11, 4483-4490.
31. On the Reactivity of Platina-β-diketones - Synthesis and Characterization of Acylplatinum(II) Complexes  
Dirk Steinborn, Tobias Hoffmann, Michael Gerisch, Clemens Bruhn, Harry Schmidt, Karsten Nordhoff, Julian A. Davies, Kristin Kirschbaum, Ingo Jolk  
*Z. Anorg. Allg. Chem.* **2000**, 626, 661-666.
32. Trigonal Prismatic vs Octahedral Coordination Geometry(I): Syntheses and Structural Characterization of Hexakis(arylthiolato) Zirconate Complexes  
Jan C. Friese, Arndt Krol, Carsten Puke, Kristin Kirschbaum, Dean M. Giolando  
*Inorg. Chem.* **2000**, 39, 1496-1500.
33. Polymeric structures containing self-assembled Li-dioxane networks; syntheses and crystal structures of [{Li(dioxane)}<sub>2.5</sub>TaCl<sub>4</sub>S]<sub>n</sub>.n/2 dioxane and [{Li<sub>2</sub>(dioxane)}<sub>3</sub>Cl]<sub>n</sub>][TaCl<sub>6</sub>]<sub>n</sub>  
Sven Hasche, Christian Mock, Jens Otto, Florian Schweppe, Kristin Kirschbaum, Bernt Krebs, A. Alan Pinkerton  
*Inorg. Chim. Acta*, **2000**, 298, 9-15.
34. 2-Phenylglycerol: crystal structure and conformational considerations pertaining to formation of its related oxetane

Paul W. Erhardt, Wieslaw A. Klis, Peter I. Nagy, Kristin Kirschbaum, Nan Wu, Anthony Martin, and A. Alan Pinkerton  
*J. Chem. Crystallogr.*, **2000**, *30*, 83.

35. Linear Tricobalt Compounds with Di-(2-pyridyl)amide (dpa) Ligands: Temperature Dependence of the Structural and Magnetic Properties of Symmetrical and Unsymmetrical Forms of  $\text{Co}_3(\text{dpa})_4\text{Cl}_2$  in the Solid State.  
Rodolphe Clérac, F. Albert Cotton, Lee M. Daniels, Kim R. Dunbar, Kristin Kirschbaum, Carlos A. Murillo, A. Alan Pinkerton, Arthur J. Schultz, Xiaoping Wang  
*J. Am. Chem. Soc.* **2000**, *122*, 6226-6236.
36. Catenated Organotelluride Compounds: A facile Route to the Linear  $[(\text{TeC}_6\text{H}_5)_3]^-$  Anion  
Daniel Withaut, Kristin Kirschbaum, Olaf Conrad, Dean M. Giolando  
*Organometallics*, **2000**, *19*, 5238-5240.
37. Hydrogen Bonding in  $[\text{Me}_2\text{NHC}_2\text{H}_4\text{NHMe}_2][\text{SePh}]_2$   
Arnold A. Feldmann, Kai Schmengler, Klaus Laue, Stefan Marose, Kristin Kirschbaum, Olaf Conrad, Dean M. Giolando  
*Acta Cryst.* **2000**, *C56*, e531.
38. The pentacoordinate titanium complex  $[\text{TiCl}_2(\text{NMe}_2)_2(\text{HNMe}_2)]$   
Kristin Kirschbaum, Olaf Conrad, and Dean M. Giolando  
*Acta Cryst.* **2000**, *C56*, e541.
39. The titanium thiolate complex  $[\text{Li}(\text{C}_4\text{H}_8\text{O})_4][\text{Ti}_2(\text{SC}_6\text{H}_5)_9]$   
Carsten Puke, Kai Schmengler, Kristin Kirschbaum, Olaf Conrad, Dean M. Giolando  
*Acta Cryst.* **2000**, *C56*, e542.
40. Dimeric Phenalenyl-Based Neutral Radical Molecular Conductors  
X. Chi, M.E. Itkis, K. Kirschbaum, A.A. Pinkerton, R.T. Oakley, A.W. Cordes, R.C. Haddon  
*J. Am. Chem. Soc.* **2001**, *123*, 4041-4048.
