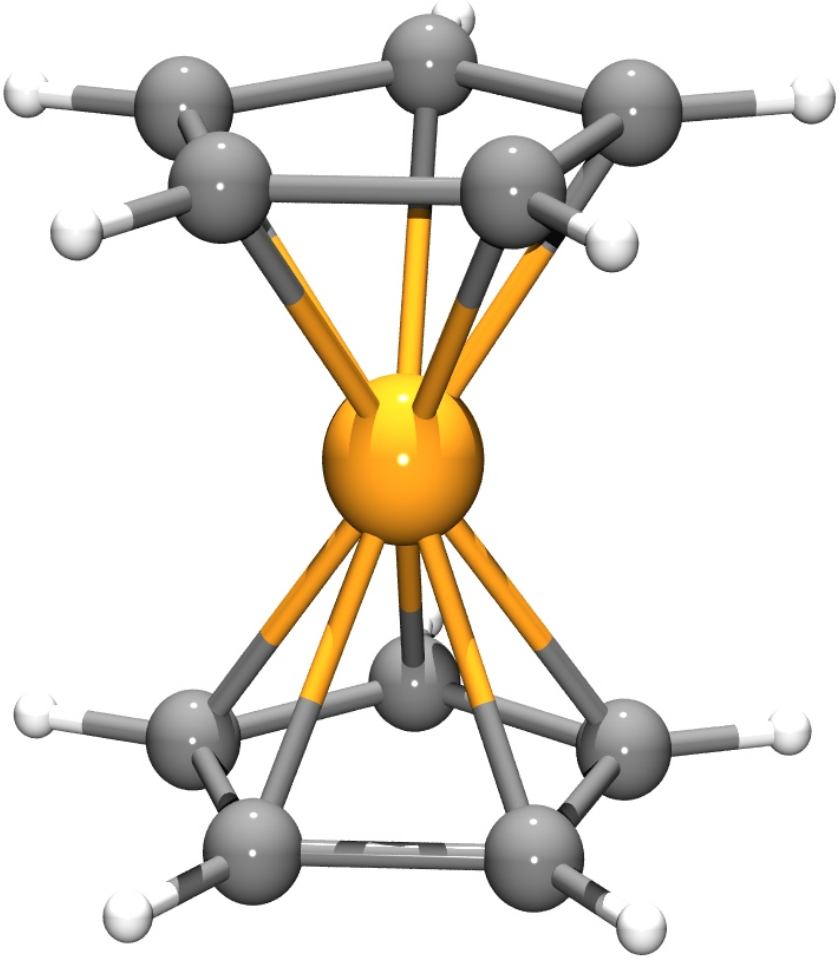
9th Ferrocene Colloquium



February 14 – 16, 2011

CHEMNITZ UNIVERSITY
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1836-2011
175 Years

Sponsors

The 9th Ferrocene Colloquium would not be possible without the generous support of our sponsors. We are grateful to:

"Die Chemie ist, abgesehen von ihrer Nützlichkeit,
die niemand bestreiten wird, eine schöne Wissenschaft."

"Chemistry is apart from its usefulness,
which no one will deny, a beautiful science."

Julius Adolph Stöckhardt (1809–1886)
1st Professor for Chemistry in Chemnitz

Table of Contents

Preface

Almost 60 years after its unintended discovery, ferrocene still arouses great interest among scientists in many areas of research. The wide spectrum of applications is reflected in many different topics the 9th Ferrocene Colloquium is dedicated to. During the next three days, young researchers along with outstanding scientists will present recent results of their research, for example the synthesis of new ferrocene molecules and materials, the application of metallocenes in catalysis or electron transfer studies as well as the investigation of hitherto unknown reactivities.

In the past years the Ferrocene Colloquium has become a full meeting primarily for young researchers in the field of organometallic chemistry with main focus on metallocenes. It gives me great pleasure to welcome more than 100 participants to the 9th Ferrocene Colloquium, who will present more than 20 lectures together with many posters.

This meeting would not be possible without the financial and material support of our sponsors. We are grateful to NILES - SIMMONS Industrieanlagen GmbH, Gesellschaft der Freunde der TU Chemnitz e. V., UVION GmbH, Fonds der Chemischen Industrie, Gesellschaft Deutscher Chemiker, Braustolz GmbH, HypoVereinsbank, Innospec Deutschland GmbH, Springer Science+Business Media, VWR International and Wiley-VCH Verlag GmbH & Co. KGaA for their assistance.

We wish all the participants and contributors a successful conference, fruitful scientific discussions and a pleasant stay in Chemnitz.

Chemnitz, February 2011

Heinrich Lang
Alexander Hildebrandt
Dieter Schaarschmidt
Sascha Tripke

Organizing Committee

Previous Meetings

1st Ferrocene Colloquium
Kassel, Germany
January 14, **2003**

2nd Ferrocene Colloquium
Würzburg, Germany
February 16–17, **2004**

3rd Ferrocene Colloquium
Heidelberg, Germany
February 24–25, **2005**

4th Ferrocene Colloquium
Frankfurt am Main, Germany
February 25–26, **2006**

5th Ferrocene Colloquium
Kaiserslautern, Germany
February 25–27, **2007**

6th Ferrocene Colloquium
Prague, Czech Republic
February 9–11, **2008**

7th Ferrocene Colloquium
Düsseldorf, Germany
February 16–18, **2009**

8th Ferrocene Colloquium
Bochum, Germany
February 17–19, **2010**

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Schedule

Monday, February 14

10:00–13:00	**Arrival and Registration**	*Altes Heizhaus*
13:00–13:20	**Opening Remarks** Prof. Dr. Dr. h.c. D.R.T. Zahn (Vice-President for Research of Chemnitz University of Technology) Prof. Dr. K. H. Hoffmann (Dean of Faculty of Sciences) Prof. Dr. H. Lang	
	Chair: H. Lang	
13:20–14:10	**C. Lapinte** (CNRS-Université de Rennes 1) *Molecular Devices Based on Electro-Switchable Organometallics*	**I1**
14:10–14:30	**A. Hildebrandt** (Chemnitz University of Technology) *Intervalence Charge Transfer in Diferrocenyl Heterocycles*	**O1**
14:30–14:50	**C. Herfurth** (Universität Potsdam) *Ferrocenyl Monomers and Controlled Radical Polymerization*	**O2**
	Coffee Break	
	Chair: W. Kläui	
15:20–15:40	**R.F. Winter** (Universität Konstanz) *Relevance of Through-space and Through-bond Pathways for Electronic Coupling in Cyclophanes*	**O3**
15:40–16:00	**D. Siebler** (Johannes Gutenberg-Universität Mainz) *Biferrocene amino acid: Synthesis, crosslinking and redox chemistry*	**O4**
16:00–16:20	**R. Breuer** (University of Siegen) *1,1'-Biferrocenylene - can it replace ferrocene ?*	**O5**
16:20–16:40	**C. Gers** (Heinrich Heine Universität Düsseldorf) *A novel synthesis of ynediones: Copper-mediated coupling of in situ generated α-oxo-acid chlorides with terminal alkynes*	**O6**
17:00–19:00	**Poster Session**	*Altes Heizhaus*

Tuesday, February 15

	Chair: M. Tamm	
09:00–09:50	**G. Erker** (Westfälische Wilhelms-Universität Münster) *Frustrated Lewis Pairs:* *Principles and Applications in Organometallic Chemistry*	**I2**

09:50–10:10 **D. Schaarschmidt** (Chemnitz University of Technology) **O7**
Chiral P,O-Ferrocenes as Ligands in the Suzuki-Miyaura Coupling

10:10–10:30 **L. Taghizadeh Ghoochany** (TU Kaiserslautern) **O8**
Novel Ruthenium Catalysts for Transfer Hydrogenation

Coffee Break

Chair: U. Siemeling

11:00–11:20 **K. Kowalski** (University of Łódź) **O9**
Friedel-Crafts reactions of $W(CO)_5$-complexes of azaferrocenes

11:20–11:40 **K. Kaleta** (Leibniz-Institut für Katalyse e. V. an der Universität Rostock) **O10**
Ferrocenyl Substituted Group 4 Metallacycles

11:40–12:00 **C. Thoms** (Universität Regensburg) **O11**
Dehydrocoupling of $PH_2BH_2{\cdot}NMe_3$ Induced by Transition Metal Fragments

12:00–12:20 **A.C. Tagne Kuate** (TU Braunschweig) **O12**
(η^5–cyclopentadienyl)(η^7–cycloheptatrienyl)titanium(IV) (Troticene): Selective Lithiation, Phosphane Functionalization, Heterobimetallic Derivatives, Ansa and Ambivalent Complexes

Lunch Break

Chair: B. Bildstein

14:00–14:50 **I. Butler** (University of Wales) **I3**
A Tour of the Simplest Ferrocene Chemistry over 25 Years

14:50–15:10 **B. Hildebrandt** (Heinrich-Heine Universität Düsseldorf) **O13**
A New N-Heterocyclic Carbene Containing a Cationic Metallocene Backbone

15:10–15:30 **C. Färber** (Universität Kassel) **O14**
Diaminocarbenes and their reactivity towards carbon monoxide; Novel and easy: Instant N-Heterocyclic Carbenes

Coffee Break

Chair: K. Heinze

16:00–16:20 **K. Rademann** (Humboldt-Universität zu Berlin) **O15**
FERROCEN assisted formation of noble metal nano-structures at the oil/water interface

16:20–16:40 **S. Pandey** (Universität Leipzig) **O16**
Chiral Polyferrocenes with Phosphorus-Based Backbones

16:40–17:00 **M. Gawron** (Technische Universität Dortmund) **O17**
An Asymmetrically Substituted Phosphorus-Containing O,C-Coordinating Ferrocene Ligand and its Organotin Derivatives: Synthesis and Reactivity

17:00–17:20	**A.D. Russell** (University of Bristol) *Studies of the Bond Cleavage Mechanisms for Ring-Opening Reactions of Strained [2]Dicarbaferrocenophanes*	**O18**
18:00	**Conference Dinner (BBQ)**	*Altes Heizhaus*

Wednesday, February 16

Chair: H. Butenschön

09:00–09:50	**I. Manners** (University of Bristol) *Strained Ferrocenophanes and Metalloring Analogues - New Reactivity and Utility as Precursors to Functional Metallopolymers*	**I4**
09:50–10:10	**G. Lackner** (University Duisburg-Essen) *Infiltration study of vertically-aligned Carbon Nanotube forest (va-CNT) with different organic semiconductor materials forming a composite*	**O19**
10:10–10:30	**A. Glöckner** (TU Braunschweig) *Open Indenyl — More Than Just Another Pentadienyl Ligand?!*	**O20**

Coffee Break

Chair: W. Thiel

11:00–11:20	**A. Korotvička** (Charles University Prague) *Synthesis of Polyaromatics with Ferrocene Substituents*	**O21**
11:20–11:40	**M. Braun** (Heinrich-Heine Universität Düsseldorf) *Electron Poor NHC-Ligands: A Five-Membered N,N'-Diamidocarbene*	**O22**
11:40–12:00	**D. Weismann** (TU Kaiserslautern) *Dinitrogen Activation with Cyclopentadienyl Complexes*	**O23**
12:00–12:30	**Closing Remarks, Prizes** Prof. Dr. H. Lang, Prof. Dr. M. Tamm Award for best posters Award for best lecture	

Invited Speakers

Molecular Devices Based on Electro-Switchable Organometallics

Claude Lapinte

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The design, preparation, and characterization of new electro-functional materials containing transition metals hybridized with other substances containing various elements constitute a very active field of basic and applied research. A particularly appealing class of composite molecules can be obtained by linking two redox-active inorganic building blocks with unsaturated organic ligands [1]. These molecules can be isolated in several oxidation states, each of them exhibiting different physical properties, like for example, photoluminescence [2], photo-induced electron transfer, hyperpolarizability or magnetic properties [3]. These physical properties can be easily switched on or off by a single electron transfer.

Very recently, we prepared and investigated new molecules that incorporate redox active building blocks into carbon-rich bridges between the terminal iron centers with d^5 and d^6 electronic configurations [4–5]. Physical properties of these new compounds were investigated in regard to their merit to mediate electron transfer and magnetic coupling interactions

[1] Paul, F.; Lapinte, C. *Coord. Chem. Rev.* **1998**, *427*, 178.

[2] Samoc, M.; Gauthier, N.; Cifuentes, M.P.; Paul, F.; Lapinte, C.; Humphrey, M.G. *Angew. Chem. Int. Ed.* **2006**, *45*, 7376.

[3] Paul, F.; Lapinte, C. in *Unusual Structures and Physical Properties in Organometallic Chemistry*; Gielen, M.; Willem, R.; Wrackmeyer, B., Eds.; John Wiley & Sons: London, 2002; p 220.

[4] Lohan, M.; Justaud, F.; Roisnel, T.; Ecochard P.; Lang, H.; Lapinte, C. *Organometallics* **2010**, *29*, 4804.

[5] Miyazaki, A.; Ogyu, Y.; Justaud, F.; Ouahab, L.; Cauchy, T.; Halet, J.-F.; Lapinte, C. *Organometallics* **2010**, *29*, 4628.

Frustrated Lewis Pairs:
Principles and Applications in Organometallic Chemistry

Gerhard Erker

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Non-quenched pairs of bulky Lewis acids and bases ("frustrated Lewis pairs") show interesting new properties. Often cooperative behaviour is observed. This is used in small molecule activation. Both intramolecular and intermolecular frustrated Lewis pairs can often be used for heterolytic dihydrogen activation. Many examples subsequently transfer the resulting proton/hydride pair to specific substrates. This has been used to develop metal-free catalytic hydrogenation reactions of e.g. enamines, silyl enolethers or bulky imines. In this lecture some recent examples of reactions of frustrated Lewis pairs with a variety of small molecules are presented. Frustrated Lewis pairs have also been used in Organometallic Chemistry. They provide very mild conditions for functional group conversions at sensitive organometallic substrates. Some specific examples from ferrocene chemistry and Group 4 bent metallocene chemistry will be discussed.

