

The Danish Chemical Society Annual Meeting 2017



15th of June 2017, Odense
University of Southern Denmark

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Mission and history of The Danish Chemical Society

The Danish Chemical Society has been founded in 1879 as a society for Danish chemists and has since focused on the advancement of chemistry and the improvement of the public recognition of chemistry. This mission has not changed and is of even more importance today, where modern life is entirely dependent on chemical achievements like materials research (e.g. polymers), and medicinal chemistry (e.g. drug discovery), to name just a few. The public recognition of chemistry needs more young students and researchers in the various branches of chemistry to engage in discussions on important questions in our society. Many global problems are strongly linked to chemistry (e.g. green energy, affordable health care, clean water or the protection of our environment).

Become a member of The Danish Chemical Society and:

- ✓ Participate in scientific meetings organized or supported by our society
- ✓ Write articles and essays in the society journal – *Dansk Kemi*
- ✓ Apply for travel grants
- ✓ Find job offers within the society network
- ✓ Receive society awards for outstanding contributions in chemistry (e.g. PhD prizes)
- ✓ Organize local meetings for your chemistry division with support from your society
- ✓ Promote your career as an invited speaker at our national meetings

Sign up at chemsoc.dk and become a member (1st year of your membership is free)

[annual membership fee - student members: 225 Kr - full members: 450 Kr]

Famous Danish chemists



W. C. Zeise, 1789-1847

New metal-organic compounds (e.g. Zeise's salt).



J.N. Brønsted, 1879-1947

Key acid-base definition (Brønsted theory).



N. J. Bjerrum, 1879-1958

Theory of strong electrolytes and applied IR spectroscopy.

Program Agenda

Time		Room
09.30 – 10.00	Registration	Outside U45
10.00 – 10.05	Welcome	U45
10.05 – 10.50	Plenary lecture by Prof. Dr. Evamaria Hey-Hawkins University of Leipzig, Germany “Carboranes – Highly Versatile Scaffolds in Ligand and Drug Design”	U45
10.55 – 12.25	Session lectures I <i>The Division of Organic Chemistry I</i> <i>The Division of Inorganic Chemistry</i> <i>The Division of Pharmaceutics and Biopharmaceutics I</i>	U45 U47 U46
12.25 – 13.10	Lunch and Poster session	“Old Fridaybar”
13.10 – 14.40	Session lectures II <i>The Division of Medicinal Chemistry I</i> <i>Danish Society of Molecular Spectroscopy</i> <i>Chemical Engineering / IDA Kemi – Kemiingeniørgruppen I</i> <i>The Division of Pharmaceutics and Biopharmaceutics II</i>	U45 U47 U44 U46
14.40 – 15.00	Coffee break	“Old Fridaybar”
15.00 – 16.30	Session lectures III <i>The Division of Organic Chemistry II</i> <i>The Division of Medicinal Chemistry II</i> <i>Chemical Engineering / IDA Kemi – Kemiingeniørgruppen II</i> <i>The Division of Theoretical Chemistry</i>	U46 U45 U44 U47
16.30 – 17.15	Bjerrum-Brønsted-Lang lecture awarded by The Royal Danish Academy of Sciences and Letters	U45
17.15 – 18.30	Poster session	“Old Fridaybar”
18.30 –	Dinner and poster awards	SDU restaurant
20.30	Departure for participants from Copenhagen and Aarhus	

Session lectures I	10.55 – 12.25	room
The Division of Organic Chemistry / Sektionen for Organisk Kemi		U45
Studies of dehaloperophoramidine: Evolution of a total synthesis Peter Somfai Centre for Analysis and Synthesis, Department of Chemistry, Lund University, Sweden	10.55 – 11.25	
Learning to love CO₂ Jiwoong Lee Department of Chemistry, University of Copenhagen	11.25 – 11.55	
Synthetic oligosaccharides as tool compounds to study glycan-protein interactions Mads H. Clausen DTU Chemistry, Technical University of Denmark	11.55 – 12.25	
The Division of Inorganic Chemistry / Sektionen for Uorganisk Kemi		U47
Point defect chemistry of internal interfaces in ferroic oxides Sverre Magnus Selbach Department of Materials Science and Engineering, Norwegian University of Science and Technology (NTNU), Norway	10.55 – 11.35	
Power at the atomic scale – designing new materials for rechargeable batteries Dorthe Bomholdt Ravnsbæk Department of Physics, Chemistry and Pharmacy, University of Southern Denmark	11.35 – 12.00	
Magnetic anisotropy in single molecule magnets determined using neutron and X-ray diffraction Jacob Overgaard Center for Materials Crystallography, Department of Chemistry, Aarhus University	12.00 – 12.25	

