

## List of publications Kenneth Wärnmark

- 1) “Ring Expansions of N-Acylisatins to N-Oxidoquinazoline-4-Carbohydroxamic acid Derivatives Induced by Hydroxylamine” Bergman, J.; Engelhardt, P.; Kiss, A. I.; Lindström, J; Wärnmark, K. in *Stud.Org. Chem.*; Kovác, J. and Zálupsky, P., Eds.; Vol 35; Wiley, 1988; pp 1-11.
- 2) “Synthesis and Structure of Macrocyclic Amides Containing a 2,2’-Dipyridylmethane Unit. A New Class of Chiral macrocyclic Ligands” Moberg, C.; Wärnmark, K.; Csöreg, I.; Ertan, A. *J. Org. Chem.* **1991**, *56*, 3339-3344.
- 3) “Structures of Novel Macrocyclic Dipyridylmethaneamides” Csöreg, I.; Ertan, A.; Moberg, C.; Wärnmark, K. *Acta Crystallogr., Sect. C: Cryst. Struct. Commun.* **1991**, *C47*, 2171-2176.
- 4) “Enantiomerically Pure C<sub>3</sub>-Symmetric Tripodal Pyridine Ligands” Adolfsson, H.; Wärnmark K.; Moberg C. *J. Chem. Soc., Chem. Commun.* **1992**, 1054-1055.
- 5) “The Coordination Chemistry of Macrocyclic 13- and 14-membered Dipyridylmethaneamides; Crystal Structure of the Deprotonated Ni(II) Complex of 3,15-Dioxo-9-Ethyl-9-Methoxy-1,4,5,6,7,8,10,11,12,13,14,17,18,19,20,21,22,23-octadecadehydro-2,16,22,23-Tetraazatetracyclo[15.4.0.14,8.110,14]tricosane” Ertan, A.; Csöreg, I.; Wärnmark, K.; Moberg, C. *Inorganica Chimica Acta* **1993**, *203*, 21-27.
- 6) “The Strength of the Metal-Olefin Bond in Titanium Complexes Related to Ziegler-Natta Catalysis. A Theoretical Model Study of an Octahedral Active Center Postulated to be Found in Titanium Halide Based Catalysts” Jensen, V. R.; Ystenes, M.; Wärnmark, K.; Åkermark, B.; Svensson, M.; Siegbahn, P. E. M.; Blomberg, M. R. A. *Organometallics* **1994**, *13*, 282-288.
- 7) “The Metal-Alkene Bond in Rh(I)( $\beta$ -diketonato)(alkene)<sub>2</sub> Complexes. Correlation of <sup>103</sup>Rh-NMR Shifts with Stability Constants, Alkene Excitation Energies and d-d Absorption Bands. An Experimental and Theoretical Study” Åkermark, B.; Glaser, J.; Öhrström, L.; Wahlberg, S.; Wärnmark, K.; Zetterberg, K.; Blomberg, M. R. A. *J. Am. Chem. Soc.* **1994**, *116*, 3405-3413.
- 8) “Synthesis and Coordination Properties of Pendant Arm Dipyridylmethane Derivatives” Adolfsson, H.; Wärnmark, K.; Moberg, C. *J. Org. Chem.* **1994**, *59*, 2004-2009.
- 9) “A New Dipyridylmethane Ligand with Hard and Soft Coordination Sites” Cernerud, M.; Wärnmark, K.; Moberg, C. *Tetrahedron Letters* **1994**, *35*, 5473-5476.

- 10) "Unusual Conformational Determining Interactions in Oxymethyl Pyridines. An ab Initio Study and Refined molecular Mechanics (MM2) Parameters" Wärnmark, K.; Moberg, C.; Åkermark, B; Norrby, P.-O. *Journal of Computational Chemistry* **1995**, *16*, 620-627.
- 11) "Pyridineamides in Asymmetric Catalysis" Moberg, C.; Adolfsson, H.; Wärnmark, K. *Acta Chem. Scand.* **1996**, *50*, 195-202.