A Tour of the Simplest Ferrocene Chemistry over 25 Years

Ian Butler

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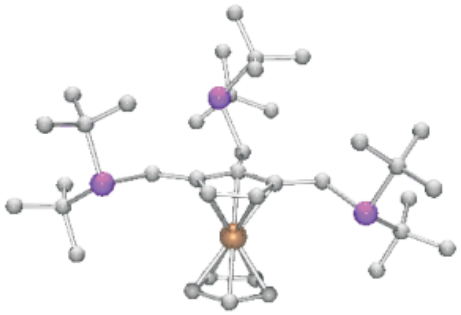
The talk will give a personal perspective on developing simple synthetic methodology for the preparation of substituted ferrocenes, exploring the idea that it takes more time to develop simple synthetic strategies than it does more complicated ones. The focus will primarily be on the development of lithiation as a route to substituted ferrocenes beginning with 1,1'-dilithioferrocene and ending with 1,2-dilithioferrocene. The talk is not intended to be a research seminar but a look at ferrocene chemistry from the perspective of a synthetic chemist looking back over 25 years with personal anecdotes. Applications in the synthesis of ferrocene-based ligands will be discussed together with complementary work carried out with collaborating research groups. Finally an example of the use of bulky ferrocene based ligands such as **1**, in the palladium-catalysed preparation of acrylic intermediates in the Lucite α-process will be used to highlight how the basic synthetic chemistry can be applied to an industrial problem.



1

Strained Ferrocenophanes and Metalloring Analogues - New Reactivity and Utility as Precursors to Functional Metallopolymers

Ian Manners

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This lecture will focus on the synthesis, structures, reactivity and ring-opening polymerization of strained metallorings such as ferrocenophanes and analogous species containing elements such as V, Cr, Ru and Co and also Si, P, Sn, Ni, and Pt [1]. The presence of the metal center allows access to remarkable reactivity that can often also be exploited to prepare functional metallopolymers via ring-opening polymerization [1,2]. Properties and applications of the new polymeric materials containing metal centers such as polyferrocenylsilanes will be noted, for example, in new types of displays, and as block copolymers in nanoscience [3].

[1] Herbert, D.E.; Mayer, U.F.J.; Manners, I. *Angew Chem. Int. Ed.* **2007**, *46*, 5060.

[2] See, for example: (a) Tanabe, M.; Vandermeulen, G.W.M.; Chan, W.-Y.; Cyr, P.W; Vanderark, L.; Rider, D.A.; Manners, I. *Nat. Mater.* **2006**, *5*, 467; (b) Matas Ruiz, I.; Whittell, G.R.; Partridge, B.M.; Holland, J.P.; Haddow, M.F.; Green, J.C.; Manners, I. *J. Am. Chem. Soc.* **2010**, *132*, 279.

[3] (a) Arsenault, A.C.; Puzzo, D.P.; Manners, I.; Ozin, G.A. *Nat. Photonics*, **2007**, *1*, 468; (b) Wang, X.; Guerin, G.; Wang, H.; Wang, Y.; Manners, I.; Winnik, M.A. *Science*, **2007**, *317*, 644; (c) Whittell, G.R.; Hager, M.D.; Schubert, U.S.; Manners, I. *Nat. Mater.* **2011**, *10*, in press.

Oral Presentations

O1	A. Hildebrandt	Chemnitz University of Technology
O2	C. Herfurth	Universität Potsdam
O3	R.F. Winter	Universität Konstanz
O4	D. Siebler	Johannes Gutenberg-Universität Mainz
O5	R. Breuer	University of Siegen
O6	C. Gers	Heinrich Heine Universität Düsseldorf
O7	D. Schaarschmidt	Chemnitz University of Technology
O8	L. Taghizadeh Ghoochany	TU Kaiserslautern
O9	K. Kowalski	University of Łódź
O10	K. Kaleta	Universität Rostock
O11	C. Thoms	Universität Regensburg
O12	A.C. Tagne Kuate	TU Braunschweig
O13	B. Hildebrandt	Heinrich-Heine Universität Düsseldorf
O14	C. Färber	Universität Kassel
O15	K. Rademann	Humboldt-Universität zu Berlin
O16	S. Pandey	Universität Leipzig
O17	M. Gawron	Technische Universität Dortmund
O18	A.D. Russell	University of Bristol
O19	G. Lackner	University Duisburg-Essen
O20	A. Glöckner	TU Braunschweig
O21	A. Korotvička	Charles University Prague
O22	M. Braun	Heinrich-Heine Universität Düsseldorf
O23	D. Weismann	TU Kaiserslautern

Intervalence Charge Transfer in Diferrocenyl Heterocycles

Alexander Hildebrandt, Dieter Schaarschmidt, Heinrich Lang*

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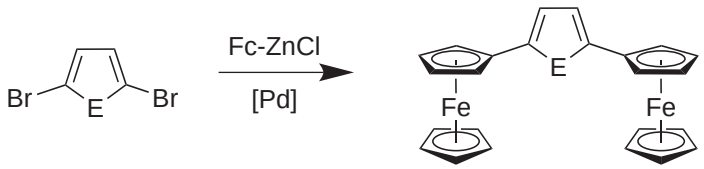
A series of 2,5-diferrocenyl-substituted heterocycles including thiophene, furan and pyrroles were synthesized using Negishi *C,C* cross-coupling reactions. The electronic and electrochemical properties of these compounds were investigated by cyclovoltammetry (CV), square wave voltammetry (SWV), and *in situ* UV-Vis/NIR spectroscopy. The ferrocenyls could independently be oxidized giving two reversible responses for the appropriate diferrocenyl-substituted heterocyclic species. The NIR measurements confirm electronic communication as IVCT absorptions were found in the corresponding monocationic mixed valent systems.



E = S, O, NMe, NPh

A linear relationship between $\Delta E_{1/2}$ and the IVCT oscillator strength f could be shown for the first time in organometallic chemistry. This was possible because the series of molecules exhibit analogous geometries and hence, similar electrostatic properties. This correlation was confirmed by electro- and spectro-electrochemical measurements.

[1] Hildebrandt, A.; Rüffer, T.; Erasmus, E.; Swarts, J.C.; Lang, H. *Organometallics* **2010**, *29*, 4900–4905.

[2] Hildebrandt, A.; Schaarschmidt, D.; Lang, H. *Organometallics* **2011**, *30*, 556–563.

Ferrocenyl Monomers and Controlled Radical Polymerization

Christoph Herfurth,[a] Jens Buller,[a] Jan Weiß,[a] Jörg Bohrisch,[b] André Laschewsky*[,a,b]

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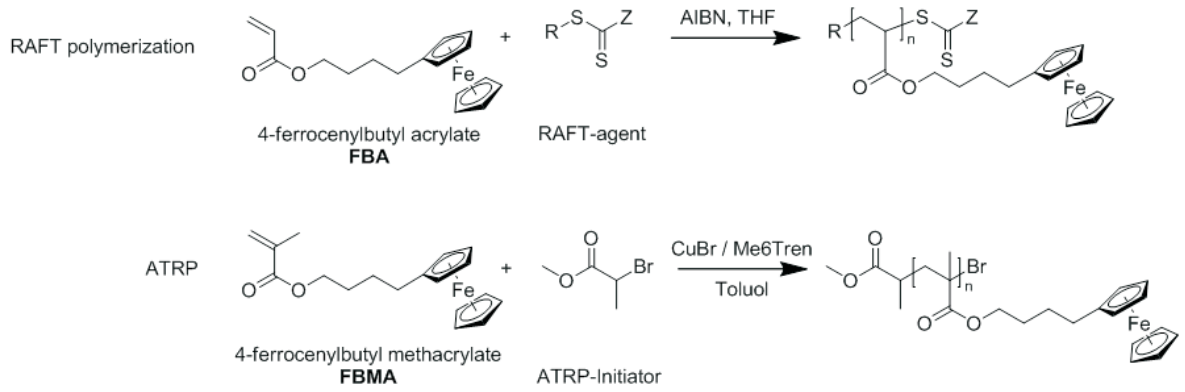
The synthesis of ferrocenyl acrylate and methacrylate monomers and their free radical homo- and co-polymerization were first reported in the 1970s by Pittman and coworkers [1]. However, even then it was noted that the polymerization of these monomers does not always obey to the expected kinetics [2]. With the advent of controlled radical polymerization techniques like atom transfer radical polymerization (ATRP) or radical addition fragmentation chain transfer (RAFT) polymerization, these interesting monomers reappeared in the focus of polymer scientists [3,4].



We synthesized two new ferrocenyl monomers: 4-ferrocenylbutyl acrylate (FBA) and 4-ferrocenylbutyl methacrylate (FBMA). Both were successfully polymerized using free and controlled radical polymerization techniques. However, the RAFT polymerizations revealed unwanted chain transfer reactions taking place during the polymerization. When the monomers were subjected to ATRP, similar problems were encountered. It seems that these difficulties are inherent to ferrocenyl monomers, as will be discussed.

[1] Pittman, C.U.; Lai, J.C.; Vanderpool, D.P. *Macromolecules* **1970**, *3*, 105–107.

[2] Pittman, C.U.; Voges, R.L.; Jones, W.B. *Macromolecules* **1971**, *4*, 291–297.

[3] Sakakiyama, T. et al. *Chem. Letters* **2005**, *34*, 1366–1367.

[4] Shi, M.; Li, A.-L.; Liang, H.; Lu, J. *Macromolecules* **2007**, *40*, 1891–1896.

Relevance of Through-space and Through-bond Pathways for Electronic Coupling in Cyclophanes

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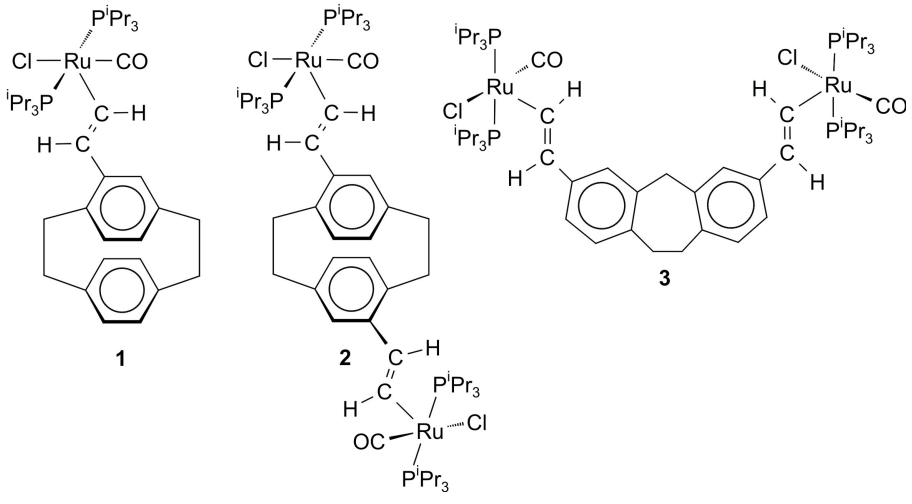
Cyclophanes are important model compounds for studying through-space conjugation between stacked arene rings. Studies on organic derivatives have revealed that electron transfer occurs on timescales faster than or equivalent to the EPR timescale and that through-bond and through-space pathways both contribute to overall delocalization [1–3]. We report here on vinylruthenium substituted cyclophanes which, owing to the spectroscopic labels offered by the {Ru}CH=CH subunits, allow for addressing the issue of intrinsic delocalization down to the fast vibrational timescale. Comparison of the *para*- and the *ortho*-cyclophane **2** and **3** (Chart 1) provides us with the opportunity to estimate the relative contributions of through-bond and through-space pathways to the overall delocalization in these systems.



[1] Wartini, A.; Staab, H.A.; Neugebauer, F.A. *Eur. J. Org. Chem.* **1998**, 1161.

[2] Wartini, A.; Valenzuela, J.; Staab, H.A.; Neugebauer, F.A. *Eur. J. Org. Chem.* **1998**, 139.

[3] Kattnig, D.R.; Mladenova, B.; Grampp, G.; Kaiser, C.; Heckmann, A.; Lambert, C. *J. Phys. Chem. C* **2009**, *113*, 2983.

Biferrocene amino acid: Synthesis, crosslinking and redox chemistry

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[a]*Institute of Inorganic Chemistry and Analytical Chemistry, Duesbergweg 10-14, 55128, Mainz, Germany;* [b]*Institute of Inorganic Chemistry and Analytical Chemistry, Staudingerweg 9, 55128, Mainz, Germany.*

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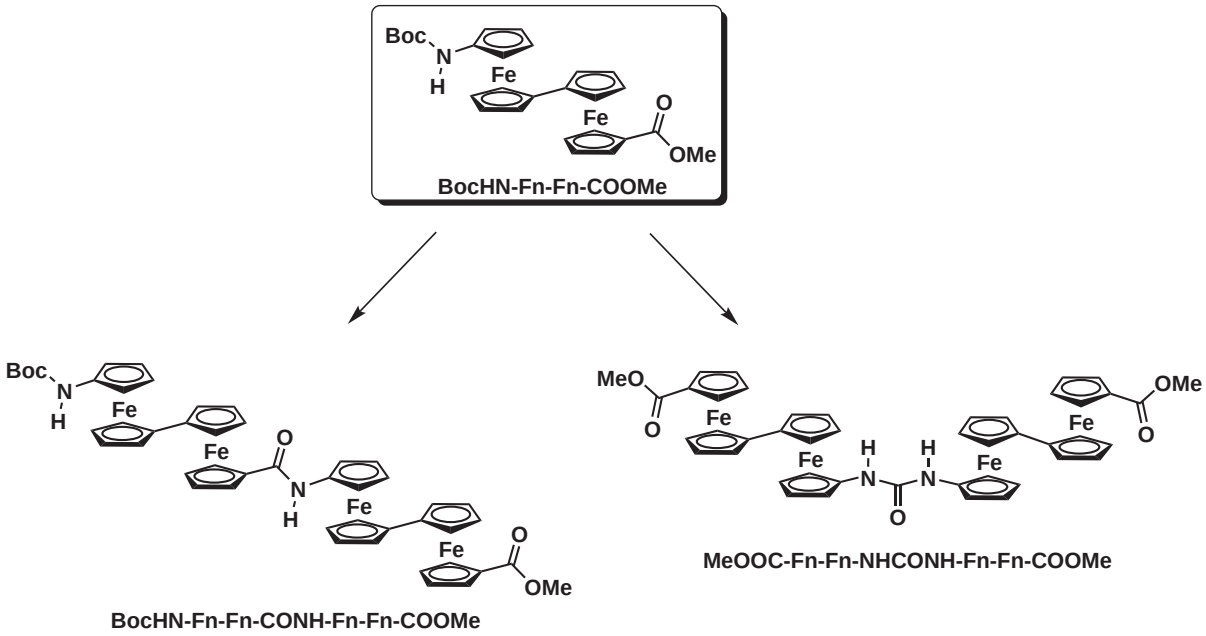
We address a novel donor/acceptor substituted biferrocene system H_2N-Fn-Fn-COOH (Fn = 1,1'-ferrocenylene) as ferrocenylogous amino acid and describe routes to the Boc-protected biferrocene amino acid methyl ester Boc-HN-Fn-Fn-COOMe, to its head-head dimer with ureylene bridge MeOOC-Fn-Fn-NHCONH-Fn-Fn-COOMe and to its head-tail dimer with an amide bridge BocHN-Fn-Fn-CONH-Fn-Fn-COOMe. Site selective oxidations of ferrocene subunits in these biferrocenes and bis(biferrocenes) and the interaction between electronically coupled ferrocene/ferrocenium subunits are investigated. By designing differences in zero-point energies with different bridging types (direct link, amide bridge, ureylene bridge) we aim at site-selective oxidation of individual ferrocene units and influencing the degree of interaction between subunits in oligomers of such building blocks.



