

List of publications Kenneth Wärnmark

- 128) “Highly-Destabilized Ligand Field Excited States of Iron Carbene Complexes and Their Relation to Charge Transfer State Lifetimes” Hooper, R. X.; Poulter, B. I.; Schwarz, J.; Barakat, M.; Kunnus, K.; Nelson, K. J.; Ilic, A.; García-Mateos, C.; Chowdhury, R.; Uhlig, J.; Wärnmark, K.; Jakubikova, E.; Cordones, A. A.; Gaffney, K. J. *Chem. Sci.* **2026**, *in press*. DOI: 10.1039/D5SC07843A
- 127) “Design, Synthesis and Aggregation of Amphiphilic Monomers—Cyclic and Tubular Hydrogen-Bonded Self-assembly in Conventional and Polar Media” Lidskog, A.; Neniškis, A.; Edin, S.; Takács, Z.; Klimkevičius, V.; Orentas, E.; Wärnmark, K. *Chem. Eur. J.* **2025**, e02804 <https://doi.org/10.1002/chem.202502804>
- 126) “Iron N-Heterocyclic Carbene Photoactive Complexes with Rigid Phenylethynyl Substituents as Ligand π -System Extensions” Persson, S.; Koninti, R. J.; Barakat, M.; Mishra, A.; Lindgren, F.; Ericsson, T.; Häggström, L.; Lidin, S.; Gonzalez, A.; Jakubikova, E.; Lomoth, R.; Wärnmark, K. *Inorg. Chem.* **2025**, *64*, 12120–12131. <https://doi.org/10.1021/acs.inorgchem.5c01461>
- 125) “Push-Pull Amino-substituted Heteroleptic Iron N-Heterocyclic Carbene Photosensitizers in Dye-Sensitized Solar Cells: Optimization and Characteristics” Persson, S.; Benesperi, I.; Goriya, Y.; Kand, D.; Rayavarapu, S.; Keller, T.; Freitag, M.; Wärnmark, K. *Sustainable Energy Fuels* **2025**, *9*, 2389–2395. DOI: 10.1039/d4se01772b.
- 124) “Base-Promoted Homolytic Aromatic Substitution (BHAS) Reactions and Hydrodehalogenations Driven by Green Light and an Iron(III)-NHC Photoredox Catalyst”. de Groot, L. H. M.; García-Mateos, C.; Johnson, C. E.; Freyr Hlynsson, V.; Sharma, A. K.; Lomoth, R.; Wärnmark, K. *Chem. Eur. J.* **2025**, e202500409. <https://doi.org/10.1002/chem.202500409>
- 123) “Shining light on the ferrous analogue: Excited state dynamics of an Fe(II) hexa-carbene scorpionate complex” Johnsson, C. E.; Deegbey, M.; Ilic, A.; Kaul, N.; Prakash, O.; Wärnmark, K.; Jakubikova, E.; Lomoth, R. *Dalton Trans.* **2025** accepted.
- 122) “Diastereospecific Synthesis of Vicinally Substituted 2-Oxazolidinones via Oxidative Rearrangement of α,β -Unsaturated γ -Lactams” Lidskog, A.; Li, Y.; Kumar Gupta, A.; Mishra, A.; Sundin, A.; Wärnmark, K. *J. Org. Chem.* **2025**, *90*, 1209–1213. <https://pubs.acs.org/doi/10.1021/acs.joc.4c02653>.
- 121) “Aminomethylations of electron-deficient compounds-bringing iron photoredox catalysis into play” Ilic, A.; Strückner, B. R.; Johnson, C. E.; Hainz, S.; Lomoth, R.; Wärnmark, K. *Chem. Sci.* **2024**, *15*, 12077–12085. DOI: 10.1039/d4sc02612h.