41. Macromolecular data collection with cryogenic helium  
B. Leif Hanson, Joel M. Harp, Kristin Kirschbaum, Damon A. Parrish, David E. Timm, Andrew Howard, A. Alan Pinkerton, Gerard J. Bunick  
*Journal of Crystal Growth* **2001**, *232*, 536-544.
42. Refinement of the crystal structure of digallium trisulfide,  $\text{Ga}_2\text{S}_3$   
C.Y.Jones, J.C.Bryan, K.Kirschbaum, J.G.Edwards  
*Z. Kristallogr. NCS* **2001**, *216*, 327-328.
43. A novel cage organotellurate(IV) macrocyclic host encapsulating a bromide anion guest:  
 $[\text{Li}(\text{THF})_4][\{\text{Pr}_3\text{Te}\}_{12}\text{O}_{16}\text{Br}_4\{\text{Li}(\text{THF})\text{Br}\}_4]\text{Br}.2\text{THF}$   
Hélène Citeau, Kristin Kirschbaum, Olaf Conrad, Dean M. Giolando  
*J. Chem. Soc. Chem. Commun.* **2001**, 2006-2007.

44. Experiments Testing the Abatement of Radiation Damage in D-Xylose Isomerase Crystals with Cryogenic Helium  
B. Leif Hanson, Joel M. Harp, Kristin Kirschbaum, Constance A. Schall, Ken DeWitt, Andrew Howard, A. Alan Pinkerton and Gerard J. Bunick  
*J. Synchrotron Rad.* **2002**, *9*, 375-381.
45. Resonance Stabilized 1,2,3-Dithiazolo-1,2,3-dithiazolyls as Neutral  $\pi$ -Radical Conductors  
Leanne Beer, Jaclyn L.Brusso, A.Wallace Cordes, Robert C. Haddon, Mikhail E. Itkis, Kristin Kirschbaum, Douglas S. MacGregor, Richard T.Oakley, A.Alan Pinkerton, Robert W. Reed  
*J. Am. Chem. Soc.* **2002**, *124*, 9498-9509.
46. Homoleptic Phenolate Complexes of Zirconium(IV): Syntheses and Structural Characterization of the First Six Coordinate Complexes  
Thomas C. Rosen, Dean M. Giolando, Kristin Kirschbaum  
*J. Chem. Soc., Dalton Trans.* **2003**, *1*, 120-125.
47. Structures of divalent transition metal salts of 4-aminonaphthalene-1-sulfonate: unexpected variation in layering pattern  
Jill E. Morris, Phillip J. Squattrito, Kristin Kirschbaum, A. Alan Pinkerton  
*J. Chem. Crystallogr.* **2003**, *33*, 307-321.
48. Di- and Triindolylmethanes: Molecular Structures and Spectroscopic Characterization of Potentially Bidentate and Tridentate Ligands  
Mark R. Mason, Thomas S. Barnard, Mawuto F. Segla, Baohan Xie, Kristin Kirschbaum  
*J. Chem. Crystallogr.* **2003**, *33*, 531-540.
49. A Standard Local Coordinate System for Multipole Refinements of the Estrogen Core Structure  
Kristin Kirschbaum, Damon A. Parrish, Kumar Poomani, A. Alan Pinkerton, E.A. Zhurova,  
*J. Appl. Crystallogr.* **2003**, *36*, 1464-1466.
50. Titanium and Zirconium Amido Complexes Ligated by Scorpionate 2,2'-Di(3-methylindolyl)-methanes: Synthesis, Characterization, and Ethylene Polymerization Activity  
Mark R. Mason, Bassam N. Fneich, and Kristin Kirschbaum  
*Inorg. Chem.* **2003**, *42*, 6592-6594.