[1] Siebler, D.; Förster, C.; Gasi, T.; Heinze, K. *Organometallics* **2011**, *30*, 313–327.

1,1'-Biferrocenylene - can it replace ferrocene ?

Rochus Breuer, Michael Schmittel*

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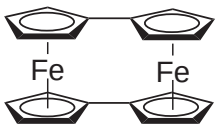
Over the last 60 years ferrocene has been established as "the standard" for various redox applications. Whenever a redox tag in biomedical chemistry [1], a signaling unit in sensorics or a redox-active terminal group on a self-assembled monolayer is needed [2], the ferrocene/ferrocinium couple belongs to the first choice. The undeniable advantages of ferrocene, like the facile access to numerous derivatives, the air-stability and the fully reversible redox chemistry may have contributed to such an outstanding position of ferrocene among all organometallic compounds.

Surprisingly only a few groups explicitly reported about the crucial disadvantage of the ferrocene system: the low stability of the ferricinium cation towards nucleophiles, e.g. hydroxide or chloride [3]. Even in acidic aqueous solution the oxidized ferrocene will be rapidly decomposed, what in fact limits the reliable usage of the ferrocene/ferrocinium couple especially under physiological conditions.

Herein we will report about 1,1'-biferrocenylene (BFD) as a stable redox system, able to serve in long-time applications. Even under strong alkaline aqueous conditions the BFD-monocation demonstrates far superior redox-stability than the corresponding ferrocinium cation, investigated through electroanalytical methods at the SAM/water interface. Furthermore we present spectroelectrochemical data of several BFD-derivatives, proving the mixed-valence class III properties of BFD.



1,1´-Biferrocenylene
(BFD)

[1] van Staveren, D.R.; Metzler-Nolte, N. *Chem. Rev.* **2004**, *104*, 5931.

[2] Abbott, N.L.; Whitesides, G.M. *Langmuir* **1994**, *10*, 1493.

[3] Prins, R.; Korswagen, A.R.; Kortbeek, A.G.T.G. *J. Organomet. Chem.* **1972**, *39*, 335.

A novel synthesis of ynediones: Copper-mediated coupling of in situ generated α-oxo-acid chlorides with terminal alkynes

Charlotte Gers, Eugen Merkul, Janis Dohe, Thomas J. J. Müller*

Heinrich Heine Universität Düsseldorf, Institut für Organische Chemie und Makromolekulare Chemie, Geb. 26.43.00.24, Universitätsstraße 1, 40225, Düsseldorf, Germany.

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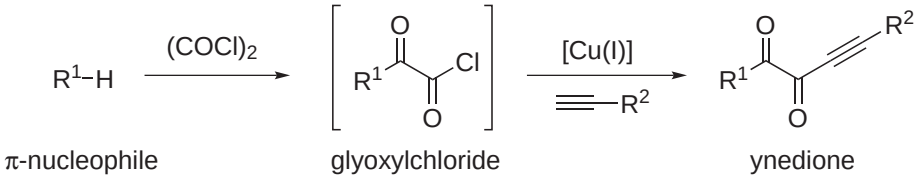
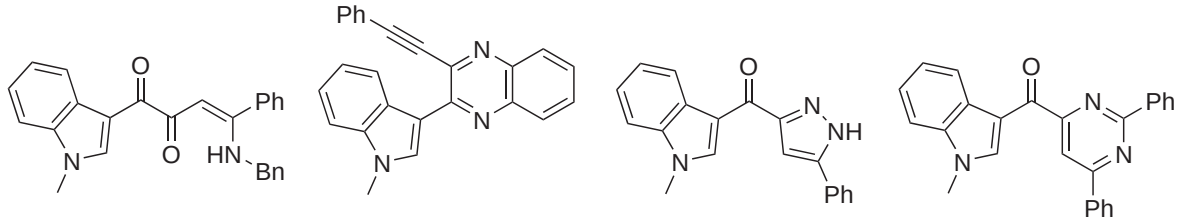
In the past years, we reported different catalytic accesses to generate ynones, which are highly potent building blocks in the organic synthesis of heterocycles. Based on the recent work upon the formation of ynones via a glyoxylation – decarbonylative *Sonogashira* coupling sequence [1], we now report the synthesis of ynediones via a glyoxylation – *Stephens-Castro* coupling sequence [2].



Ynediones are highly electrophilic and offer, due to their *Michael*-acceptor system and dione motif, a variety of possibilities for the synthesis of heterocycles. We were able to show that both functionalities can be adressed in a one-pot fashion with different mono- and binucleophiles, thus leading to the formation of enaminediones, quinoxalines, indoloyl pyrazoles and indoloyl pyrimidines.



[1] Merkul, E.; Oeser, T.; Müller, T.J.J. *Chem. Eur. J.* **2009**, *15*, 5006–5011.

[2] Merkul, E.; Dohe, J.; Gers, C.; Rominger, F.; Müller, T.J.J. *Angew. Chem.* **2011**, Article in Press.

Chiral *P,O*-Ferrocenes as Ligands in the Suzuki-Miyaura Coupling

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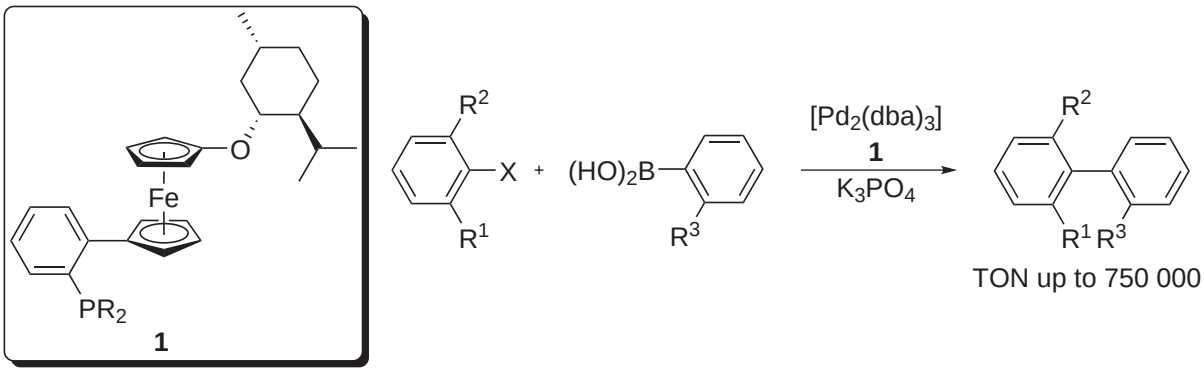
The Suzuki-Miyaura coupling is undoubtedly among the most essential catalytic transformations in organic chemistry; in the last decades there have been major efforts to develop efficient catalysts for this reaction [1]. However, the ability to synthesize sterically hindered biaryls in an enantioselective manner by Suzuki-Miyaura coupling is still a challenge. Catalysts that can perform such transformations under mild conditions are of great interest and will found numerous applications, *e. g.* natural product synthesis or production of pharmaceuticals [2].



Herein we report on the synthesis of chiral *P,O*-Ferrocenes (**1**) starting from enantiopure ferrocenyl ethers [3] and their application as ligands in the Suzuki-Miyaura coupling.

[1] (a) Miyaura, N.; Suzuki, A. *Chem. Rev.* **1995**, *95*, 2457; (b) Suzuki, A. *Proc. Jpn. Acad., Ser. B* **2004**, *80*, 359.

[2] (a) Schaarschmidt, D.; Lang, H. *Eur. J. Inorg. Chem.* **2010**, 4811; (b) Schaarschmidt, D.; Lang, H. DE Patent 10 2010 001 364.1, 2010.

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Novel Ruthenium Catalysts for Transfer Hydrogenation

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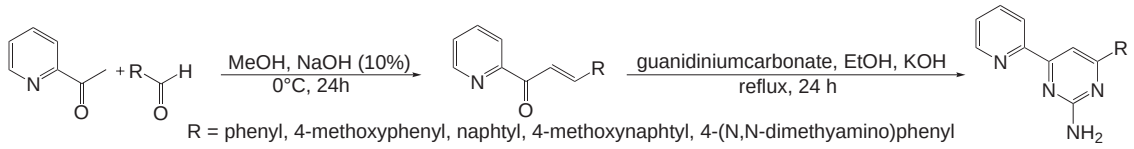
Catalytic transfer hydrogenation of ketons makes accessible a wide range of alcohols, including chiral ones [1]. Under basic conditions and mainly with iPrOH as the solvent, ruthenium(II) complexes turned out to be the most active systems. Thus, a broad variety of different areneruthenium complexes have been investigated for (enantioselective) transfer hydrogenation reactions [2,3].

Since the N-H protons of a 2-aminopyrimidine ligand are slightly acidic, they might be involved in the proton transfer during a keton hydrogenation. We therefore synthesized a series of 2-amino-4-aryl-6-(pyridin-2-yl)pyrimidines and tested the activities of their ruthenium complexes for the transfer hydrogenation of acetophenone in isopropanol.



The corresponding complexes were synthesized from the $[(\eta^6\text{-}p\text{-cymene})RuCl(\mu^2\text{-}Cl)]_2$ and characterized by means of NMR spectroscopy, elemental analysis and single crystal x-ray diffraction. Their catalytic activity for the transfer hydrogenation of the acetophenone was investigated.

[1] (a) Ohkuma, T.; Ooka, H.; Ikariya, T.; Noyori, R. *J. Am. Chem. Soc.* **1995**, *117*, 10417; (b) Wu, X.; Xiao, J. *Chem. Commun.* **2007**, 2449; (c) Blaser, H.-U.; Malan, C.; Pugin, B.; Spindler, F.; Steiner, H.; Studer, M. *Adv. Synth. Catal.* **2003**, *345*, 103.

[2] (a) Ghebreyessus, K.Y.; Nelson, J.H. *J. Organomet. Chem.* **2003**, *669*, 48; (b) Ikariya, T.; Blacker, A.J. *Acc. Chem. Res.* **2007**, *40*, 1300.

[3] (a) Ohkuma, T.; Utsumi, N.; Tsutsumi, K.; Murata, K.; Sandoval, C.; Noyori, R. *J. Am. Chem. Soc.* **2006**, *128*, 8724; (b) Sandoval, Ch.A.; Ohkuma, T.; Utsumi, N.; Tsutsumi, K.; Murata, K.; Noyori, R. *Chem. Asian J.* **2006**, *1*, 102.

Friedel-Crafts reactions of $W(CO)_5$-complexes of azaferrocenes

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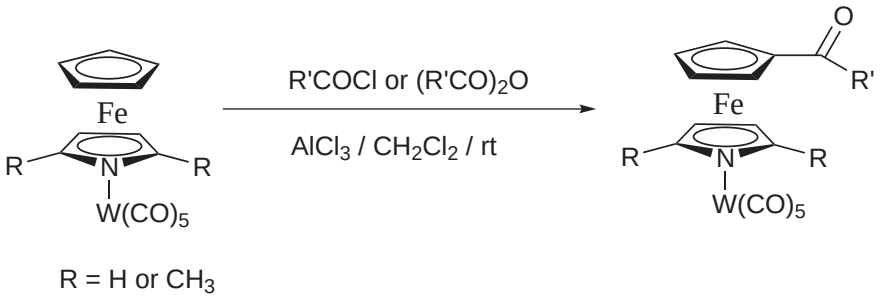
Over the past six decades, the Friedel-Crafts reactions has evolved into an efficient synthetic tool in the chemistry of ferrocene and group 15 heteroferrocenes (phospa- and arsaferrocenes) [1,2]. In contrast, the Friedel-Crafts reaction of azaferrocenes has not been reported for over 40 years. The nucleophilic character of nitrogen atom leads to the formation of unstable *N*-acyl drerivatives instead of expected electrophilic substitution products. Since discovery that the coordination of the neutral $W(CO)_5$ fragment to the azaferrocenes eliminates the electronic influence of the lone pair of nitrogen electrons, protected by the $W(CO)_5$ moiety azaferrocenes were found to easily undergo electrophilic substitution reactions [3,4].



R = H or CH_3

This presentation depicts Friedel-Crafts acylation reactions of azaferrocenes. In addition, the importance of the obtained by "Friedel-Crafts approach" azaferrocene derivatives in biology will be shown [4].

[1] Woodward, R.B.; Rosenblum, M.; Whiting, M.C. *J. Am. Chem. Soc.* **1952**, *74*, 3458.

[2] De Lauzon, G.; Deschamps, B.; Fischer, J.; Mitschler, J.; Mathey, F. *J. Am. Chem. Soc.* **1980**, *102*, 994.