- 12) "Stereoisomerically Controlled Inorganic Architectures: Synthesis of Enantio- and Diastereomerically Pure Ruthenium-Palladium Molecular Rods from Enantiopure Building Blocks" Wärnmark, K; Thomas, J. A.; Heyke, O.; Lehn, J.-M. *J. Chem. Soc., Chem. Commun.* **1996**, 701-702.
- 13) "Conformational Preferences of 2-(Halomethyl)- and 2-(Oxymethyl)pyridines. Microwave Spectrum, Ab Initio and MM3 Studies of 2-(Fluoromethyl)pyridine" Moberg, C; Adolfsson, H.; Wärnmark, K.; Norrby P.-O.; Marstokk, K.-M.; Möllendal, H. *Chemistry - A European J.* **1996**, *2*, 516-522.
- 14) "Novel 2-(Hydroxyalkyl)pyridines Derived from the Chiral Pool" Adolfsson, H.; Nordström, K.; Wärnmark, K.; Moberg, C., *Tetrahedron: Asymmetry* **1996**, *7*, 1967-1972.
- 15) "Stereoisomerically Controlled Inorganic Architectures: Synthesis of Extended Enantio- and Diastereomerically pure Tris-ruthenium Disks from Enantiopure Building Blocks" Wärnmark, K; Heyke, O.; Thomas, J. A.; Lehn, J.-M. *J. Chem. Soc., Chem. Commun.* **1996**, 2603-2604.
- 16) "Application of (2'R,5'R)-2-[(2',5'-Dimethylpyrrolidinyl)methyl]pyridine and (2'R,5'R)-2-[(2',5'-Diphenylpyrrolidinyl)methyl]pyridine to the Palladium Catalyzed Allylic Alkylation" Wärnmark, K; Stranne, R.; Cernerud, M.; Terien, I.; Rahm, F.; Nordström, K.; Moberg, C. *Acta Chem. Scand.* **1998**, *52*, 961-963.
- 17) "Stereoselective Synthesis of Linear Bipyridyl-Phenylene Based Ruthenium Rods from Enantiopure Building Blocks" Wärnmark, K.; Baxter, P. N. W.; Lehn, J.-M. *J. Chem. Soc., Chem. Commun.* **1998**, 993-994.
- 18) "A Bis(Crown-Ether) Analogue of Tröger's Base: Recognition of Achiral and Chiral Primary Ammonium Salts" Hansson, A. P. H.; Norrby, P.-O.; Wärnmark, K. *Tetrahedron Letters* **1998**, *39*, 4565-4568.
- 19) "Tetranuclear Copper(I)-bisphenanthroline Gridwork: Violation of the Principle of Maximal Donor Coordination Caused by Intercalation and CH-to-N Forces" Toyota, S.; Woods, C. R.; Benaglia, M.; Haldiman, R.; Wärnmark, K.; Hardcastle, K. and Siegel, J. S. *Angew. Chem.* **2001**, *40*, 751-754.
- 20) "Synthesis of Halogen Substituted Analogues of Tröger's Base" Jensen, J. and Wärnmark, K. *Synthesis* **2001**, 1873-1877.
- 21) "General Protocols for the Synthesis of C<sub>2</sub>-Symmetric and Asymmetric

- 2,8-Disubstituted Analogues of Tröger's Base via Efficient Bromine-Lithium Exchanges of 2,8-Dibromo-6*H*,12*H*-5,11-methanodibenzo[*b,f*]diazocine" Jensen, J.; Tejler, J.; Wärnmark, K. *J. Org. Chem.* **2002**, *67*, 6008-6014.
- 22) "Introduction of Terminal Alkynes into the 2,8-positions of the Tröger's Base Core via Sonogashira Coupling of 4,10-Dimethyl-2,8-diiodo-6*H*,12*H*-5,11-methanodibenzo[*b,f*](1,5)diazocine" Jensen, J.; Strozyk, M.; Wärnmark, K. *Synthesis* **2002**, 2761-2765.
- 23) "Influence of Scale, Stoichiometry and Temperature on the Synthesis of 2,8-Dihalo Analogues of Tröger's Base from the Corresponding Anilines and Paraformaldehyde" Jensen, J.; Strozyk, M.; Wärnmark, K. *J. Het. Chem.* **2003**, *40*, 373-375.