The Division of Pharmaceutics and Biopharmaceutics / Sektion for Farmaci og Biofarmaci	U46
Recent developments in co-processed excipients: Technical and regulatory insight Christian Nowak Meggler GmbH, Germany	10.55 – 11.25
Recent developments in amorphous drug formulation Korbinian Löbmann Department of Pharmacy, University of Copenhagen	11.25 – 11.55
Nucleation, Growth and Characterization of Triolein Nanoparticles Prepared in the Absence and Presence of Phospholipids by Rapid Solvent Shifting Technique Anders Utoft and Prasad Walke Department of Physics, Chemistry and Pharmacy, University of Southern Denmark	11.55 – 12.25

Session lectures II	13.10 – 14.40	room
Danish Society of Pharmacology, Toxicology and Medicinal Chemistry / Dansk Selskab for Farmakologi, Toksikologi og Medicinalkemi		U45
The I B Kinase Project - From hits to clinical candidates: Dead ends, detours and successes! Olaf Ritzeler Sanofi, Research and Development, Frankfurt, Germany		13.10 – 13.40
Presentations from finalists for Denmark's Young Medicinal Chemist Symposium candidate		
Lighting up atherosclerosis Mario Ficker Department of Chemistry, University of Copenhagen		13.40 – 13.55
Development of modulators and tool compounds for the short-chain fatty acid receptor FFA2 Anders Højgaard Hansen Department of Physics, Chemistry and Pharmacy, University of Southern Denmark		13.55 – 14.10
DNA nucleobases with extended ring systems: Promising new players in antisense therapeutics Mick Hornum Department of Physics, Chemistry and Pharmacy, University of Southern Denmark		14.10 – 14.25
LEGO®-inspired drug design and the discovery of novel C-H functionalization difluoromethylation reaction for drug discovery Truong Thanh Tung Department of Drug Design and Pharmacology, University of Copenhagen		14.25 – 14.40

**The Danish Society of Molecular Spectroscopy /
Dansk Forening for Molekylspektroskopi****U47****3D Alignment in helium droplets: a route to ultrafast diffraction of large molecules**

13.10 – 13.40

Adam Simon Chatterley

Department of Chemistry, Aarhus University

Reliable structural characterization of ZnAl₄ layered double hydroxides

13.40 – 14.10

Nicholai Daugaard Jensen

Department of Physics, Chemistry and Pharmacy, University of Southern Denmark

Dealumination of ZSM-5 zeolites investigated by solid-state NMR spectroscopy and complementary techniques

14.10 – 14.40

Julian Holzinger

iNANO and Department of Chemistry, University of Aarhus

**The Division of Pharmaceutics and Biopharmaceutics /
Sektion for Farmaci og Biofarmaci****U46****Cubosomes and hexosomes as versatile platforms for drug delivery**

13.10 – 13.40

Anan Yagmur

Department of Pharmacy, University of Copenhagen

Cochleate cylinders as parenteral depot formulations

13.40 – 14.00

Søren Kristensen

Department of Physics, Chemistry and Pharmacy, University of Southern Denmark

Prediction of oral bioavailability using enabling formulations

14.00 – 14.20

Hanady Akram Bibi

Department of Physics, Chemistry and Pharmacy, University of Southern Denmark

Influence of nonionic surfactants on oral absorption of P-glycoprotein substrates in vitro and in vivo

14.20 – 14.40

Ahmed A. Abdulhussein

Department of Physics, Chemistry and Pharmacy, University of Southern Denmark

Chemical Engineering division / IDA Kemi – Kemiingeniørgruppen**U44****Special Session on Catalysis****Industrial gas cleaning by ionic liquid absorption and catalytic conversion**

13.10 – 13.40

Rasmus Fehrmann

CSC Research Centre, DTU Chemistry, Technical University of Denmark

Selective formation of formic acid from biomass-derived compounds over supported ruthenium hydroxide catalyst