51. Mechanisms of Exchange Modulation in Trimethylenemethane-type Biradicals: The Roles of Conformation and Spin Density  
David A. Shultz, Rosario M. Fico, Jr., Hyoyoung Lee, Jeff W. Kampf, Kristin Kirschbaum, A. Alan Pinkerton, Paul D. Boyle  
*J. Am. Chem. Soc.* **2003**, *125*, 15426-15432.
52. Synthesis and Structure of [(nitrito-O,O')bis(di-2-pyridylamine)copper(II)]nitrite  
Alvin A. Holder, Robert T. Stibrany, Martin Hall, Vince C.R. Payne, Kristin Kirschbaum, A. Alan Pinkerton, Nadeja Bolotina  
*J. Chem. Crystallogr.* **2004**, *34*, 383-386.

- 
53. An Addition to the Oxoacid Family: H<sub>2</sub>B<sub>12</sub>(OH)<sub>12</sub>  
Daniel J. Stasko, Kevin J. Perzynski, Mark A. Wasil, Julia K. Brodbeck, Kristin Kirschbaum,  
Yong Wah Kim, and Cora Lind  
*Inorg. Chem.* **2004**, *43*, 3786-3788.
54. Remarkable Room-Temperature Insertion of Carbon Monoxide into an Aluminum-Carbon Bond of Tri-*tert*-butylaluminum  
Mark R. Mason, Bingxu Song, Kristin Kirschbaum  
*J. Am. Chem. Soc.* **2004**, *126*, 11812-11813.
55. Sample size: an important parameter in choosing flash-cooling protocols for macromolecular crystallography  
Unmesh Chinte, Binal Shah, Ken DeWitt, Kristin Kirschbaum, A. Alan Pinkerton, Constanze Schall  
*J. Appl. Crystallogr.* **2005**, *38*, 412-419.
56. Deprotonated diindolylmethanes as dianionic analogues of scorpionate bis(pyrazolyl)borate ligands: synthesis and structural characterization of representative titanocene and zirconocene complexes  
Mark.R.Mason, Dough Ogrin, Bassam Fneich, ThomasS.Barnard, Kristin Kirschbaum  
*J. Organomet. Chem.* **2005**, *690*, 157-162.
57. Fortuitous formation of [(LiCl)<sub>6</sub>{(Me<sub>2</sub>NCH<sub>2</sub>C<sub>8</sub>H<sub>5</sub>N)<sub>3</sub>P}<sub>2</sub>]: an amine-ligated hexameric lithium chloride aggregate  
Mark R. Mason, Floyd A. Beckford, Kristin Kirschbaum, and Bradford J. Gorecki  
*Inorg. Chem. Commun.* **2005**, *8*, 331-334.
58. Design of an efficient solution grown semiorganic NLO crystal for short wavelength generation: 2-amino-5-nitropyridinium tetrafluoroborate  
S. Manivannan, S. Dhanuskodi, K. Kirschbaum, S.K. Tiwari  
*Journal of Crystal Growth and Design* **2005**, *5*, 1463-1468.
59. Synthesis of the anti and syn Isomers of Thieno[f,f']bis[1]benzothiophene.  
Comparison of the Optical and Electrochemical Properties of the *anti* and *syn* Isomers.  
Brigitte Wex, Bilal R. Kaafarani , Kristin Kirschbaum, and Douglas C. Neckers  
*J. Org. Chem.* **2005**, *70*, 4502-4505.
60. Solid State and Solution Structures of 2-Halophenolate Complexes of Lithium  
Thomas Rosen, Kristin Kirschbaum, Dean M. Giolando  
*Inorg. Chim. Acta* **2005**, *358*, 3680-3690.
61. Energetic materials:  $\alpha$ -NTO crystallizes as a 4-component triclinic twin  
Nadezhda B. Bolotina, Kristin Kirschbaum, A. Alan Pinkerton  
*Acta Cryst* **2005 B61**, 577-584.

62. Twisted, Z-Shaped Perylene Bisimide  
Faysal Ilhan, Daniel S. Tyson, Daniel J. Stasko, Kristin Kirschbaum, Michael A. Meador  
*J. Am. Chem. Soc.* **2006**, 128, 702-703.