- 24) "Synthesis of Dihalosubstituted Analogues of Tröger's Base from ortho- and meta-Substituted Anilines" Hansson, A.; Jensen, J.; Wendt, O. F.; Wärnmark, K. *Eur. J. Org. Chem.* **2003**, 3179-3188.
- 25) "Design and Synthesis of a  $C_2$ -symmetric self-complementary hydrogen-bonding cleft molecule based on the bicyclo[3.3.1]nonane and 4-oxo-5-azaindole framework. Formation of channels and inclusion complexes in the solid state" Stoncius, S.; Butkus, E.; Ilinskas, A.; Larsson, K.; Öhrström, L.; Berg, U.; Wärnmark, K. *J. Org. Chem.* **2004**, *69*, 5196-5203.
- 26) "A Dynamic Supramolecular System Exhibiting Substrate Selectivity in the Catalytic Epoxidation of Olefins" Jónsson, S.; Odille, F. G. J.; Norrby, P.-O.; Wärnmark, K. *Chem. Commun.* **2005**, 549 – 551.
- 27) "Synthesis of 2-Pyridone-fused 2,2'-Bipyridine Derivatives. An Unexpectedly Complex Solid State Structure of 3,6-Dimethyl-9*H*-4,5,9-triazaphenanthren-10-one" Jónsson, S.; Solano Arribas, C.; Wendt, O. F.; Siegel, J. S.; Wärnmark, K. *Org. Biomol. Chem.* **2005**, *3*, 996-1001.
- 28) "A Desymmetrization Route to Fused Tröger's Base Analogues: The Synthesis, Isolation and Characterization of the First *anti-anti* Diastereomer of a Fused Tris-Tröger's Base Analogue" Hansson, A.; Wixe, T.; Bergquist, K.-E.; Wärnmark, K. *Organic Letters* **2005**, *7*, 2019-2022.
- 29) "Introduction of Aromatic and Heteroaromatic Groups in the 2- and 8-Positions of the Tröger's Base Core via the Suzuki, Stille and Negishi Cross-Coupling Reactions. A Comparative Study" Solano, C.; Svensson, D.; Olomi, Z.; Jensen, J.; Wendt, O. F.; Wärnmark, K. *Eur. J. Org. Chem.* **2005**, 3510-3517.
- 30) "The Synthesis and Characterization of all Diastereomers of a Linear Symmetrically Fused Tris-Tröger's Base Analogue - New Chiral Cleft Compounds" Artacho, J.; Nilsson, P.; Bergquist, K.-E.; Wendt, O. F. and Wärnmark, K. *Chem. Eur. J.* **2006**, *12*, 2692-2701.

- 31) "Modulation of the Reactivity, Stability and Substrate- and Enantioselectivity of an Epoxidation Catalyst by Non-Covalent Dynamic Attachment of a Receptor Functionality – Aspects on the Mechanism of the Jacobsen-Katsuki epoxidation" Jónsson, S.; Odille, F. G. J.; Norrby, P.-O.; Wärnmark, K. *Org. Biomol. Chem.* **2006**, *4*, 1927 - 1948.
- 32) "An Approach to Helical Tubular Self-Aggregation Using  $C_2$ -Symmetric Self-Complementary Hydrogen-Bonding Cavity Molecules" Stoncius, S.; Orentas, E.; Butkus, E.; Öhrström, L.; Wendt, O. F.; Wärnmark, K. *J. Am. Chem. Soc.* **2006**, *126*, 8272-8285.
- 33) "On the characterization of Dynamic Supramolecular Systems: A General Mathematical Association Model for Linear Supramolecular Copolymers and Application on a Complex Two-Component Hydrogen-Bonding System" Odille, F. G. J.; Jónsson, S.; Stjernqvist, S.; Rydén, T.; Wärnmark, K. *Chem. Eur. J.* **2007**, *13*, 9617-9636.
- 34) "Genetically engineered *Saccharomyces cerevisiae* for kinetic resolution of racemic bicyclo[3.3.1]nonane-2,6-dione" Carlquist, M.; Wallentin, C. J.; Wärnmark, K.; Gorwa-Grauslund, M. F. *Tetrahedron: Asymmetry* **2008**, *19*, 2293-2295.