13.40 – 14.10

Amalie E. Modvig

CSC Research Centre, DTU Chemistry, Technical University of Denmark

Methanation of CO₂ using zeolite encapsulated nickel nanoparticles

14.10 – 14.40

Jerrick J. Mielby

CSC Research Centre, DTU Chemistry, Technical University of Denmark

Session lectures III	15.00 – 16.30	room
The Division of Organic Chemistry / Sektionen for Organisk Kemi		U46
Reactive metabolites, diabetes and biological aging – Development of chemical biological tools for discovery of functional effects Mogens Johannsen Department of Forensic Medicine, University of Copenhagen	15.00 – 15.30	
Probing HDAC and sirtuin function with fluorogenic substrates Andreas S. Madsen Center for Biopharmaceuticals and Department for Drug Design and Pharmacology, University of Copenhagen	15.30 – 16.00	
PhD prize – award lecture	16.00 – 16.30	
Danish Society of Pharmacology, Toxicology and Medicinal Chemistry / Dansk Selskab for Farmakologi, Toksikologi og Medicinalkemi		U45
<i>Plenary speakers and announcement of Denmark's YMCS candidate</i>		
Medicinal polymer chemistry: From macromolecular design to therapeutic benefits and back Alexander Zelikin Department of Chemistry, University of Aarhus	15.00 – 15.25	
Towards amplification-free nucleic acid diagnostics Kira Astahkova Department of Physics, Chemistry and Pharmacy, University of Southern Denmark	15.25 – 15.50	
Current trends in development of fluorination reactions - and a story about natural product chemistry John Nielsen Department of Drug Design and Pharmacology, University of Copenhagen	15.50 – 16.15	
Announcement of Denmark's Young Medicinal Chemist Symposium candidate	16.15 – 16.30	

Chemical Engineering section / IDA Kemi – Kemiingeniørgruppen**U44****Super-resolution localization and live-tracking analyzed by pair correlation and a novel power-spectral analysis method reveal short-term regulation of the water channel aquaporin-3**

15.00 – 15.30

Eva Arnsfang Christensen

Department of Chemical Engineering, Biotechnology and Environmental Technology, University of Southern Denmark

Upgrading Landfill Gas to Natural Gas

15.30 – 16.00

Jacob Hjerrild Zeuthen

Haldor Topsøe A/S

Natural Blue Food Colour

16.00 – 16.30

Maria Cinta Roda-Serrat

Department of Chemical Engineering, Biotechnology and Environmental Technology, University of Southern Denmark

**The Division of Theoretical Chemistry /
Sektionen for Teoretisk Kemi****U47****50 years of response function theory**

15.00 – 15.45

Poul Jørgensen

Department of Chemistry, University of Aarhus

Relativistic effects in electronic decay processes

15.45 – 16.10

Elke Faßhauer

Department of Chemistry, University of Copenhagen

Computational approach to evaluation of optical properties of membrane probes

16.10 – 16.30

Lina Nåbo

Department of Physics, Chemistry and Pharmacy, University of Southern Denmark

Plenary lecture Abstract – Prof. Dr. Evamarie Hey-Hawkins

Leipzig University, Faculty of Chemistry and Mineralogy, Institute of Inorganic Chemistry,
Johannisallee 29, D-04103 Leipzig, Germany
hey@uni-leipzig.de

Carboranes – Highly Versatile Scaffolds in Ligand and Drug Design

The chemistry of boron is highly suitable for the construction of boron-rich building blocks due to the formation of polyhedral boranes and heteroboranes. Especially dicarba-*closo*-dodecaboranes (*closo*-C₂B₁₀H₁₂, carboranes), which are highly hydrophobic icosahedral carbon-containing boron clusters, are versatile starting materials for boron-cluster-based ligand and drug design. The three isomers of dicarba-*closo*-dodecaborane (1,2- (*ortho*)) (Fig. 1), 1,7- (*meta*), 1,12- isomer (*para*)) are three-dimensional electron-poor aromatic analogues. The cage framework of these clusters can be easily modified with a variety of substituents both at the carbon and at the boron atoms.

Especially the 1,2-dicarba-*closo*-dodecaborane is a very versatile C₂ backbone for the synthesis of electron-poor ligands, e.g., bis-phosphines (Fig. 2),^[1] the transition metal complexes of which are potentially useful as catalysts.

On the other hand, boron clusters can be used in medicine as boron neutron capture therapy (BNCT) agents or as pharmacophores in which the carborane replaces the phenyl rings in drug candidates.