[3] Kowalski, K.; Zakrzewski, J.; Jerzykiewicz, L. *J. Organomet. Chem.* **2005**, *690*, 1474.

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Ferrocenyl Substituted Group 4 Metallacycles

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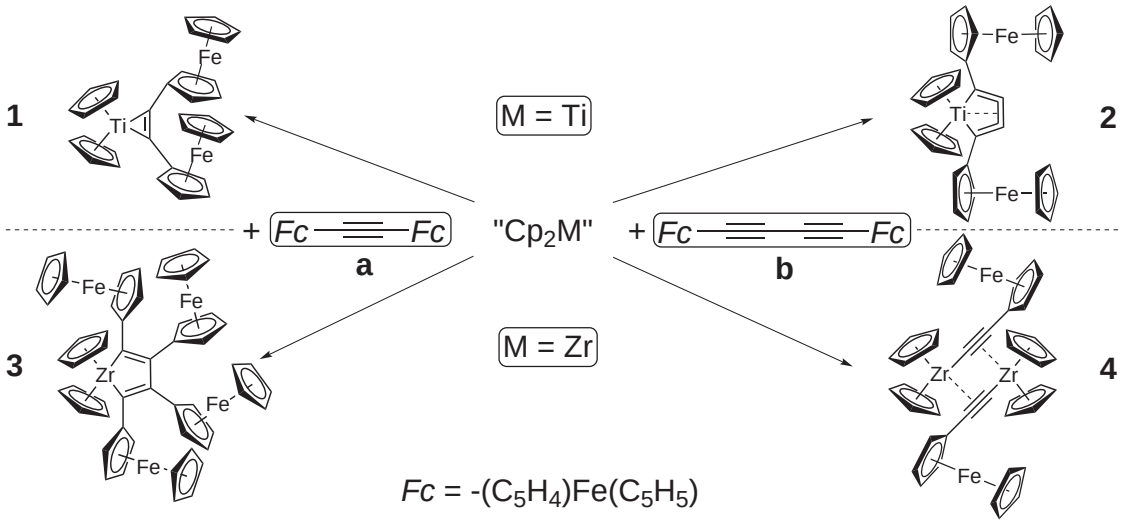
Since the discovery of the sandwich structure of ferrocene in 1952 some aesthetic complexes with this structural element were described up to now, e.g. hexaferrocenylbenzene and a penta-(ferrocenyl)cyclopentadienyl manganese complex in 2006 [1].

We studied the reaction of titanocene and zirconocene precursors with diferrocenylacetylene (**a**) and 1,4-diferrocenyl-buta-2,3-diyne (**b**), respectively, yielding attractive oligocyclopentadienyl complexes.



By a simple ligand addition to the titanocene fragment three (**1**) and five membered metallacycles (**2**) were formed. On the other hand in the reaction of the zirconocene under similar conditions the coupling of two alkynes (**3**) or a C-C bond cleavage (**4**) was observed.

[1] Yu, Y.; Bond, A.D.; Leonard, P.W.; Lorenz, U.J.; Timofeeva, T.V.; Vollhardt, K.P.C.; Whitener, G.D.; Yakovenko, A.A. *Chem. Commun.* **2006**, 2572–2574; and cited references.

Dehydrocoupling of $PH_2BH_2{\cdot}NMe_3$ Induced by Transition Metal Fragments

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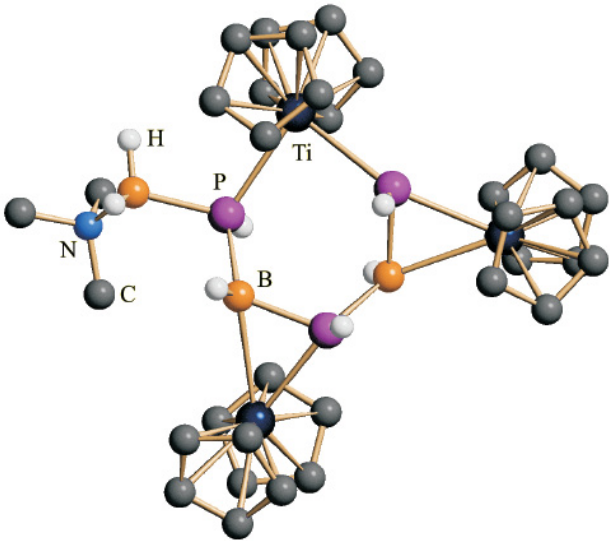
Compounds containing Group 13/15 elements have become very popular in recent years because of their possible use as hydrogen storage materials. The ammonia borane complex $NH_3{\cdot}BH_3$ is of special interest due to its high hydrogen content. However, also phosphorus- and boron-containing compounds play a significant role in the field, as shown by the work of Stephan et al. [1]. We are interested in the reactivity of the Lewis-base-stabilized monomeric compound $PH_2BH_2{\cdot}NMe_3$ (**1**), which has potential use as a hydrogen storage material [2]. We have found that the reaction of **1** with the in situ generated dehydrocoupling reagent $[Cp_2Ti]^{\ddagger}$ led, depending on the reaction conditions, to novel oligomeric compounds (Figure; carbon-bound hydrogen atoms are omitted for clarity).



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(η^5–cyclopentadienyl)(η^7–cycloheptatrienyl)titanium(IV) (Troticene): Selective Lithiation, Phosphane Functionalization, Heterobimetallic Derivatives, Ansa and Ambivalent Complexes

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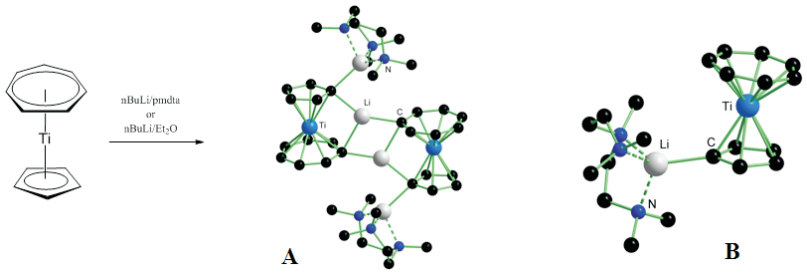
The functionalization of heteroleptic sandwich compounds, such as (η^5–C_5H_5)M(η^7–C_7H_7) (M = group 4–6 transition metals) is, in contrast to the well established chemistry of ferrocene, much less developed. This latency is probably due to the rather poor synthetic methods that allow the selective lithiation of this class of metallocene. In the last decade, our research group has been intensively involved in the chemistry of (η^5–C_5H_5)Ti(η^7–C_7H_7) (troticene) [1]. In this contribution, we will demonstrate that using a mixture of *n*BuLi/pmdta or *n*BuLi/Et_2O and depending of the experimental conditions, the selective lithiation of troticene either at the Cp, Cht or both rings can be quantitatively achieved and the lithiated species characterized in the solid state (see structures **A** and **B**) [2].



These compounds represent precious intermediates for the development of a rich chemistry based on troticene. Important troticenyl derivatives will be presented [2,3].

[1] Tamm, M. *Chem. Commun.* **2008**, 3089–3100.

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[3] Tagne Kuate, A.C.; Mohapatra, S.K.; Daniliuc, C.; Jones, P.G.; Tamm, M. *J. Organomet. Chem.*, Manuscript submitted.

A New *N*-Heterocyclic Carbene Containing a Cationic Metallocene Backbone

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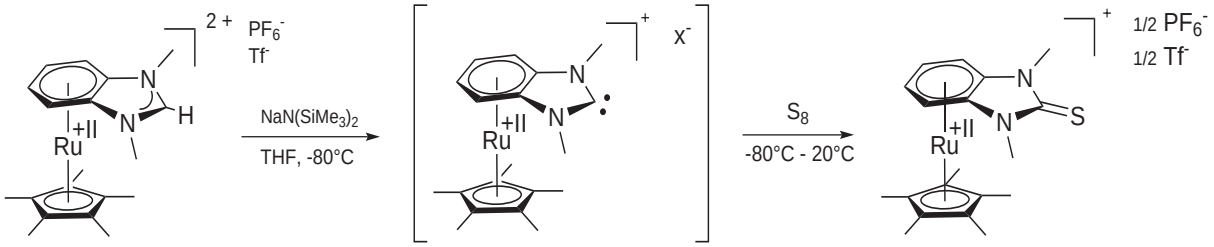
N-Heterocyclic carbene chemistry continues to be an attractive research area. Since the isolation of a free, heteroatomic-stabilized carbene in the early 1990´s by Arduengo et al. [1], a rapid expansion of a hole new research area took place and, although twenty years later, many aspects in carbene chemistry remain uninvestigated. Here, we describe the development of a new cationic *N*-heterocyclic carbene containing an anellated metallocene in the backbone.



There are only few examples of *N*-heterocyclic carbenes in literature in which the carbene center is in a direct conjugation with the electronic system of the metallocene [2–5]. Some aspects of further investigations might be the electronic properties of the new carbene, referring to its potential to be an π-acceptor-ligand, and its catalytic activity in aqueous cross-coupling reactions.

[1] Arduengo, A.J.; Harlow, R.L.; Kline, M. *J. Am. Chem. Soc.* **1991**, *113*, 361.

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Diaminocarbenes and their reactivity towards carbon monoxide; Novel and easy: Instant N-Heterocyclic Carbenes

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Due to their stabilization mode, diaminocarbenes belong to the class of push-push carbenes revealing a four-electron three-centre π-system. The vacant p-type orbital of the divalent carbene centre is involved in this π-system (LUMO). The lone pair of electrons generates the σ-type orbital orientated perpendicular to the empty p-orbital (HOMO). For these reasons, diaminocarbenes are classified as singlet carbenes with high σ-donicity and nucleophilicity, but with a particulary low degree of electrophilicity [1]. Commonly, these carbenes are employed as organocatalysts and ligands for transition-metal chemistry and, in stark contrast to (alkyl)(amino)carbenes, have been judged to be not sufficiently electrophilic to add small molecules like H_2 and CO.

In this context we will describe the unprecedented reactivity of a ferrocene-based, cyclic diaminocarbene and the simplest stable acyclic diaminocarbene, C(N*i*Pr$_2$), towards carbon monoxide [2].

In a second part of this presentation we will introduce for the first time a new class of N-heterocyclic carbenes with exceedingly easy access. These instant carbenes even provide the possibility of tuning the electronic properties of the carbene centre by a deprotonation process in the carbene backbone.

[1] Martin, D.; Soleilhavoup, M.; Bertrand, G. *Chem. Sci.* **2011**, Article in Press, DOI: 10.1039/C0SC00388C

[2] Siemeling, U.; Färber, C.; Bruhn, C.; Leibold, M.; Selent, D.; Baumann, W.; von Hopffgarten, M.; Goedecke, C.; Frenking, G. *Chem. Sci.* **2010**, *1*, 697–704.

FERROCEN assisted formation of noble metal nano-structures at the oil/water interface

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Ferrocen in microemulsions of water and fluorobenzene is preferentially dissolved in the oil phase and directly present at the oil/water-interface. When an acidified solution of Au(III) salts is added to the aqueous phase, the formation of gold nano-structures occurs directly at the interface. The growth and ripening processes of elemental gold at the interface occur all the way up from the cation Au(III) as a precursor material for atoms, dimers, clusters, nanoparticles. After further ripening, a thicker shiny gold film can be observed at the interface via optical reflectivity. Applications for surface functionalizations will be discussed.

As for gold growth mechansisms, definitive determination of core size and size distribution within a nanoparticle sample, requires the application of several techniques in combination with TEM, as has been shown for gold nanoparticle reference materials. Small-angle X-ray scattering (SAXS) has shown promise as a rapid method for precisely determining the size, shape, and polydispersity of a variety of nanoparticles in solution. Of particular interest in previous work, SAXS has been demonstrated to be a fast and precise method for determining the sizes and size distribution of a series of gold nanoparticle reference materials [1]. The in situ application of a wide range of X-ray techniques, using a variety of cells and reactors, has facilitated the study of structural reorganization processes at the nanoscale. In particular time-resolved reaction data have provided insights into intermediate species, reaction kinetics, and nanoparticle growth mechanisms [2].

[1] Bienert, R.; Emmerling, F.; Thunemann, A.F. *Anal. Bioanal. Chem.* **2009**, *395*, 1651–1660.

[2] Polte, J.; Erler, R.; Thunemann, A.F.; Sokolov, S.; Ahner, T.T.; Rademann, K.; Emmerling, F.; Kraehnert, R. *ACS Nano* **2010**, *4*, 1076–1082.

Chiral Polyferrocenes with Phosphorus-Based Backbones

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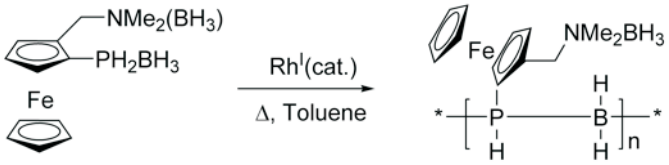
Macromolecules containing chiral ferrocenyl moieties in the main chain or as side groups, which are either directly connected to the main chain or via a spacer, are of special interest. For several applications, incorporation of the ferrocenyl moiety in the main chain is desirable. We have chosen dehydrocoupling reactions (ferrocenyl moiety as side chain) and ring opening polymerization (ROP) (ferrocenyl moiety in backbone) as synthetic methods for the preparation of such polymers.

We have synthesized several chiral monomers, one of which is *N*,*N*-dimethylamino-methylferrocenylphosphine–borane adduct, and a few achiral building blocks, e.g., 1,1'-ferrocenylphosphine–borane adduct.



Catalytic dehydrocoupling reaction of *N*,*N*-dimethylaminomethylferrocenylphosphine–borane adduct resulted in a polymer with a P–B-based backbone (Scheme 1). Introduction of a chiral ferrocenyl moiety should facilitate interesting properties, such as electrical conductivity, magnetic behaviour, thermal stability, unusual optical properties and possibly superconductivity [1], which are significantly different from those of conventional organic polymers. IR, multi-nuclear NMR spectroscopy, XRD, mass spectrometry, and thermal analysis has been chosen for characterization of monomers and polymers and showed satisfactory resemblance with previously reported P-based polymers [2].