- 35) "Baker's Yeast for Sweet Dough Enables Large Scale Synthesis of Enantiomerically Pure Bicyclo[3.3.1]nonane-2,6-dione" Wallentin, C. J.; Orentas, E.; Butkus, E.; Wärnmark, K. *Synthesis* **2009**, 864-867.
- 36) "rac-4,8-Divinyl-bicyclo[3.3.1]nonane-2,6-dione" Orentas, E., Wendt, O. F.; Wärnmark, K.; Butkus, E., Wallentin, C.-J. *Acta Cryst. E.* **2009**, E65, o1357.
- 37) "On the Synthesis of mono- and diamino analogues of Tröger's base" Artacho, J; Wärnmark, K, *Synthesis* **2009**, 3120-3126.
- 38) "Network analysis of bicyclo[3.3.1]nonanes: the diol, the dione and the acetal" Wallentin, C.-J.; Orentas, E., Johnson, M.; Butkus, E., Wendt, O.-F.; Öhrström, L.; Wärnmark, K. *Cryst. Eng. Commun.* **2009**, *11*, 1837-1841.
- 39) "Chirality – a never ending source of confusion" Wallentin, C.-J.; Orentas, E.; Wärnmark, K.; Wendt, O. F. *Z. Kristallogr.* **2009**, *224*, 607-608.
- 40) "Synthesis and Self-Aggregation of Enantiopure and Racemic Molecular Tweezers Based on the Bicyclo[3.3.1]nonane Framework" Wallentin, C.-J.; Wixe, T.; Bergquist, K.-E.; Wärnmark, K. *Chem. Eur. J.* **2010**, *16*, 3994-4002.
- 41) "Dynamic Supramolecular SalenCrCl Complexes as Efficient Catalysts for or Ring Opening of Epoxides" Ma, D.-Y.; Nourouzi-Arasi, H.; Sheibani, E.; Wärnmark, K. *ChemCatChem* **2010**, *2*, 629-632.
- 42) "Formation of an heterochiral supramolecular cage by diastereomer self-discrimination: Fluorescence enhancement and C60 sensing" Arribas, C.

- S.; Carling, C.-J.; Lemieux, R. P.; Sundin, A.; Wang, R.; Wendt, O. F.; Wärnmark, K. *Chem. Commun.* **2010**, *46*, 4381-4383.
- 43) "Highlight article: Mechano-Assisted Supramolecular Catalysis in Solid State Synthesis" Ma, D.-Y.; Wärnmark, K. *ChemCatChem* **2010**, *2*, 1059-1060.
- 44) "Topology Selection and Tautoleptic Aggregation: Formation of an Enantiomerically Pure Supramolecular Belt over a Helix" Orentas, E.; Wallentin, C.-J.; Bergquist, K.-E.; Lund, M.; Butkus, E.; Wärnmark, K. *Angew. Chem, Int. Ed.* **2011**, *50*, 2071-2074.
- 45) "Synthetic and Crystallographic studies of bicyclo[3.3.1]nonane derivatives: from strong to weak hydrogen bonds and the stereochemistry of network formation" Wallentin, C.-J., Orentas, E.; Johnson, M. T.; Bathori, N. B.; Butkus, E.; Wendt, O. F.; Wärnmark, K.; Öhrström, L. *CrystEngComm* **2012**, *14*, 178-187.
- 46) "Twisted Amide Analogues of Tröger's Base" Artacho, J., Ascic, E.; Rantanen, T.; Karlsson, J.; Wallentin, C.-J.; Wang, R.; Wendt, O. F.; Harmata, M.; Snieckus, V.; Wärnmark, K. *Chem. Eur. J.* **2012**, *18*, 1038-1042.
- 47) "Conformationally Restricted Dynamic Supramolecular Catalysts for Substrate Selective Epoxidations" Sheibani, E., Wärnmark, K. *Org. Biomol. Chem.* **2012**, *10*, 2059-2067.