63. Synthesis, structural, thermal and optical studies of 1-ethyl-2,6-dimethyl-4-hydroxy pyridinium halides  
S. Dhanuskodi, S. Manivannan, K. Kirschbaum  
*Spectrochimica Acta. Part A* **2006**, 64, 504-511.
64. Structural, thermal and dielectric studies on a new solution grown 4-dimethylaminopyridinium dihydrogen phosphate crystal  
S.Dhanuskodi, S.Manivannan, K.Kirschbaum, J.Philip, S.Selladurai  
*Journal of Crystal Growth and Design* **2006**, 290, 1463-1468.
65. The twinned crystal structure of  $\mu$ -2,2'-bipyrimidine-1 $\kappa^2$ N<sup>1</sup>,N<sup>1'</sup>: 2 $\kappa^2$ N<sup>3</sup>,N<sup>3'</sup>-bis{tris[4,4,4-trifluoro - 1 - (2 - thienyl )butane – 1,3 - dionato -  $\kappa^2$ O,O']}terbium(III)} ethyl acetate solvate  
Kristin Kirschbaum, Albert Fratini and Shawn Swavey  
*Acta Cryst. C* **2006**, C62, m186-187.
66. Role of Anions in Inducing Noncentrosymmetry in 4-dimethylaminopyridinium Salts for Quadratic Nonlinear Optics  
S. Manivannan, S. Dhanuskodi, K. Kirschbaum, S.K. Tiwari,  
*Crystal Growth & Design* **2006**, 6, 1285-1290.
67. Origin of the second harmonic generation in a supramolecular inclusion complex between *p*-nitroaniline and  $\beta$ -cyclodextrin  
Ali N. Rashid, Kristin Kirschbaum, Richard K. Shoemaker  
*Journal of Molecular Structure* **2006**, 785, 1-6.
68. Order-disorder twinning model and stacking faults in  $\alpha$ -NTO  
Dieter Schwarzenbach, Kristin Kirschbaum, A.Alan Pinkerton  
*Acta Cryst. B* **2006**, B62, 944-948.
69. Experimental Charge Density Study of Estrogens: 17 $\alpha$ -Estradiol·Urea  
Damon Parrish, Elizabeth A. Zhurova, Kristin Kirschbaum, A. Alan Pinkerton  
*J. Phys. Chem. B* **2006**, 110, 26442-26447.
70. A Luminescent Charge Transfer Platinum(II) Metallacycle  
Fei Hua, Solen Kinayigit, Elena A. Shikhova, Sebastien Goeb, John R. Cable, Christopher J. Adams, Kristin Kirschbaum, A. Alan Pinkerton, Felix N. Castellano  
*Inorg. Chem.* **2007**, 46, 8771-8773.
71. Non-merohedral Twin Crystal of 2,3,9,10-Tetrakis(triisopropylsilylethynyl)-6,13-bis(trimethylsilylethynyl)pentacene

- Jiang, J.; Kaafarani, B. R.; Kirschbaum, K.; Hu, Y.; Neckers, D. C.,  
*Acta Cryst.* **2007**, E63, o3760–o3761.
72. Hexaaquacobalt(II) 3-ammonionaphthalene-1,5-disulfonate tetrahydrate  
Dane J. Genther, Philip J. Squattrito, Kristin Kirschbaum, A. Alan Pinkerton  
*Acta Cryst.* **2007**, E63, m2260–m2261.
73. Hexaaquazinc(II) 3-ammonionaphthalene-1,5-disulfonate tetrahydrate  
Dane J. Genther, Philip J. Squattrito, Kristin Kirschbaum, A. Alan Pinkerton  
*Acta Cryst.* **2007**, E63, m2262.
74. 5-Aminonaphthalene-1-sulfonic acid and its manganese, nickel and cobalt salts  
Dane J. Genther, Philip J. Squattrito, Kristin Kirschbaum, Eric J. Yearley, A. Alan Pinkerton  
*Acta Cryst.* **2007**, C63, m604–m609.