[1] *Ferrocenes*; Togni, A.; Hayashi, T., Eds.; VCH: Weinheim, 1995.

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An Asymmetrically Substituted Phosphorus-Containing O,C-Coordinating Ferrocene Ligand and its Organotin Derivatives: Synthesis and Reactivity

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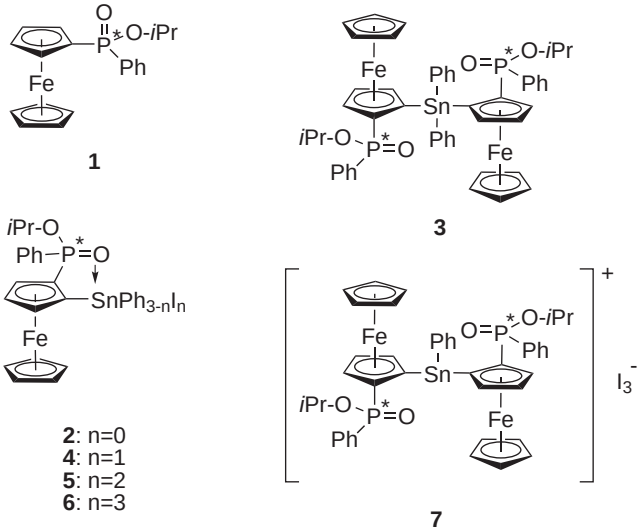
In continuation of our ongoing interest in phosphorus-containing donor ligands [1,2] we report the synthesis of the chiral ferrocene derivative **1**, as its racemate. This ferrocene ligand can easily be metallated by the reaction with *t*-BuLi/KO*t*Bu and, by reaction with triphenyltin chloride and diphenyltin dichloride, respectively, transformed into the diastereomeric organotin compounds **2** and **3**. Compound **2** was functionalized at the tin atom by the reaction with iodine to provide the corresponding organotin iodides **4** – **6**. Most remarkably, the reaction of compound **3** with iodine exclusively gave the trioganostannylium triodide **7** rather than the diorganotin diiodide $[FcP(O)R_2]_2SnI_2$.



All compounds are characterized by *state of the art* analytical methods.

[1] Fischer, J.; Schürmann, M.; Mehring, M.; Zachwieja, U.; Jurkschat, K. *Organometallics* **2006**, *25*, 2886.

[2] Henn, M.; Deáky, V.; Krabbe, S.; Schürmann, M.; Prosenc, M.H.; Herres-Pawlis, S.; Mahieu, B.; Jurkschat, K. *Z. Anorg. Allg. Chem.* **2011**, Article in Press, DOI: 10.1002/zaac.201000387

Studies of the Bond Cleavage Mechanisms for Ring-Opening Reactions of Strained [2]Dicarbaferrocenophanes

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Metal-containing polymers have emerged as an exciting new class of functional materials [1], with a plethora of applications including those in semiconductor and photonic crystal display devices and nanolithography. [n]Metallocenophanes are attractive monomeric targets as precursors to these materials as bond cleavage releases the strain inherent in the ring and provides a thermodynamic driving force for ring-opening and subsequent polymerisation [2]. Several different methods of polymerisation have been developed [3], with mechanistic understanding of these polymerisations essential to end-group control, chain length control, block copolymer synthesis.

In this presentation a series of studies will be described for [2]dicarbaferrocenophanes that aim to help elucidate the mechanism for their thermal ring-opening polymerisation (ROP). In addition, we report the effects of changing the nature and substitution pattern for the C2 bridging species on the location and mechanism of bond cleavage.

[1] (a) Manners, I. *Synthetic Metal Containing Polymers*; VCH: Weinhiem, 2004; (b) Eloi, J.; Chabanne, L.; Whittell, G. R.; Manners, I. *Mater. Today* **2008**, *11*, 28.

[2] (a) Whittell, G.R.; Manners, I. *Adv. Mater.* **2007**, *19*, 3439; (b) Rehahn, M.; Bellas, V. *Angew. Chem. Int. Ed.* **2007**, *46*, 5082.

[3] (a) Herbert, D.E.; Mayer, U.F.J.; Manners, I. *Angew. Chem. Int. Ed.* **2007**, *46*, 5060; (b) Herbert, D.E.; Gilroy, J.B.; Staubitz, A.; Haddow, M.F.; Harvey, J.N.; Manners, I. *J. Am. Chem. Soc.* **2010**, *132*, 1988.

Infiltration study of vertically-aligned Carbon Nanotube forest (va-CNT) with different organic semiconductor materials forming a composite

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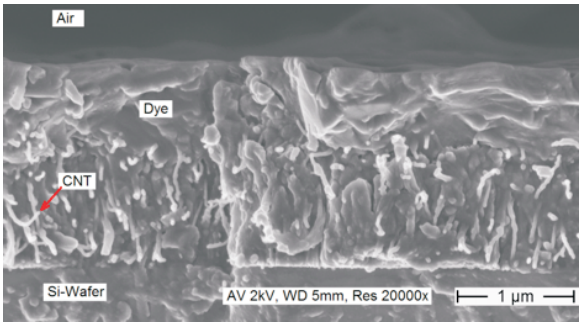
The infiltration of a vertically-aligned Carbon Nanotube forest (va-CNT) with different organic semiconductors is presented. Dyes like ferrocene, P3HT and a copper phthalocyanine derivate are used as filling material. The surface of these va-CNT arrays has been reported to have super-hydrophobic properties [1]. For a liquid phase infiltration adequate solvents were chosen using goniometric contact angle measurements and a heterogeneous wetting regime is expected to take place [2]. During an evaporation process the solved dye precipitates. This precipitated dye bears the CNT, conserves the vertical alignment of the forest and forms a composite material with the CNT. Parameters like dye concentration, amount of solvent, height of the va-CNT and sample size determine the height of the resulting composite material. In order to correlate these parameters FE-SEM analysis was used.



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Open Indenyl — More Than Just Another Pentadienyl Ligand?!

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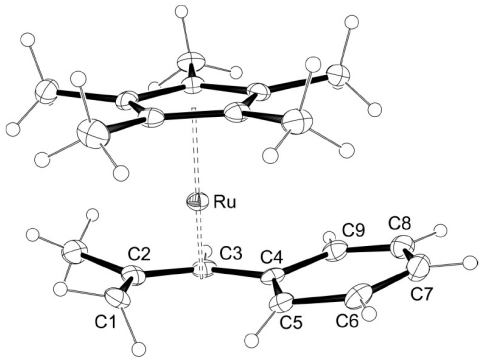
The ubiquitous cyclopentadienyl (Cp) ligand and its derivatives have found numerous applications in fundamental and applied organometallic chemistry. By formally breaking a C-C bond in the Cp ligand, a pentadienyl ligand, often referred to as "open Cp", is obtained. This class of ligands has some unique properties, e.g. η^1, η^3 and η^5 bonding modes are often easier accessible [1]. However, it was noted that the interconversion between different bonding modes appear to be more facile for heteropentadienyl ligands due to a relatively weak C-X π-bond [2]. As part of our interested in pentadienyl systems [2], we have now applied the concept of the indenyl effect to the pentadienyl chemistry and have developed a novel open indenyl ligand. Corresponding complexes of iron and ruthenium have shown that this ligand can switch its hapticity significantly more facile than corresponding heteropentadienyl or "normal" pentadienyl ligands. This enhanced reactivity might eventually allow for the use of the open indenyl ligand in catalytic applications, since a coordination site can be opened up for an incoming substrate.



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Synthesis of Polyaromatics with Ferrocene Substituents

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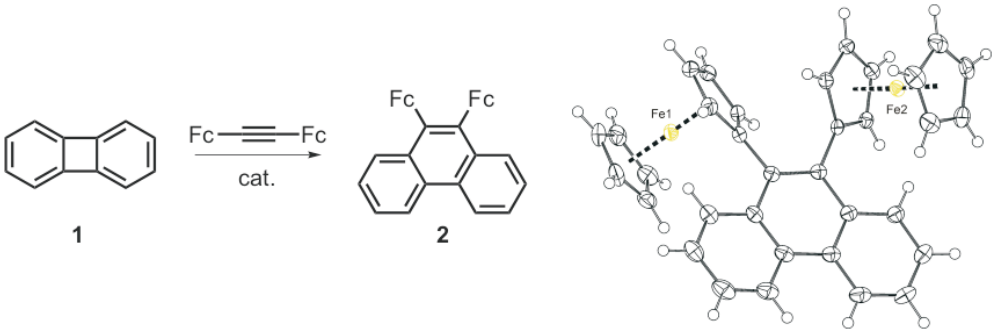
Biphenylene **1** is a relatively stable compound bearing the strained 4-membered carbocyclic ring, which is fused on two benzene rings. Transition metal complexes based on Ir, Rh, Ni, Co, Pd, Pt, Fe compounds with electron rich phosphines can oxidatively add to the C–C bond in biphenylene [1] to create dibenzometallacyclopentane intermediates, which undergo insertion of unsaturated compounds to give rise to phenanthrene derivatives.

We found that catalytic systems based on $[IrCl(cod)]_2$ or $[RhCl(cod)]_2$ and simple bidentate phosphines (e.g. dppe) were also able to create the metallacyclopentane intermediates. The formed metallacycles reacted not only with alkynes, but also nitriles to give the corresponding substituted phenanthrenes and 9-azaphenanthrenes. Gratifyingly, the reaction proceeded also with sterically hindered alkynes such as those bearing the ferrocene moiety. As a typical example may serve preparation of 9,10-diferrocenylphenanthrene **2**.



1 2

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Electron Poor NHC-Ligands: A Five-Membered N,N'-Diamidocarbene

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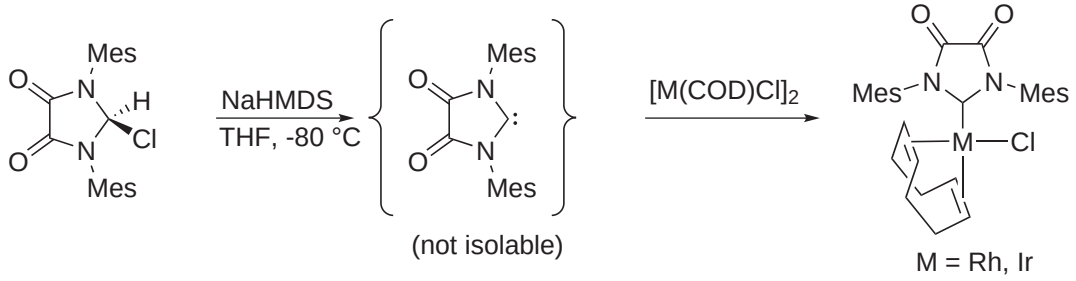
Since their isolation by Arduengo [1] in 1991, N-heterocyclic carbenes (NHCs) have found widespread and spectacular applications as ligands in transition-metal catalysis [2] and as organocatalysts [3]. In addition to application, understanding and modifying the electronic structure of NHCs is an attracting field of current research. The net donor properties of NHCs have been modified, for example, by introduction of electron releasing or withdrawing groups to either the N-bonded aryl groups or the C4 and C5 atoms of imidazol-2-ylidene rings [4]. In addition to the typical NHC-behaviour as nucleophilic ligands towards transition metal fragments, some π-acceptor character was also observed for some of these carbenes [6]. In contrast to a very recent study by Roesler [7], we were able to isolate and examine the reactivity and electronic properties of a new type of NHC ligand with an oxalamide backbone.



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Dinitrogen Activation with Cyclopentadienyl Complexes

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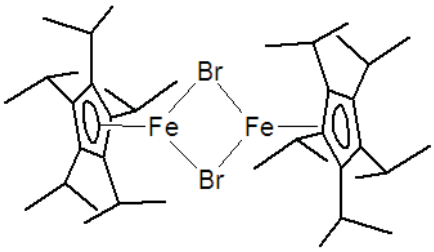
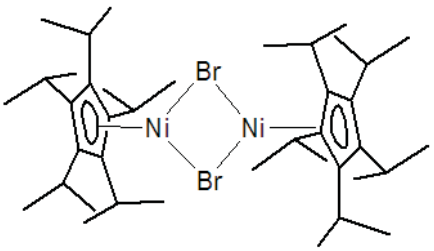
In the last three years we established the complexes of **1** and **2** using the very bulky pentaisopropylecyclopentadienide (^{5}Cp) [1]. Reducing these complexes with Na_3Sb_7 in the presence of nitrogen we obtain green crystals. Analytic and spectroscopic characterization shows a nitrogen containing dinuclear complex.

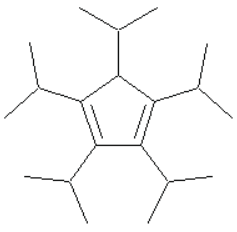


1

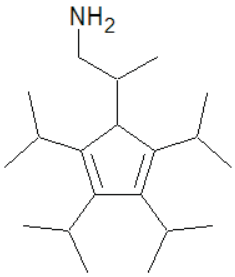


2

A pentane solution of the nitrogen complex reacts with dihydrogen at room temperature and ambient pressure with a color change of the reaction mixture from green to brownish red. After hydrolysis we obtain a mixture of the ligand **3** and the aminated species **4**. In case of the iron complex we find a ratio of 50:50, using the nickel complex we find a ration of 70:30.



3



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Poster Presentations

P1	T. Arnold	Universität Würzburg
P2	J. Mies	Universität Würzburg
P3	N. Krauße	Leibniz Universität Hannover
P4	G. Werner	Leibniz Universität Hannover
P5	Y. Melomedov	Johannes Gutenberg-University
P6	J.R.F. Pritzwald-Stegmann	Universität Leipzig
P7	D. Schmid	Eberhard Karls Universität Tübingen
P8	F. Justaud	CNRS-Université de Rennes 1
P9	G. Lackner	University Duisburg-Essen
P10	K. Wójcik	Chemnitz University of Technology
P11	A. Alrawashdeh	Chemnitz University of Technology
P12	S. Heider	Chemnitz University of Technology
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P17	K. Chen	University of Siegen
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P20	S. Nalchigar	Technische Universität of Kaiserslautern
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P23	P. Mücke	Universität Konstanz
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P26	M. Lohan	Chemnitz University of Technology
P27	B. Milde	Chemnitz University of Technology
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P1

Synthesis and structure of distanna-[2]metallocenophanes

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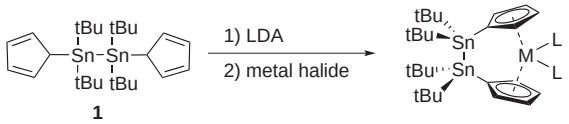
The first distanna-[2]ferrocenophane was published by Herberhold and co-workers in 1996 and the reactivity towards platinum complexes, a number of alkynes and group 16 elements is well established [1,2]. Recently, we reported on the synthesis of the first distanna *ansa* half-sandwich complexes of molybdenum and tungsten, which show analog reaction behavior as the aforementioned compound [3].