- 48) "Pseudo-C<sub>2</sub>-Symmetric Bimetallic Bissalen Catalysts for Efficient and Enantioselective Ring Opening of meso-Epoxides" Da-You Ma, Ze-Yun Xiao, Julen Etxabe, and Kenneth Wärnmark *ChemCatChem* **2012**, *4*, 1321-1329.
- 49) "Tröger's Base Twisted Amides: *Endo* functionalization and Synthesis of an Inverted Crown Ether" Artacho, J., Ascic, E.; Rantanen, T.; Wallentin, C.-J., Harmata, M.; Snieckus, V., Wärnmark, K. *Org. Lett.* **2012**, *16*, 4706-4709.
- 50) "The 125th Anniversary of the Tröger's Base Molecule: Synthesis and Applications of Tröger's Base Analogues" Rúnarsson, Ö. V.; Artacho, J.; Wärnmark, K. *Eur. J. Org. Chem.* **2012**, 7015-7041.

- 51) "Toward Highlighting the Ultrafast Electron Transfer Dynamics at the Optically Dark Sites of Photocatalysis" Canton, S. E.; Zhang, X.; Zhang, J.; van Driel, T. B.; Kjaer, K. S.; Haldrup, K.; Chabera, P.; Harlang, T.; Suarez-Alcantara, K.; Liu, Y.; Pérez, J.; Bordage, A.; Pápai, M.; Vankó, G.; Jennings, G.; Kurtz, C. A.; Rovezzi, M.; Glatzel, P.; Smolentsev, G.; Uhlig, J.; Dohn, A. O.; Christensen, M.; Galler, A.; Gawelda, W.; Bressler, C.; Lemke, H. T.; Møller, K. B.; Nielsen, M. M.; Lomoth, R.; Wärnmark, K.; Sundström, V. *J. Phys. Chem. Lett.* **2013**, *4*, 1972-1976.
- 52) "Towards Longer-Lived Metal-to-Ligand Charge Transfer States of Iron(II) Complexes: An *N*-Heterocyclic Carbene Approach" Liu Y.; Harlang, T.; Canton, S. E.; Chábera, P.; Suárez-Alcántara, K.; Fleckhaus, A. Vithanage, D. A.; Göransson, E.; Corani, A.; Lomoth, R.; Sundström, V.; Wärnmark, K. *Chem. Commun.* **2013**, *49*, 6412-6414.
- 53) "Synthesis of An Orthogonal Topological Analogue of Helicene" Wixe, T.; Wallentin, C. J.; Johnson, M. T.; Fristrup, P., Lidin, S.; Wärnmark, K. *Chem. Eur. J.* **2013**, *19*, 14963-1496.
- 54) "Composition- and Size-controlled Cyclic Self-Assembly by Solvent- and C<sub>60</sub>-Responsive Self-sorting" Shi, Q.; Bergquist, K.-E.; Huo, R.; Li, J.; Lund, M.; Vacha, R.; Sundin, A.; Butkus, E.; Orentas, E.; Wärnmark, K. *J. Am. Chem. Soc.* **2013**, *135*, 15263-15268.
- 55) Probing the Anisotropic Distortion of Photoexcited Spin Crossover Complexes with Picosecond X-ray Absorption Spectroscopy" Canto, S. E.; Zhang, X.; Lawson Daku, L. M., Smeigh, A. L.; Zhang, J.; Liu, Y.; Wallentin, C.-J.; Attenkofer, K.; Jennings, G.; Kurtz, C. A.; Gosztola, D.; Wärnmark, K.; Hauser, A.; Sundström; V. *J. Phys. Chem, C.* **2014**, *118*, 4536-4545.
- 56) "Exceptional excited state lifetime of an iron(II) N-heterocyclic carbene complex explained" Lisa A. Fredin, Mátyás Pápai, Emese Rozsalyi, György Vankó, Kenneth Wärnmark, Villy Sundström, Petter Persson *J. Phys. Chem. Lett.* **2014**, *5*, 2066-2071.