75. *N*-(*n*-Decyl)-4-nitroaniline  
Matthew M. Yonkey, Christopher P. Walczak, Philip J. Squattrito, Dillip K. Mohanty, Kristin Kirschbaum  
*Acta Cryst.* **2008**, E64, o549.
76. 1,3-Bis(ethylamino)-2-nitrobenzene, 1,3-bis(*n*-octylamino)-2-nitrobenzene and 4-ethyl-amino-2-methyl-1H-benzimidazole  
Christopher P. Walczak, Matthew M. Yonkey, Philip J. Squattrito, Dillip K. Mohanty, Kristin Kirschbaum  
*Acta Cryst.* **2008**, C64, o248–o251.
77. Characterization of Tin(IV) Oxide Thin Films Prepared by Atmospheric Pressure Chemical Vapor Deposition of *cis*-[SnCl<sub>4</sub>{OC(H)OC<sub>2</sub>H<sub>5</sub>}<sub>2</sub>]  
Nari N. Talaty, Kristina Beck, Helene Citeau, Kristin Kirschbaum, Dean M. Giolando  
*Z. Anorg. Allg. Chem.* **2009**, 635, 53–63.
78. 4,6-Dinitro-N,N'-di-*n*-octylbenzene-1,3-diamine, 4,6-dinitro-N,N'-di-*n*-undecylbenzene-1,3-diamine and N,N'-bis(2,4-dinitrophenyl)octane-1,8-diamine  
Gary Teng, Christopher P. Walczak, Philip J. Squattrito, Dillip K. Mohanty, William Scharer, Mark R. Giolando, Kristin Kirschbaum  
*Acta Cryst.* **2009**, C65, o76–o80.
79. Gold-Catalyzed Transannular [4+3] Cycloaddition Reactions  
Benjamin W. Gung, Derek T. Craft, Lauren N. Bailey, Kristin Kirschbaum  
*Chemistry – A European Journal* **2010**, 16, 639 – 644.
80. Relative substituent position on the strength of  $\pi$ – $\pi$  stacking interactions  
Benjamin W. Gung, Bright U. Emenike, Celeste N. Alvarez, John Rakovan, Kristin Kirschbaum, Nirbhay Jain  
*Tetrahedron Letters*, **2010**, 51, 1648–1650.

81. Luminescent Low Valent Rhenium Complexes with 1,2-Bis(alkylphosphino)ethane Ligands. Synthesis and X-ray Crystallographic, Electrochemical and Spectroscopic Characterization  
Messersmith, Stephania J.; Kirschbaum, Kristin; Kirchhoff, Jon R.  
*Inorganic Chemistry* **2010**, *49*, 3857-3865.
82. N,N'-Diethyl-4-nitrobenzene-1,3-diamine, 2,6-bis(ethylamino)-3-nitrobenzonitrile, and bis(4-ethylamino-3-nitrophenyl)sulfone  
Thomas J. Payne, Chad R. Thurman, Hao Yu, Qian Sun, Dillip K. Mohanty, Philip J. Squattrito\*, Mark-Robin Giolando, Christopher R. Brue, Kristin Kirschbaum  
*Acta Cryst.* **2010**, *C66*, o369-o373.
83. Preparation and Characterization of Two New N-Heterocyclic Carbene Gold(I) Complexes and Comparison of Their Catalytic Activity to Au(IPr)Cl  
Benjamin W. Gung, Derek T. Craft, Lauren N. Bailey, Kristin Kirschbaum  
*Organometallics* **2010**, *29*, 3450-3456.
84. Quantification of CH- $\pi$  Interactions: Implications on How Substituent Effects Influence Aromatic Interactions  
Benjamin W. Gung, Bright U. Emenike, Michael Lewis, Kristin Kirschbaum  
*Chemistry – A European Journal* **2010**, *16*, 12352-12362.