High and selective accumulation in tumour cells is an important requirement for a BNCT agent. We have shown that the tumour selectivity of BNCT agents can be increased by, e.g., incorporating carboranes into breast-tumour-selective modified neuropeptide Y^[2] (Fig. 3).

The use of carboranes as pharmacophores is up to now limited to just a few examples. We are developing drug mimetics of specific enzyme inhibitors, e.g., cyclooxygenase (COX) and lipoxygenase (LOX) inhibitors (Fig. 4).^[3]

The versatility of the carborane scaffold for these various modifications and applications will be presented.

References

- [1] P. Coburger, J. Schulz, J. Klose, B. Schwarze, M. B. Sárosi, E. Hey-Hawkins, *Inorg. Chem.* **2017**, *56*, 292
 [2] V.M. Ahrens, R. Frank, S. Boehnke, C. L. Schütz, G. Hampel, D.S. Iffland, N.H. Bings, E. Hey-Hawkins, A.G. Beck-Sickingler, *ChemMedChem* **2015**, *10*, 164.
 [3] M. Scholz, E. Hey-Hawkins, *Chem. Rev.* **2011**, *111*, 7035. W. Neumann, S. Xu, M.B. Sárosi, M.S. Scholz, B.C. Crews, K. Ghebreselasie, S. Banerjee, L.J. Marnett, E. Hey-Hawkins, *ChemMedChem* **2016**, *11*, 175.

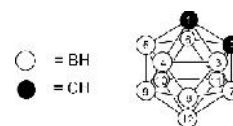


Figure 1. 1,2-Dicarba-*closo*-dodecaborane

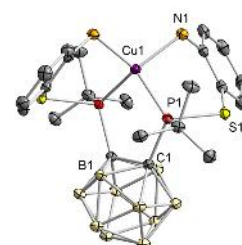


Figure 2. Cationic Cu^I complex of a tetradentate carborane-based ligand (anion and H atoms not shown)

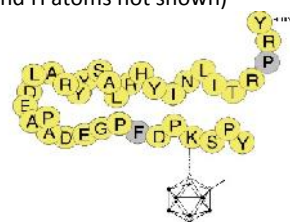


Figure 3. Carborane-modified neuropeptide Y ([Phe⁷,Pro³⁴] NPY)

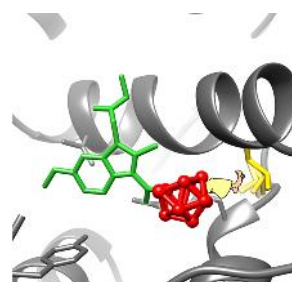


Figure 4. *nido*-Indoborin as selective COX-2 inhibitor

Biographical Information



Evamarie Hey-Hawkins studied chemistry at the University of Marburg, Germany, where she completed her PhD thesis in 1983. As recipient of a Liebig scholarship, she then spent a one-year in the group of Prof. M. F. Lappert at the University of Sussex, England. In 1988 she obtained her Habilitation and *venia legendi* in inorganic chemistry from the University of Marburg. In 1993 she became full Professor, C4 at Leipzig University. From 2001-2005 she was Dean/Vice Dean of the faculty of Chemistry and Mineralogy at Leipzig University.

Her scientific work has been published in more than 440 publications in refereed journals; more than 300 plenary, keynote and invited oral presentations (national and international).

Evamarie Hey-Hawkins has received several awards such as IUPAC Distinguish Woman in Chemistry (2013), Doctor Honoris Causa by Babes-Bolyai University, Romania (2014), Elhuyar-Goldschmidt Lecture (2015), Costin Nenitzescu-Rudolf Criegee Lecture (2016), Doctor Honoris Causa (Dr. h.c.) by Ss. Cyril and Methodius University, Republic of Macedonia (2016), Costin Nenitescu Medal (2016), and she received the Order of Merit of the Free State of Saxony, Germany (2017).

Evamarie Hey-Hawkins Research Topics

Transition metal complexes and their application in catalysis and materials science; organophosphorus compounds; biologically active boron compounds (reagents for boron-neutron capture therapy (tumour therapy), enzyme inhibitors (inflammation, progression of cancer)).



Bjerrum – Brønsted – Lang award lecture

Prof. Christine Mckenzie

Department of Chemistry, Physics and Pharmacy
University of Southern Denmark

The Royal Danish Academy of Sciences and Letters



University of Southern Denmark (SDU) campus map and conference site



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