- 57) "Highly Accurate Excited-State Structure of [Os(bpy)<sub>2</sub>dc bpy]<sup>2+</sup> Determined by X-ray Transition Spectroscopy" Zhang, X.; Canton, S. E.; Smolentsev, G.; Wallentin, C.-J.; Liu, Y.; Kong, Q.; Attenkofer, K.; Stickrath, A. B.; Mara, M. W.; Chen, L. X.; Wärnmark, K.; Sundström, V. *J. Am. Chem. Soc.* **2014**, *136*, 8804-8809.
- 58) "Substrate-Selective Catalysis" Lindbäck, E.; Dawaigher, S.; Wärnmark, K. *Chem. Eur. J.* **2014**, *20*, 13432-13481.
- 59) "A Short Designed Semi-Aromatic Organic Nanotube - synthesis, chiroptical characterization, and host properties" Torbjörn Wixe, Niels Johan Christensen, Sven Lidin, Peter Fristrup and Kenneth Wärnmark *Org. Biomol. Chem.* **2014**, *12*, 8930-8941.
- 60) "A Double Conformationally Restricted Dynamic Supramolecular System for the Substrate-Selective Epoxidation of Olefins - a Comparative Study on the Influence of Pre-Organization" E. Lindbäck, S. Cherraben, J-P. Francoia, E. Sheibani, B. Lukowski, A. Proñ, H. Norouzi-Arasi, K.

- Månsson, P. Bujalowski, A. Cederbalk, T. H. Pham, T. Wixe, S. Dawaigher; K. Wärnmark *ChemCatChem* **2015**, *7*, 333-348.
- 61) "A Heteroleptic Ferrous Complex with Mesoionic Bis(1,2,3-triazol-5-ylidene) Ligands: Taming the MLCT Excited State of Fe(II)" Yizhu Liu, Kasper S. Kjær, Lisa A. Fredin, Pavel Chábera, Tobias Harlang, Sophie E. Canton, Sven Lidin, Jianxin Zhang, Reiner Lomoth, Karl-Erik Bergquist, Petter Persson, Kenneth Wärnmark, and Villy Sundström *Chem. Eur. J.* **2015**, *21*, 3628-3639.
- 62) "Visualizing the Nonequilibrium Dynamics of Photoinduced Intramolecular Electron Transfer with Femtosecond X-ray Pulse" Sophie E. Canton, Kasper S. Kjær, György Vankó, Tim B. van Driel Shin-ichi Adachi, Amélie Bordage, Christian Bressler, Pavel Chabera, Morten Christensen, Asmus O. Dohn, Andreas Galler, Wojciech Gawelda, David Gosztola, Kristoffer Haldrup, Tobias Harlang, Yizhu Liu, Klaus B. Møller, Zoltán Németh, Shunsuke Nozawa, Mátyás Pápai, Tokushi Sato, Takahiro Sato, Karina Suarez-Alcantara, Tadashi Togashi, Kensuke Tono, Jens Uhlig, Dimali A. Vithanage, Kenneth Wärnmark, Makina Yabashi, Jianxin Zhang, Villy Sundström and Martin Nielsen *Nature Commun.* **2015**, *6*:6359.
- 63) "A Remarkably Complex Supramolecular Hydrogen-Bonded Decameric Capsule from an Enantiopure  $C_2$ -Symmetric Monomer by Solvent-Responsive Aggregation" Račkauskaitė, Dovilė; Bergquist, Karl-Erik; Shi, Qixun; Sundin, Anders; Butkus, Eugenijus; Wärnmark, Kenneth; Orentas, Edvinas *J. Am. Chem. Soc.* **2015**, *137*, 10536–10546.
- 64) "Watching the dynamics of electrons and atoms at work in solar energy conversion" S. E. Canton, X. Zhang, Y. Liu, J. Zhang, M. Pápai, A. Corani, A. L. Smeigh, G. Smolentsev, K. Attenkofer, G. Jennings, C. A. Kurtz, F. Li, T. Harlang, D. Vithanage, P. Chabera, A. Bordage, L. Sun, S. Ott, K. Wärnmark, V. Sundström *Faraday Discuss.* **2015**, *185*, 51–68.