85. Confirmation of Bridging *N*-Indolides in 3-Methylindole and Di- and Tri(3-methylindolyl)methane Complexes of Dimethyl-, Diethyl-, and Di-*iso*-butylaluminum  
Nicholas B. Kingsley, Kristin Kirschbaum, and Mark R. Mason  
*Organometallics* **2010**, *28*, 5927-5935.
86. Planar, Three-Coordinate Boron Monohydrides Ligated by Bis(3-methylindolyl)methanes  
BingXu Song, Kristin Kirschbaum, Mark R. Mason  
*Organometallics*, **2012**, *31*, 191-196.
87. Synthesis and Calorimetric, Spectroscopic, and Structural Characterization of Isocyanide Complexes of Trialkylaluminum and Tri-*tert*-butylgallium  
Nicholas B. Kingsley, Kristin Kirschbaum, Joseph A. Teprovich, Jr., Robert A. Flowers II, Mark R. Mason  
*Inorg. Chem.* **2012**, *51*, 2494-2502.
88. Electron Paramagnetic Resonance Spectroscopic Study of Copper Hopping in Doped bis(L-histidinato)Cadmium Dihydrate  
Colaneri, Michael; Vitali, Jacqueline; Kirschbaum, Kristin  
*The Journal of Physical Chemistry* **2013**, *117*, 3414-3427.
89. Ultrastable silver nanoparticles  
Desireddy, Anil; Conn, Brian E.; Guo, Jingshu; Yoon, Bokwon; Barnett, Robert N.; Monahan, Bradley M.; Kirschbaum, Kristin; Griffith, Wendell P.; Whetten, Robert L.; Landman, Uzi; Bigioni, Terry P.

*Nature* **2013**, *501*, 399-402.

90. A series of *N*-(2-phenylethyl) nitroaniline derivatives as precursors for slow and sustained nitric oxide release agents  
Wade, Colin B.; Mohanty, Dillip K.; Squattrito, Philip J.; Amato, Nicholas J.; Kirschbaum, Kristin  
*Acta Cryst.* **2013**, *69*, 1383-1389.
91. Bio-Based Bisfuran: Synthesis, Crystal Structure and Low Molecular Weight Amorphous Polyester  
Gaitonde Vishwanath; Lee Kyunghee; Kirschbaum Kristin; Suseck Steven  
*Tetrahedron Letters* **2014**; *55*, 4141–4145.
92. Mono- and Bimetallic Aluminum Alkyl, Aryl, and Hydride Complexes of a Bulky Dipyrromethene Ligand  
Gianopoulos, Christopher; Kirschbaum, Kristin; Mason, Mark R.  
*Organometallics* **2014**, *33*, 4503-4511.
93. Synthesis, Characterization and Crystal Structures of Mono and Dinuclear Macroyclic Cobalt(II) Complexes with a new tetraaza m-xylyl-based macrocyclic ligand  
Khandar, Ali Akbar; Kirschbaum, Kristin; Abedi, Marjan; Mock, Kristi; Tracy, Greg; V. Spasojevic, V.; Hosseini-Yazdi, Seyed Abolfazl  
*New Journal of Chemistry* **2015**, *39*, 2822.
94. Structural patterns at all scales in a nonmetallic chiral Au<sub>133</sub>(SR)<sub>52</sub> nanoparticle  
Chenjie Zeng, Yuxiang Chen, Kristin Kirschbaum, Kannatassen Appavoo, Matthew Y. Sfeir, and Rongchao Jin  
*Science Advances* **2015**, *1*, e1500045.  
<http://dx.doi.org/10.1126/sciadv.1500045>
95. Crystal Structure of Barrel-Shaped Chiral Au<sub>130</sub>(p-MBT)<sub>50</sub> Nanocluster  
Yuxiang Chen, Chenjie Zeng, Chong Liu, Kristin Kirschbaum, Chakicherla Gayathri, Roberto R. Gil, Nathaniel L. Rosi, and Rongchao Jin  
*J. Am. Chem. Soc.* **2015**, *137*, 10076-10079.