Until now, further distanna-[2]metallocenophanes, especially of early transition metals, are not published. Due to the fact that dilithiated metallocene precursors of early transition metals are not feasible, a new distanna ligand bearing two cyclopentadienyl-rings is needed. For this purpose, distannan **1** was prepared by treating Cl*t*Bu$_2$Sn–Sn*t*Bu$_2$Cl with Na[η^1-C$_5$H$_5$]. Dilithiation of **1** and subsequent reaction with suitable metal halides lead to the formation of new distanna-[2]metallocenophanes.



We now present the synthesis and characterization, as well as the crystal structures of the first group 4 and 6 distanna-[2]metallocenophanes.

Our main focus is put on the reactivity of the Sn–Sn bond towards insertion reactions. In particular, we are interested in the intramolecular insertion of the metal center into the Sn–Sn bond as already demonstrated for a disila-[2]metallocenophane [4].

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P2

Synthesis, Structure and Reactivity of stanna-bridged *ansa*-halfsandwich complexes of Group 8 Metals

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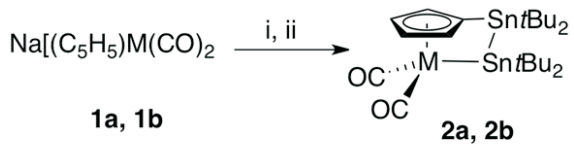
In contrast to *carba*–bridged *ansa*–halfsandwich complexes, which have been intensivly studied over the past decades [1], the knowledge of other main group elements as briding moieties is rather limited. We present the synthesis and characterization of the first stanna-bridged *ansa*-halfsandwich complexes of iron and ruthenium. These compounds exhibit high ring strain within the *ansa*-bridge, which is the key factor for the insertation of elemental chalcogens. Furthermore, late transition metal complexes react with the bridging moity by an oxidative addition [2–3].



i: $Sn_2tBu_4Cl_2$, THF, –78°C
ii: LDA, THF, –78°C
M = Fe, Ru

Their propensity to undergo thermal or catalytical ring-opening polymerisation reactions is of considerable interest for further experiments.

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P3

Synthesis of Ferrocene-based Molecular Wires

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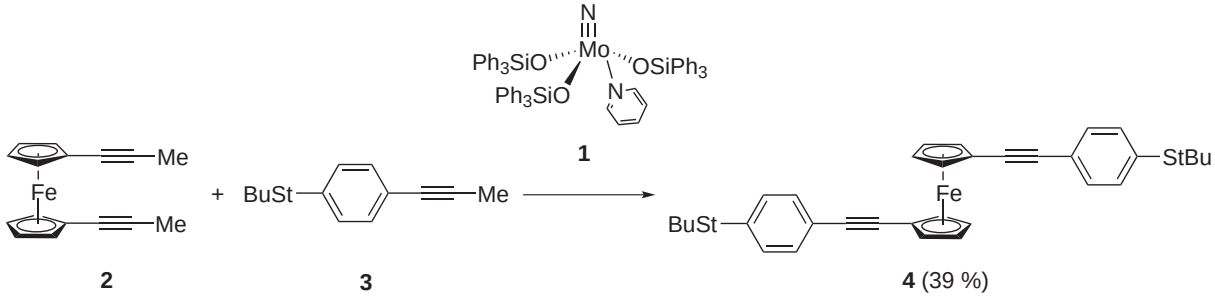
Molecular wires of the oligo(phenylene ethynylene) (OPE) type have rigid structures with fixed molecular lengths. To introduce limited conformational flexibility we are interested in replacing some 1,4-phenylene units by 1,1'-ferrocenylidene groups. Different molecular wires with two or three ferrocene units were obtained via Sonogashira coupling reaction or Negishi coupling reaction [1,2].

In search for different tools for the construction of the key elements of molecular wires we considered alkyne cross metathesis to be of interest. Catalyst **1** [3] was used in this field. The reactions were carried out in the microwave reactor.



We anticipate that manganese-catalyzed oxidative cross coupling reactions may be useful for the synthesis of ferrocene-based molecular wires [4].

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P4

The first anionic thia-Fries rearrangements at ferrocene: Extremely high interannular stereoinduction between cyclopentadienyl ligands

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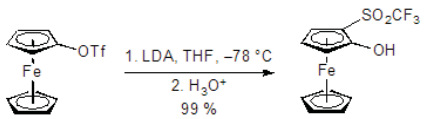
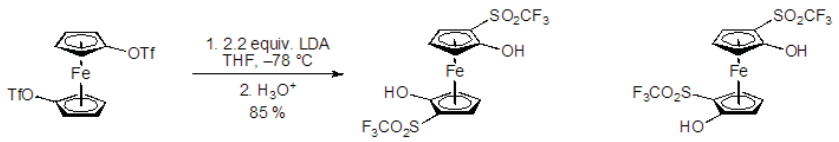
Upon *ortho* metallation (aryltriflate)tricarbonylchromium complexes do not undergo triflate elimination with formation of (aryne) species, but react in an anionic thia-Fries rearrangement with formation of 2-(trifluormethylsulfonyl)phenol complexes [1], presumably as a result of the electron withdrawal exerted by the $Cr(CO)_3$ group [2]. This result gave rise to try the reaction with the more electron rich ferrocene system with the perspective to obtain ferrocyne or ferrocenediyne. However, treatment of ferrocenyl triflate (**1**) with LDA gave in an instantaneous reaction at –78 °C (2-trifluoromethylsulfonyl)ferrocenol (**2**) as the result of an anionic thia-Fries rearrangement, the first case of this reaction at a five membered ring.



1 2

Even more surprising, 1,1'-ditriflate **3** reacted twice in the same way with full diastereoselectivity: This reaction constitutes a very rare case of an extremely high transannular stereoinduction in a ferrocene system [3].



3 **4** *meso* **5** *rac* not formed

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P5

Artificial Photosynthetic Reaction Centers with Ferrocene as Primary Electron Donor

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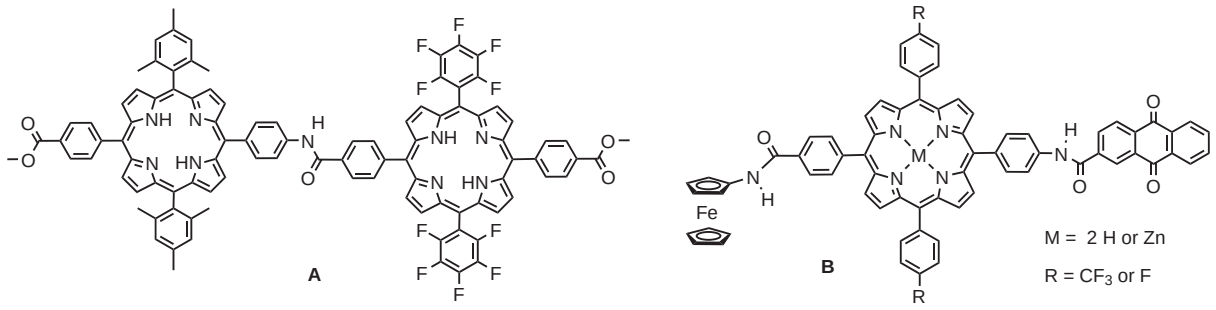
Synthetic porphyrins in redox-active dyads and triads are very useful in understanding porphyrin-based energy and electron transfer processes in photosynthesis [1,2].

With *trans*-AB_2C-tetraphenylporphyrin amino acids as building blocks and amide connectors a series of porphyrin dyads designed to facilitate vectorial interporphyrin energy has been synthesized and studied using absorption and emission spectroscopy. Electron donating (e.g. mesityl) and electron withdrawing substituents (e.g. pentafluorphenyl) were combined in porphyrin dyads **A** and their electrochemical and optical properties were investigated. DFT calculations were employed to rationalize the experimental results.



Electron donor (ferrocene) and electron acceptor moieties (quinones) were attached to the porphyrine core by sequential amide coupling (**B**). The electrochemical and optical behaviour of these redoxactive multifunctional systems were investigated by voltammetric analysis and absorption and emission spectroscopy.

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P6

Novel Ferrocenyl Phosphine Precursors for the Synthesis of New Hybrid Materials

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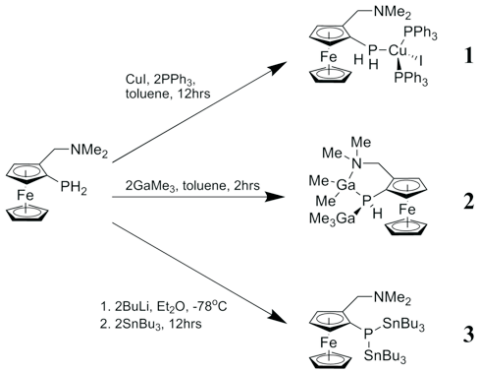
Recent advances in technology demand extraordinary properties from materials which traditional materials, such as polymers and ceramics, cannot provide. This has spurred the development of advanced hybrid materials which combine the best attributes of different worlds into one system. As part of a continuing investigation into the development of new smart molecules for use as building blocks for hybrid materials, a series of ferrocenyl phosphine compounds have been synthesised as precursors.

The copper(I) complex **1** was synthesised from a combination of copper(I) iodide, triphenylphosphine and (*N*,*N*-dimethylaminomethyl)phosphanylferrocene under mild conditions. The treatment of (*N*,*N*-dimethylaminomethyl)phosphanylferrocene with one mole of trimethylgallium results in the formation of an adduct which upon the addition of a second mole of trimethylgallium forms **2** via the elimination of methane. In addition to gallium, organyl tin compounds have been treated with the appropriate starting materials to form stannyl functionalised ferrocenyl phosphine such as compound **3**, other related compounds will also be presented. Compounds **1**, **2** and **3** will be used for the formation of well-defined, *in situ* functionalised, inorganic/organometallic building blocks which can be used for the preparation of novel hybrid materials through the bottom-up approach. The strategies currently under investigation to form other precursors will also be discussed.



P7

Synthesis and Characterisation of Imidazolium Salt Substituted Metallocenes

Dominic Schmid,[a] Erik Johnsen,[b] Birgit Monsler,[b] Frank Rominger,[b] Doris Kunz*,[a]

[a]*Institut für Anorganische Chemie, Eberhard Karls Universität Tübingen, Auf der Morgenstelle 18, 72076 Tübingen; Germany;* [b]*Organisch-Chemisches Institut, Ruprecht-Karls-Universität Heidelberg, Im Neuenheimer Feld 270, 69120 Heidelberg, Germany.*

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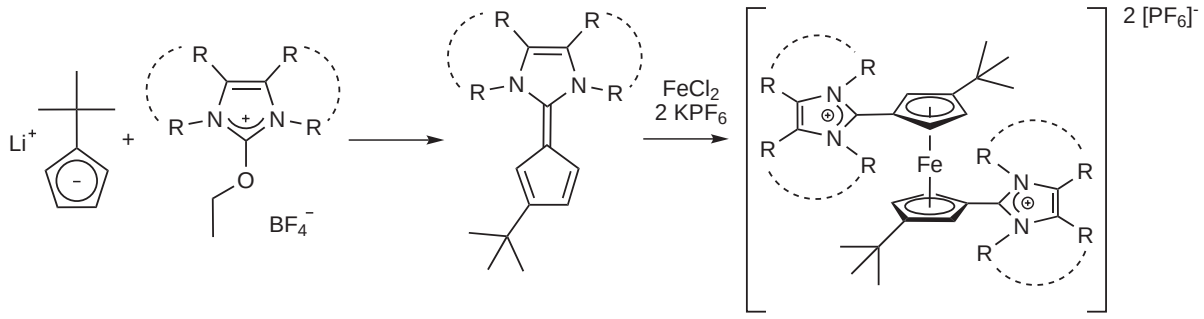
N,*N*-Dimethylaminofulvenes (**3**) show an elongated exocyclic double bond and can be converted to dicationic $FeCp_2$–derivatives at elevated temperatures [1]. Imidazoline-derived fulvenes prepared from lithiumcyclopentadienides (**1**) and ethoxyimidazolium tetrafluoroborates (**2**) show the highest ylidic character of all known 6,6-diaminofulvenes [2]. This is displayed in the extraordinary long exocyclic double bond of 1.430 Å. Therefore these fulvenes exhibit cyclopentadienyl anion-like reactivity, namely, protonation to cyclopentadienes and reaction with Fe(II) chloride to Cp-substituted 2-imidazolium ferrocenes (**4**) already at room temperature.

Similar results are achieved with dipyrido anellated imidazoline-derived fulvenes prepared from **1** and **2**. It is expected that they will show an even longer exocyclic "double" bond due to an enhanced stabilization of the imidazolium character by the aromatic dipyrido backbone [3].