- 65) "Resolution and Determination of the Absolute Configuration of a Twisted Bis-Lactam Analogue of Tröger's Base: A Comparative Spectroscopic and Computational Study" Ögmundur Vidar Ruñarsson, Christian Benkhäuser, Niels Johan Christensen, Josep Artacho Ruiz, Erhad Ascic, Michael Harmata, Victor Snieckus, Kari Rissanen, Peter Fristrup, Arne Lützen, and K. Wärnmark *J. Org. Chem.* **2015**, *80*, 8142-8149.
- 66) "Iron sensitizer converts light to electrons with 92% yield" Tobias C. B. Harlang, Yizhu Liu, Olga Gordivska, Lisa A. Fredin, Carlito S. Ponseca, Jr., Ping Huang, Pavel Chábera, Kasper S. Kjaer, Helena Mateos, Jens Uhlig, Reiner Lomoth, Reine Wallenberg, Stenbjörn Styring, Petter Persson, Villy Sundström, Kenneth Wärnmark *Nature Chemistry* **2015**, *7*, 883-889.
- 67) "A protocol for the exo-mono and exo,exo-bis functionalization of the diazocine ring of Tröger's base." Dawaigher, Sami; Månsson, Kristoffer; Ascic, Erhad; Artacho, Josep; Mårtensson, Roger; Loganathan, Nagarajan;

Wendt, Ola; Harmata, Michael; Snieckus, Victor; Wärnmark, Kenneth J. *Org. Chem.* **2015**, 80, 12006-120014.

- 68) “An Enantiopure Hydrogen-Bonded Octameric Tube: Self-Sorting and Guest-Induced Rearrangement” Dovilė Račkauskaitė, Rokas Gegevičius, Yutaka Matsuo, Kenneth Wärnmark, Edvinas Orentas, *Angew. Chem, Int. Ed.* **2016**, 55, 208-212.
- 69) “Molecular and Interfacial Calculations of Fe(II) Light Harvesters” Lisa Fredin, Kenneth Wärnmark, Villy Sundström and Petter Persson, *ChemSusChem* **2016**, 9, 667-675.
- 70) “Synthesis of Cr(III) Salen Complexes as Supramolecular Catalytic Systems for Ring-Opening Reactions of Epoxides” Emil Lindbäck, Hassan Norouzi-Arasi, Esmail Sheibani, Dayou Ma, Sami Dawaigher, Kenneth Wärnmark *ChemistrySelect* **2016**, 1, 1789-1794.
- 71) “Femtosecond X-Ray Scattering Study of Ultrafast Photoinduced Structural Dynamics in Solvated  $[\text{Co}(\text{terpy})_2]^{2+}$ ” Elisa Biasin, Tim Brandt van Driel, Kasper S. Kjær, Asmus O. Dohn, Morten Christensen, Tobias Harlang, Pavel Chabera, Yizhu Liu, Jens Uhlig, Mátyás Pápai, Zoltán Németh, Robert Hartsock, Winnie Liang, Jianxin Zhang, Roberto Alonso-Mori, Matthieu Chollet, James M. Glowonia, Silke Nelson Dimosthenis Sokaras, Tadesse A. Assefa, Alexander Britz, Andreas Galler, Wojciech Gawelda, Christian Bressler, Kelly J. Gaffney, Henrik T. Lemke, Klaus B. Møller, Martin M. Nielsen, Villy Sundström, György Vankó, Kenneth Wärnmark, Sophie E. Canton, and Kristoffer Haldrup *Phys. Rev. Lett.* **2016**, 117, 013002.
- 72) “Fe N-Heterocyclic Carbene Complexes as Promising Photosensitizers” Y. Liu, P. Persson, V. Sundström, K. Wärnmark *Acc. Chem. Res.* **2016**, 49, 1477-1485.
- 73) “Manipulating Charge Transfer Excited State Relaxation and Spin Crossover in Iron Coordination Complexes with Ligand Substitution” Wenkai Zhang, Kasper S. Kjær, Roberto Alonso-Mori, Uwe Bergmann, Matthieu Chollet, Lisa A. Fredin, Ryan G. Hadt, Robert W. Hartsock, Tobias Harlang, Thomas Kroll, Katharina Kubiček, Henrik T. Lemke, Huiyang W. Liang, Yizhu Liu, Martin M. Nielsen, Petter Persson, Joseph S. Robinson, Edward I. Solomon, Zheng Sun, Dimosthenis Sokaras, Tim B. van Driel, Tsu-Chien Weng, Diling Zhu, Kenneth Wärnmark, Villy Sundström, Kelly J. Gaffney *Chem. Sci.* **2017**, 8, 515-521.