96. Synthesis, Characterization and Crystal Structure of Dinuclear Cobalt(II) Macroyclic Complexes, Containing Thiocyanate and Azide Groups  
Marjan Abedi, Kristin Kirschbaum, Amir Nasser Shamkhali, Christopher R. Brue, Ali Akbar Khandar  
*Polyhedron* **2016**, *109*, 176-181.
97. Gold Quantum Boxes: On the Periodicities and the Quantum Confinement in the Au<sub>28</sub>, Au<sub>36</sub>, Au<sub>44</sub>, and Au<sub>52</sub> Magic Series

Chenjie Zeng, Yuxiang Chen, Kenji Iida, Katsuyuki Nobusada, Kristin Kirschbaum, Kelly J. Lambright, and Rongchao Jin  
*J. Am. Chem. Soc.* **2016**, 138, 3950-3953.

98. Heavily doped Au<sub>25-x</sub>Ag<sub>x</sub>(SC<sub>6</sub>H<sub>11</sub>)<sub>18-</sub> nanoclusters: silver goes from core to surface  
Qi Li, Shuxin Wang, Kristin Kirschbaum, Kelly J. Lambright, Anindita Das, Rongchao Jin  
*Chem. Commun.* **2016**, 52, 5194 DOI: 10.1039/c6cc01243d
99. Synthesis and Properties of “Sandwich” Diimine-Coinage Metal Ethylene Complexes  
Kristine Klimovica,<sup>†</sup> Kristin Kirschbaum,<sup>‡</sup> and Olafs Daugulis  
*Organometallics* **2016**, 35, 2938-2943
100. Aluminum Alkoxide, Amide and Halide Complexes Supported by a Bulky Dipyrromethene Ligand: Synthesis, Characterization, and Preliminary ε-Caprolactone Polymerization Activity  
Christopher G. Gianopoulos, Nishant Kumar, Yihong Zhao, Li Jia, Kristin Kirschbaum, Mark R. Mason  
*Dalton Trans.* **2016**, 45, 13787-13797
101. Emergence of hierarchical structural complexities in nanoparticles and their assembly  
C. Zeng, Y. Chen, K. Kirschbaum, K. J. Lambright, R. Jin  
*Science* **2016**, 354, 1580-1584  
<http://science.sciencemag.org/content/354/6319/1580>
102. *N*-Benzylnicotinamide and *N*-benzyl-1,4-dihydronicotinamide: Useful models for NAD<sup>+</sup> and NADH  
John M. Moore, Jasmine M. Hall, Anton W. Jensen, Philip J. Squattrito, Patrick Giolando and Kristin Kirschbaum  
*Acta Cryst.* **2017**, C73, 531-535.  
<https://doi.org/10.1107/S2053229617008877>
103. Site-selective Substitution of Gold Atoms in the Au<sub>24</sub>(SR)<sub>20</sub> Nanocluster by Silver  
Qi Li, Michael G. Taylor, Kristin Kirschbaum, Kelly Lambright, Xiaofan Zhu, Giannis Mpourmpakis, Rongchao Jin  
*Journal of Colloid & Interface Science* **2017**, 505, 1202-1207.  
<https://doi.org/10.1016/j.jcis.2017.06.049>
104. Reconstructing the Surface of Gold Nanoclusters by Cadmium Doping  
Li, Qi; Lambright, Kelly ; Taylor, Michael; Kirschbaum, Kristin; Luo, Tian-Yi; Zhao, Jianbo; Mpourmpakis, Giannis; Mokashi-Punekar, Soumitra; Rosi, Nathaniel; Jin, Rongchao  
*J. Am. Chem. Soc.* **2017**, 139, 17779–17782.  
<https://pubs.acs.org/doi/10.1021/jacs.7b11491>

105. Sharp Transition from Nonmetallic Au<sub>246</sub> to Metallic Au<sub>279</sub> with Nascent Surface Plasmon Resonance  
Tatsuya Higaki, Meng Zhou, Kelly J. Lambright, Kristin Kirschbaum, Matthew Y. Sfeir, Rongchao Jin  
*J. Am. Chem. Soc.*, **2018**, 140, 5691–5695.  