1 **2** **3** **4**

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P8

Novel Sterically Crowded 2,2'-Bipyridine Containing Two "(η^2-dppe)(η^5-C_5Me_5)Fe-C≡C-" Redox-Active Units: Synthesis, Properties and Reactivity with Copper(I) Complexes

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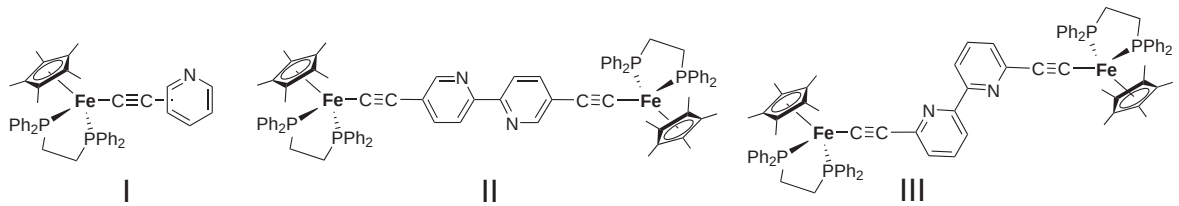
Judicious spatial or topologic arrangements of redox-active end groups can lead to molecular architectures presenting unique properties for information storage or information processing at the molecular level [1–2]. We recently prepared and investigated redox-active metalloligands **I** and **II** which incorporate the "(η^2-dppe)(η^5-C_5Me_5)Fe-C≡C-" unit stable both in the Fe^{II} and Fe^{III} oxidation states [3–4].



I II III

In this contribution we report the synthetic access, characterization, and redox properties of the metallo-ligand **III**. Reactions of compound **III** with copper(I) complexes will be also depicted.

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P9

Infiltration of vertically-aligned Carbon Nanotube forest

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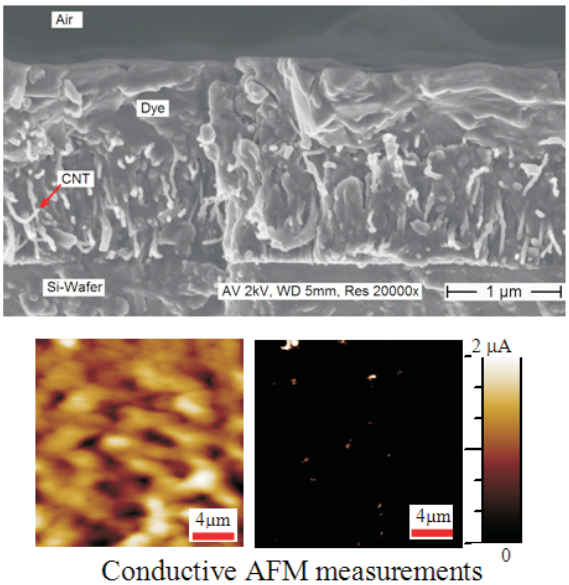
The infiltration of a vertically-aligned Carbon Nanotube forest (va-CNT) with different organic semiconductors is presented. Dyes like ferrocene, P3HT, or a copper phthalocyanine derivate are used as filling material. For a liquid phase infiltration adequate solvents were chosen using goniometric contact angle measurements and a heterogeneous wetting regime is expected to take place [1]. During the evaporation process the solved dye precipitates and bears the CNT. That process conserves the vertical alignment of the forest. The infiltration properties were investigated with FE-SEM analysis. Furthermore, the electrical properties of the resulting composite were studied with conductive AFM analysis.



Conductive AFM measurements

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P10

Cyclopentadienyl Iron-Bismuth Compounds — Synthesis, Structure and Reactivity

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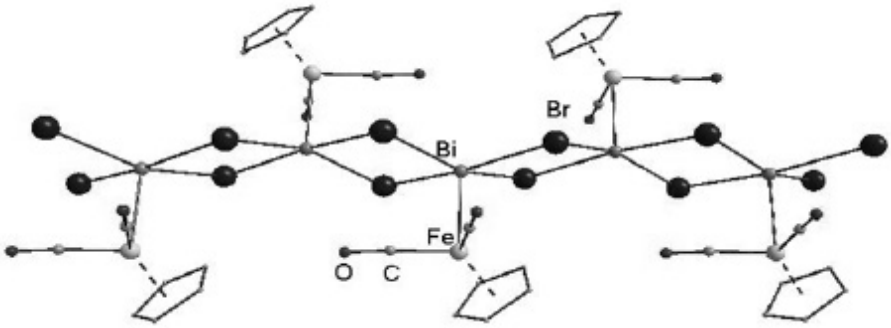
Over the last decades there has been considerable interest in the coordination chemistry of bismuth with transition metals which is based on the often observed unusual coordination behaviour of strongly Lewis-acidic bismuth compounds [1]. Currently, the "green" element bismuth is also attracting growing interest with regard to applications in medicine, materials science and catalysis [2]. Among the heterometallic bismuth transition metal complexes those with iron belong to the most intensively studied examples. Cyclopentadienyl iron-bismuth compounds such as [{$(C_5H_5)(CO)_2Fe$}$BiCl_2$] were reported as early as 1971 [3], but detailed structural analyses, e.g. on [{1,3-$^tBu_2$-$C_5H_3(CO)_2Fe$}$BiCl_2$], are more recent [4]. Over the last years, we have also contributed to the knowledge about structure and reactivity of this interesting class of compounds [5]. Here we present the synthesis, structure and reactivity of cyclopentadienyl iron compounds of the type [{$Cp^y(CO)_2Fe$}BiX_2] (Cp^y = C_5H_5, 1,3-$^tBu_2$-C_5H_3, C_5Me_5; X = Cl, Br, I).



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P11

New Biaryl Phosphine Ligands in Palladium Catalyzed Suzuki Cross-Coupling Reaction.

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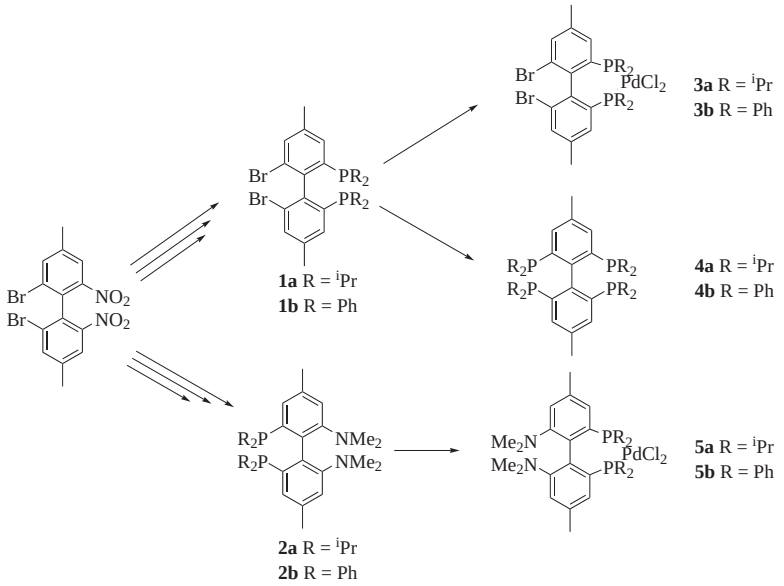
In the early studies most catalysts for the Suzuki cross coupling reaction employed triarylphosphine ligands [1]. More recently, new 2-monophosphine and 2,2'-bisphosphine biaryles have been studied, as supporting ligands they dramatically improve the efficiency and selectivity of Pd(II) catalyzed cross-coupling reactions [2–3]. We are currently investigating 2,2'-bisphosphinebiphenyls that are decorated with bulky substituent in the 6,6'-position (Scheme 1). In contrast to most of the known system employing 2,2'-bisphosphinebiaryl ligands; the most stable conformer of the resulting Pd(II)/Pt(II) complexes are non C_2-symmetric but interchange via a C_2-symmetric intermediate between two C_1-symmetric symmetry related conformers.



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P12

Synthesis of Transition Metal Complexes with Tuneable N6-Coordination Sphere

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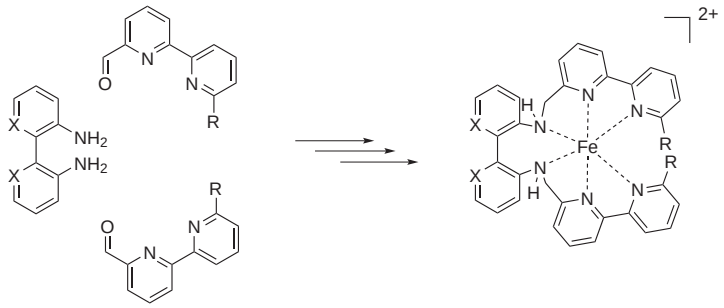
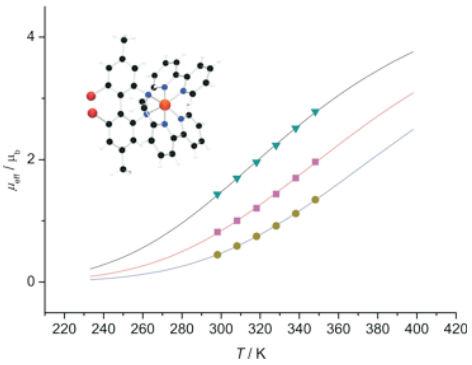
The properties (redox potential, magnetism or colour) of transition metal complexes can be influenced by choice of appropriate ligands. We have gained access to a series of polyamine-pyridyl compounds which feature a hexadentate coordination environment. Those easily accessible and stable amines are the basis for the construction of iron(II) complexes, that either show Spin-Crossover (SCO) behaviour or exist only in high-spin configuration, depending on the substituion pattern.



The ligands of the shown complexes exhibit an AB_2-structure, which is based on a diamine and two aldehydes (Figure 1). Thereby versatile substitution patterns are feasible. Peculiarly interesting is the change of the corresponding transition temperature $T_{1/2}$ for the spin transition upon variation of the functionalities X and R (Figures 1 and 2) [1].



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P13

1,1'-Diaminoferrocene as an unusual N,N'-bridge for bis(oxamato) complexes

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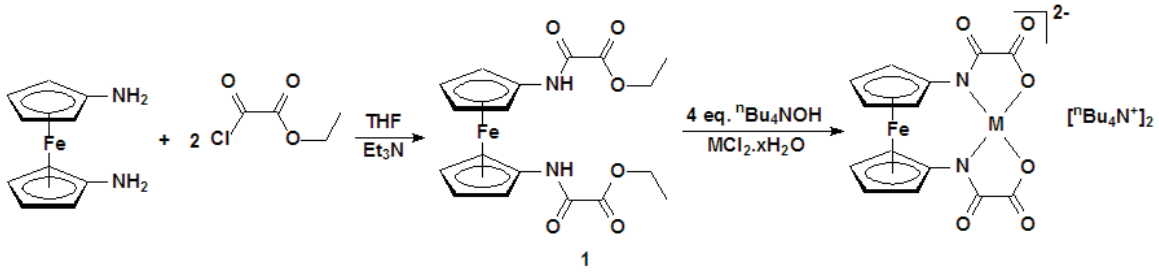
N,N'-bridged bis(oxamato) complexes have been already shown as useful starting materials for the syntheses of polymetallic transition metal complexes due to their flexidentate properties [1,2]. The polymetallic complexes obtained thereby are valuable materials for the study of magnetic properties with respect to the magnetic superexchange [3].

So far, these polymetallic bis(oxamato) complexes did not include any functionality which allows oxidation and reduction, respectively, and thus an electrochemically induced change of the magnetic properties. In a first study 1,1'-Diaminoferrocene has been synthesized according to the literature [4] and was used according to Scheme 1 for the synthesis of novel bis(oxamato) complexes via compound **1**. The behaviour of **1** against the treatment with four equivalent of OH^- and the *in situ* addition of transition metal salts will be shown together with the solid state structure of isolated materials. In addition the results of cyclovoltammetric measurements of obtained complexes will be presented and discussed.



1

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P14

Synthesis, NMR-Spectroscopic Characterization and Structural Survey of a New Class of Ferrocene Containing Cobalt Hydrides

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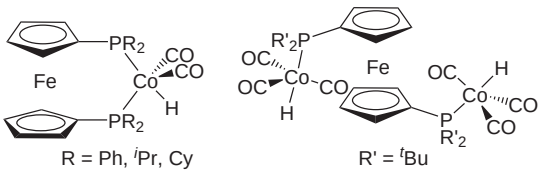
Currently, there is intense research in the synthesis, structure, bonding and reactivity of transition metal hydride compounds [1]. Transition metal hydride species are often involved in small-molecule activation [2]. Sustainable elements like cobalt are more and more brought into focus in this growing field [3,4].

The synthesis provides access to a new class of ferrocene containing cobalt(I) hydrides. A series of three neutral heterodimetallic cobalt(I) hydride complexes $[CoH(dpf)(CO)_2]$ where dpf are the diphosphinoferrocenes 1,1'-bis(diphenylphosphino)ferrocene (dppf), 1,1'-bis(di*iso*propylphosphino)ferrocene (dippf) and 1,1'-bis(dicyclohexylphosphino)ferrocene was synthesized and characterized by different NMR-spectroscopic methods but also by X-ray diffraction showing the first examples of cobalt hydrides containing a ferrocene backbone. Also the first example of a ferrocene-bridged trinuclear cobalt dihydride complex $(\mu\text{-dtbpf})[CoH(CO)_3]_2$ was obtained using the bulky 1,1'-bis(di*tert*butylphosphino)ferrocene (dtbpf) as ligand.



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P15

Copper(I) Complexes with Quinonoid Ligands: Unusual Bonding Situations and Valence Tautomerism

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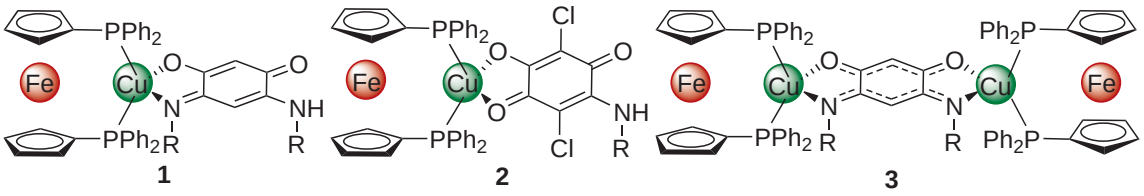
Reaction of N,N´-di-*n*-butyl-2-amino-5-alcoholate-1,4-benzoquinonemonoiminium $\mathbf{H_2L^1}$, or 2,5-dichloro-3-((2,6-di*iso*propylphenyl)amino)-6-hydroxycyclohexa-2,5-diene-1,4-dione $\mathbf{H_2L^2}$ with $[\{(dppf)Cu\}_2(\mu\text{-}Cl)_2]$ (dppf = 1,1´-bis(diphenylphosphino)ferrocene) led to the formation of the heterodinuclear complexes $[(dppf)(Cu\mathbf{HL^1})]$ (**1**) [1], $[(dppf)(Cu\mathbf{HL^2})]$ (**2**) [3] and the heterotetranuclear complex $[\{Cu(dppf)\}_2(\mu\text{-}\mathbf{L^1})]$ (**3**) [2], respectively. The crystal structures of **1** and **3** were determined by X-ray diffraction and show distorted tetrahedral coordination for the Cu(I) centres in both complexes. The dinuclear complex **3** shows the $6\pi + 6\pi$ form of $\mathbf{L^1}$ that also exists in the free ligand and a more localized π-system in **1** [1,2].