- 120) "How substituents tune quantum interference in *meta*-OPE3 molecular junctions to control thermoelectric transport" Yan, S.; Luan, Y., Xu, H.; Martin, L.; Kumar Gupta, A.; Linke, H.; Meyhofer, E.; Reddy, P.; Pauly, F.; Wärnmark, K. *Nanoscale*, **2024**, *16*, 13906-13914.
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- 119) "Using Iron L-Edge and Nitrogen K-Edge X-ray Absorption Spectroscopy to Improve the Understanding of the Electronic Structure of Iron Carbene Complexes" Guo, M.; Temperton, R.; D'Acunto, G.; Johansson, N.; Jones, R.; Handrup, K.; Ringelband, S.; Prakash, O.; Fan, H.; de Groot, L. H. M.; Freyr Hlynsson, V.; Kaufhold, S.; Gordivska, O.; Velásquez González, N.; Wärnmark, K.; Schnadt, J.; Persson, P.; Uhlig, J. *Inorg. Chem.* **2024**, *63*, 12457-12468.
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- 118) "Side-group switching between metal-to-ligand charge transfer and metal centred excited state properties in iron(II) N-heterocyclic carbene complexes" Lindh, L.; Rosemann, N. W; Bolaño Losada, I.; Persson S; Yogesh Goriya, Y.; Fan H.; Gordivska, O.; Wärnmark, K.; Uhlig, J.; Chábera, P.; Yartsev, A.; Persson; P. *Coord. Chem. Rev.* **2024**, *506*, article 215709.
<https://www.sciencedirect.com/science/article/pii/S0010854524000559>
- 117) "How Rigidity and Conjugation of Bidentate Ligands Affect the Geometry and Photophysics of Iron N-heterocyclic Complexes — A comparative Study"
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- 116) Tailoring the Photophysical Properties of a Homoleptic Iron (II) tetra N-Heterocyclic carbene complex by Attaching an Imidazolium Group to the (C^NC) Pincer ligand – A Comparative Study
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- 114) "Electrical Conductance and Thermopower of β -Substituted Porphyrin Molecular Junctions – Synthesis and Transport". Xu, H.; Fan, H.; Luan, Y.; Yan, S.; Martin, L.; Miao, R.; Pauly, F.; Meyhofer, E.; Reddy, P.; Linke, H.; Wärnmark, K. *J. Am. Chem. Soc.* **2023**, *145*, 23541-23555.
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- 111) “Competing dynamics of intramolecular deactivation and bimolecular charge transfer processes in luminescent Fe(III) N-heterocyclic carbene complexes, Rosemann, N. W.; Lindh, L.; Bolaño Losada, I.; Kaufhold, S.; Prakash, O.; Ilic, A.; Schwarz, J.; Wärnmark, K.; Chábera, P.; Yartsev, A.; and Persson, P. *Chem. Sci.* **2023** *14*, 3569-3579.
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- 110) “Photophysical Integrity of the Iron(III) Scorpionate Framework in Iron(III)-NHC Complexes with Long-lived ²LMCT Excited States” Prakash, O.; Lindh, L.; Kaul, N.; Rosemann, N. W.; Bolaño Losada, I.; Johnson, C.; Chábera, P.; Ilic, A.; Schwarz, J.; Kumar Gupta, A.; Uhlig, J.; Ericsson, T.; Häggström, L.; Huang, P.; Bendix, J.; Strand, D.; Yartsev, A.; Lomoth, R.; Persson, K.; Wärnmark, K. *Inorg. Chem.* **2022**, *61*, 17515-17526.
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- 108) “Photoredox Catalysis via Consecutive ²LMCT and ³MLCT Excitation of an Fe(III/II)-N-Heterocyclic Carbene Complex” Aleksandra Ilic, Jesper Schwarz, Catherine Johnson, Lisa H. M. de Groot, Simon Kaufhold, Reiner Lomoth, and Kenneth Wärnmark *Chem. Sci.* **2022**, *13*, 9165-9175.
- 107) “Quantifying the Steric Effect on Metal–Ligand Bonding in Fe Carbene Photosensitizers with Fe 2p3d Resonant Inelastic X-ray Scattering” Kristjan Kunnus*, Meiyuan Guo, Elisa Biasin, Christopher B. Larsen, Charles J. Titus, Sang Jun Lee, Yizhu Liu, Kenneth Wärnmark, Dennis Nordlund, Amy A. Cordones, Jens Uhlig, Kelly J. Gaffney *Inorg. Chem.* **2022**, *61*, 1962-1972. . DOI: [10.1021/acs.inorgchem.1c03124](https://doi.org/10.1021/acs.inorgchem.1c03124)
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- 104) "Counter Intuitive electrostatics upon Metal Ion Coordination to a Receptor with Two Homotopic binding sites" Aspelin, V.; Lidskog, A.; Solano Arribas, C.; Hervø-Hansen, S.; Stenqvist, B.; Chudoba, R.; Wärnmark, K.;[§] Lund, M.[§] *J. Am. Chem. Soc.* **2022** accepted. [§] = equal contribution
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- 97) "Mono *endo*-6-*N,N*-Diethylcarbamoyl and Bis *endo,endo*-6,12-*N,N*-Diethylcarbamoyl Derivatives of Tröger's Base. Synthesis and *Exo-Endo* Isomerization Study" S. Dawaigher, E. Lindbäck, D. Strand, A. Cederbalk, S. Winikoff, M. Harmata, Victor Snieckus, K. Wärnmark *ARKIVOC* **2020**, part (vii), 68-81 (JB-11183KP).
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