<https://pubs.acs.org/doi/10.1021/jacs.8b02487>
106. Bidentate and Tridentate Coordination Modes of Bis(3-methylindolyl)-2-pyridylmethane in Complexes of Aluminum and Gallium: Structural Characterization of Bridging *N*-Indolide in a Dialuminum Complex  
Bassam N. Fneich, Anirban Das, Kristin Kirschbaum, and Mark R. Mason  
*J.Organomet. Chem.* **2018**, 872, 12-23  
<https://doi.org/10.1016/j.jorgancem.2018.07.024>
107. One-pot synthesis of carbohydrate *exo*-cyclic enones and hemiketals with 6, 8-dioxabicyclo-[3.2.1]octane moiety. Serendipitous formation of a spironolactone when 2-pyridinecarboxaldehyde is used as reactant. Part II  
Rachael E. Hohol, Holly Arcure, Zbigniew J. Witczak, Roman Bielski, Kristin Kirschbaum, Peter Andreana, Donald E. Mencer  
*Tetrahedron*, **2018**, 74, 7303-7309  
<https://doi.org/10.1016/j.tet.2018.10.049>
108. Models for potential dendritic nitric oxide-donors: crystal structures of two 2-nitroanilino precursors and nitric oxide-release behavior of the nitrosated derivatives  
Alec R. Badour, Corey J. Arnett-Butscher, Dillip K. Mohanty, Philip J. Squattrito, Kelly J. Lambright and Kristin Kirschbaum  
*Acta Cryst.*, **2018 C74**, 1038-1044.  
<https://doi.org/10.1107/S205322961801173>
109. Large-Scale Synthesis, Crystal Structure, and Optical Properties of the Ag<sub>146</sub>Br<sub>2</sub>(SR)<sub>80</sub> Nanocluster  
Yongbo Song, Kelly Lambright, Meng Zhou, Kristin Kirschbaum, Ji Xiang, Andong Xia, Manzhou Zhu and Rongchao Jin  
*ACS Nano* **2018**, 12, 9318-9325.  
<https://pubs.acs.org/doi/10.1021/acsnano.8b04233>
110. Syntheses and structures of zinc(tmada)di(aryltellurolato) and its facile chalcogenospecific ligand exchange reactivity  
Sandra Behr, Thorsten Bestvater, Arnold Feldmann, Kristin Kirschbaum, Olaf Conrad and Dean M. Giolando  
*Z. Anorg. Allg. Chem.* **2018**, 644, 1431–1438.  
<https://doi.org/10.1002/zaac.201800302>

111. Crystal structures of two coordination isomers of copper(II) 4-sulfobenzoic acid hexahydrate  
and two mixed silver/potassium 4-sulfobenzoic acid salts  
Squattrito, Philip J., Lambright, Kelly J., Giolando, Patrick A., Kirschbaum, Kristin  
*Acta Cryst.* **2019**, E75, 1801 – 1807.
112. New Class of Trianionic Constrained Geometry Ligands: Representative Complexes of Zirconium  
Ryan T. Rondo, Kristin Kirschbaum, and Mark R. Mason  
*J.Organomet. Chem.* **2021**, 944, 121830
113. Direct Observation of the Pressure-Induced Structural Variation in Gold Nanoclusters and The Correlated Optical Response  
Qi Li, Charles J. Zeman IV, Bora Kalkan, Kristin Kirschbaum, Christopher G. Gianopoulos, Abhinav Parakh, David Doan, Andrew C. Lee, John Kulikowski, George C. Schatz, Guoyin Shen, Martin Kunz, X. Wendy Gu  
*Nano Letters* **2022**, 23, 132-139.
114. Bidentate and Tridentate Coordination Modes of Bis(3-methylindolyl)-2-(1- methyl-imidazolyl)methane in Complexes of Aluminum and Gallium  
Anirban Das, Nicholas Kingsley, Kristin Kirschbaum, Mark Mason  
*J.Organomet. Chem.* **2023**, 984, 122554.