- 74) “A low-spin Fe(III) complex with 100 ps ligand-to-metal charge transfer photoluminescence” Pavel Chábera , Yizhu Liu, Om Prakash, Erling Thyrhaug , Amal El Nahhas , Alireza Honarfar, Sofia Essén, Lisa A. Fredin, Tobias C. B. Harlang, Kasper S. Kjær, Karsten Handrup, Fredric Ericson, Hideyuki Tatsuno, Kelsey Morgan, Joachim Schnadt, Lennart Häggström, Tore Ericsson, Adam Sobkowiak, Sven Lidin, Ping Huang, Stenbjörn Styring<sup>i</sup>, Jens Uhlig<sup>a</sup>, Jesper Bendix<sup>j</sup>, Reiner Lomoth<sup>i</sup>, Villy Sundström, Petter Persson, Kenneth Wärnmark *Nature* **2017**, *543*, 695–699.
- 75) “Stimuli-controlled self-assembly of diverse tubular aggregates form one single small monomer“ Qixun Shi, Tomas Javorskis, Karl-Erik Bergquist, Artūras Ulčinas, Gediminas Niaura, Ieva Matulaitienė, Edvinas Orentas and Kenneth Wärnmark *Nature Commun.* **2017**, *8*: 14943.
- 76) “Electronic structure and excited state properties of iron carbene photosensitizers - a combined X-ray absorption and quantum chemical investigation” F. Ericson, A. Honarfar, H. Tatsuno, K. Handrup, P. Chabera, O. Prakash, O. Gordivska, L. A. Fredin, K. S. Kjaer, Y. Liu, J. Schnadt, K. Wärnmark, V. Sundström, P. Persson, J. Uhlig *Chem. Phys. Lett.* **2017**, *683*, 559-566.
- 77) “Ligand manipulation of charge transfer excited state relaxation and spin crossover in [Fe(2,2'-bipyridine)<sub>2</sub>(CN)<sub>2</sub>]” Kjaer, K. S.; Zhang, W.; Alonso-Mori, R.; Bergmann, U.; Chollet, M., Hadt, R. G.; Hartsock, R. W.; Harlang, T.; Kroll, T., Kubicek, K.; Lemke, H. T.; Liang, H. W.; Liu, Y.; Nielsen, M. M.; Robinson, J. s.; Solomon, E. I; Sokaras, D.; van Driel, T. B.; weng, T-C, Zhu, D.; Persson, P., Wärnmark, K.; Sundström, V.; Gaffney, K. J. *Structural dynamics* **2017**, *4*, 044030.
- 78) “Tracking the Picosecond Deactivation Dynamics of a Photoexcited Iron Carbene Complex by Time-Resolved X-ray Scattering” Denis Leshchev, Tobias C. B. Harlang, Lisa A. Fredin, Dmitry Khakhulin, Yizhu Liu, Elisa Biasin, Mads G. Laursen, Gemma E. Newby, Kristoffer Haldrup, Martin M. Nielsen, Kenneth Wärnmark, Villy Sundström, Petter Persson, Kasper S. Kjær, Michael Wulff *Chem. Sci.* accepted for publication.
- 79) “A Fe<sup>II</sup> Hexa *N*-Heterocyclic Carbene Complex with a 528 ps Metal-to-Ligand Charge-Transfer Excited-State Lifetime” Pavel Chábera, Kasper S. Kjaer, Om Prakash, Alireza Honarfar, Yizhu Liu, Lisa A. Fredin, Tobias C. B. Harlang, Sven Lidin, Jens Uhlig, Villy Sundström, Reiner Lomoth, Petter Persson, and Kenneth Wärnmark *J. Chem. Phys. Lett.* accepted for publication.