Cyclic voltammetry of the complexes showed various redox processes. Monooxidation of **1** and **3** led to EPR-spectra that show ligand radicals bound to Cu(I) [1,2]. Temperature-dependent EPR-measurements of the one-electron-oxidised form of **2** show valencetautomeric behaviour between $[Cu^{I}(\mathbf{HL^{2\cdot}})]^+$ and $[Cu^{II}(\mathbf{HL^2})]^+$ [3]. UV/Vis/NIR-spectroscopy (**1**) and -spectroelectrochemistry (**2, 3**) will be reported [1–3].

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P16

Synthesis, Structure and Magnetic Properties of Complexes of the Type $[CpME(SiMe_3)_2]_2$ (M = Cr, Mn; E = P, As)

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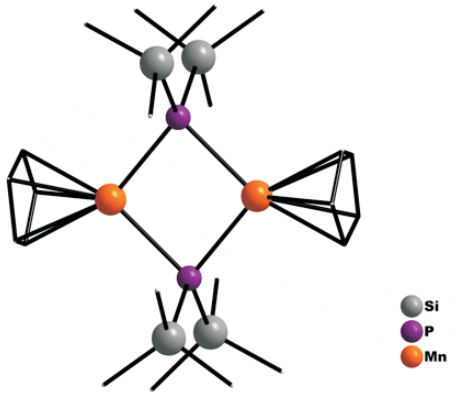
Manganese cluster compounds, particularly complexes containing oxo ligands, are of special interest because of their magnetic properties and potential applications as single molecule magnets. Similar clusters of manganese with N-containing ligands present interesting properties. Although a wide range of manganese(II)-amido, –imido and –pyrimidino [1] complexes is known, there are only few examples for the coordination of the heavier group 15 elements to manganese [2]. Hence, their chemistry and properties, specially magnetic properties are little known.

Herein we report the nucleophilic substitution reaction of Cp_2M (M = Cr, Mn) and $[LiE(SiMe_3)_2 \cdot n(thf)]$ (E = P, As) that leads to $[CpME(SiMe_3)_2]_2$ (M = Cr, Mn; E = P, As), which contains a M_2E_2 four-membered ring as central unit. The synthesis, structure, spectroscopic characterisation and magnetic properties will be presented.



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P17

Ratiometric recognition of polysulfonate anions based on electroactive biferrocenylene-SAMs in biological buffer solution

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Due to the lower oxidation potential (BFD/$BFD^{+\bullet}$ –0.28 V vs. Fc/$Fc^{+\bullet}$) [1] and better stability, biferrocenylene (BFD) [2] is highly suitable to be used as an electroactive probe in the field of sensor. Herein, we report the preparation of electroactive self-assembled monolayers (SAMs) on gold substrate starting from BFD-thiol hybrid structures and their analysis by cyclic voltammetry. The BFD-SAMs can quantitatively detect sodium polystyrene sulfonate in the Tris-buffer solution by electrostatic and hydrophobic interaction. With the addition of the polyanion, a new cathodically shifted peak appeared in the reduction. The ratio of the new peak to the old peak showed a good linear relationship with the logarithm of the concentration of the polyanion.

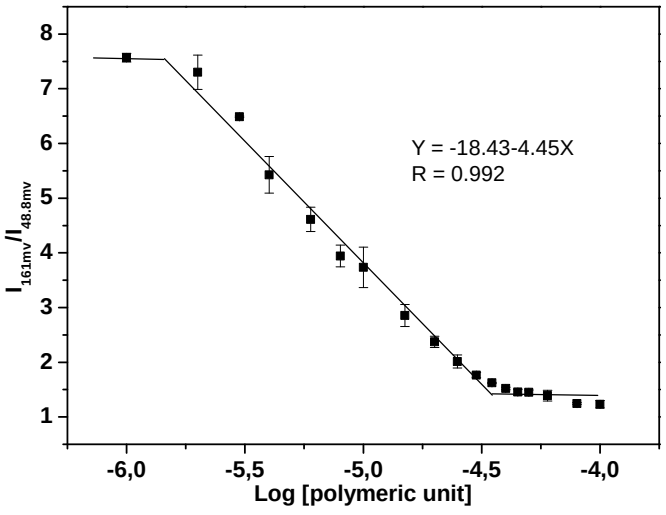

Figure 1. The titration curve of $HSC_{11}BFD/C_{10}SH$-SAM with sodium polystyrene sulfonate as evaluated by cyclic voltammetry.

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P18

A new ferrocene-based bis(guanidine) ligand

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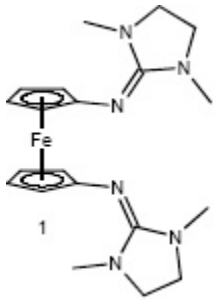
Guanidines are well known organic compounds with a rich coordination chemistry [1,2]. They are common motifs in biomolecules, in which they often serve as a proton cache [3]. There is particular current interest in bis(guanidine) systems, since these can exhibit fascinating properties such as, for example, proton-sponge behaviour [4], and may be utilised, in form of suitable Cu^{I} complexes, for biomimetic O_2 activation [5–7].



1

We present the new bis(guanidine) ligand **1** (Fig. 1), which contains a 1,1'-ferrocenediyl backbone. In contrast to known ferrocene-based bis(guanidine)s, **1** is not macrocyclic and hence more flexible [8]. Compared to the structurally similar 1,3-bis(guanidine)propane ligands [9], **1** is less flexible and the electron-rich ferrocenediyl backbone provides more electron density to the donor atoms than the propane structure. A rich coordination chemistry of **1** towards transition metals can be expected. First results will be shown.

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P19

A Cycloheptatrienyl Pogo-Stick Molecule with Imido-Type Reactivity

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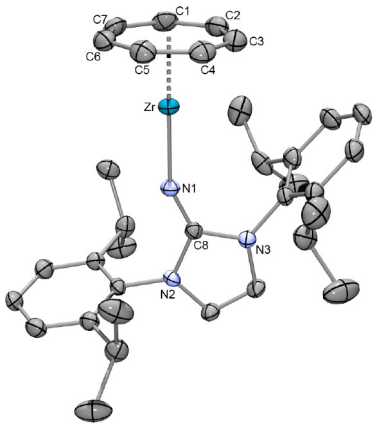
The complex [(η^7-C_7H_7)ZrCl(tmeda)] (**1**) (tmeda = N,N,N',N'-tetramethylethylene-1,2 diamine) turned out to be a fairly versatile starting-material for the incorporation of monanionic ligands into the cycloheptatrienyl zirconium coordination sphere by a transmetallation reaction. **1** has been used for the synthesis and characterization of half-open trozircenes [(η^7-C_7H_7)Zr(η^5-Pdl)] (Pdl = pentadienyl) [1], several substituted trozircenes [(η^7-C_7H_7)Zr(η^5-C_5H_4R)] [2] and also phosphatrozircenes [(η^7-C_7H_7)Zr(η^5-C_4PR_4)]. We now wish to report on our latest results concerning cycloheptatrienyl-allyl zirconium complexes. Subsequent reactions allowed for the formation of the first cycloheptatrienyl pogo-stick molecule (η^7-C_7H_7)Zr(NImDipp) (**2**) (NImDipp = 1,3-bis(2,6-diisopropylphenyl)imidazolin-2-iminato), which has a very short Zr-N bond (1.997 Å). This complex can be regarded as isoelectronic and isolobal to imido-complexes of the type [(η^8-C_8H_8)Ti(NR)] (R = *t*Bu, 2,6-*i*$Pr_2C_6H_3$) and can be expected to undergo typical imido-type reactions such as [2+2] cycloadditions or insertions. Indeed, the reaction of an appropiate substrate with **2** resulted in a four-membered metallacycle, whereas other substrates simply coordinated to **2**.



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P20

Coordination Chemistry of Pyrimidinyl Functionalized Phosphine Ligands towards Palladium(II) and Ruthenium(II)

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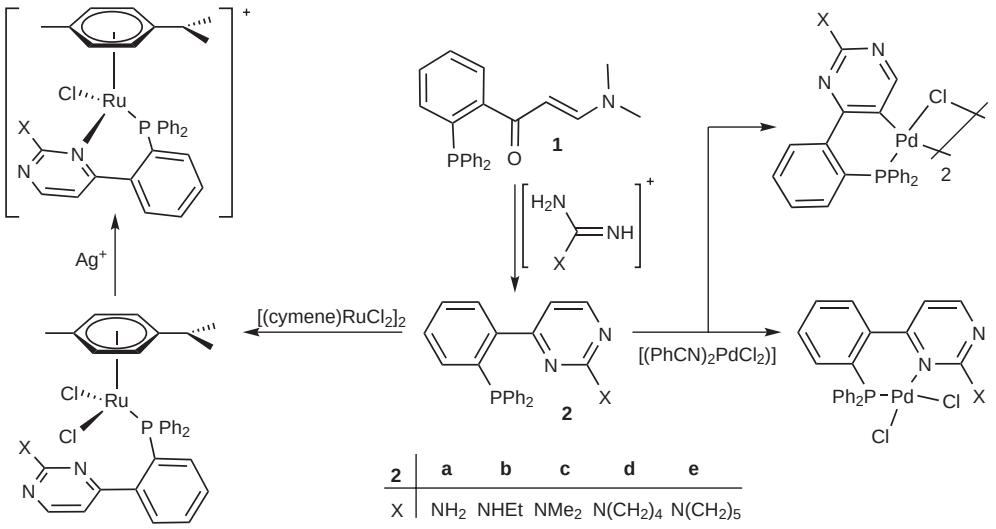
Functionalized phosphines are important ligands in coordination chemistry and are frequently applied in transition metal catalysis. Since a couple of years, our group is engaged in developing novel phosphines such as imino [1] and pyrazole functionalized phosphines [2] or enantiomerically pure *P,N*-donors [3]. On continuing our efforts to synthesize new *P,N* ligands we established the pyrimidinyl functionalized donors **2a-e** which are easily accessible by ring closure of **1** with differently substituted guanidines.



The coordination chemistry of these ligands towards palladium(II) and half-sandwich ruthenium(II) sites has been investigated and the different coordination modes are clearly expressed by ^{1}H and ^{31}P NMR spectroscopy. The solid-state structures of the resulting complexes were confirmed by single crystal x-ray diffraction studies.

[1] Sun, Y.; Ahmed, R.; Beller, M.; Thiel, W.R. *Organometallics* **2004**, *23*, 5260.

[2] Sun, Y.; Grasser, J.; Herdtweck, E.; Thiel, W.R. *J. Organomet. Chem.* **2006**, *681*, 2891.

[3] Seubert, C.; Sun, Y.; Thiel, W.R. *J. Chem. Soc., Dalton Trans.* **2009**, 4971.

P21

Synthesis of Organometallic Molybdenum Complexes for Oxidation Reactions

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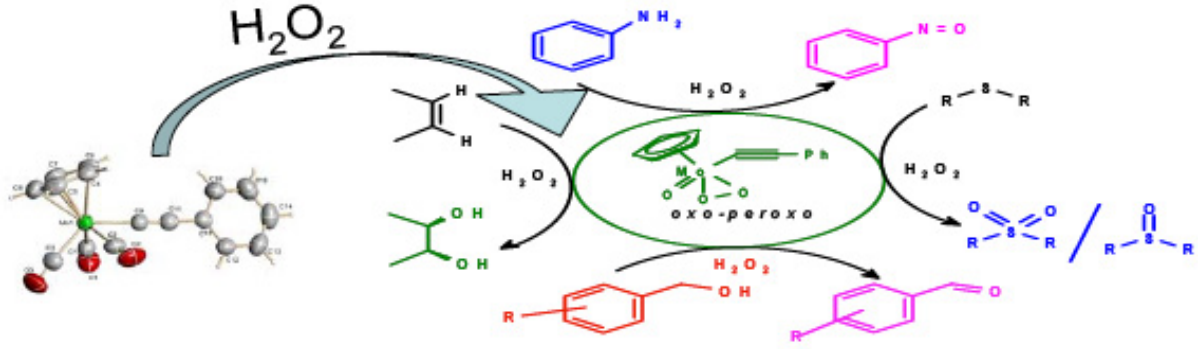
Cyclopentadienyl molybdenum tricarbonyl acetylide complexes $CpMo(CO)_3(\text{-}C{\equiv}CPhR)$ (R = H, CF_3, CH_3) have been synthesised and tested for various selective oxidation reactions using hydrogen peroxide as green oxidant. These catalysts showed very high activity for selective oxidation of olefin to *cis*-diol, anilines to nitroso derivatives at room temperature, sulphides to sulfoxides or sulfones and alcohols to aldehydes. These catalysts have shown very high turnover number in case of all the reactions [1–3].



In presence of hydrogen peroxide these catalysts form corresponding oxo peroxo complex, $CpMo(O)(O_2)(\text{-}C{\equiv}CR)$. This oxo peroxo complex is the catalytically active species and is soluble in water. It was easily separated and recycled by extraction of the organic products in organic solvent and recycling the catalyst in aqueous phase. As Mo (VI)-oxo peroxo is the catalytically active species, very simple route for synthesis of cyclopentadienyl molybdenum dioxo acetylide complex from MoO_3 instead of $Mo(CO)_6$ as precursor is being worked out and this is being used for oxidation of various organics.

[1] Biradar, A.V.; Sathe, B.R.; Umbarkar, S.B.; Dongare, M.K. *J. Mol. Catal. A* **2008**, *285*, 111.

[2] Biradar, A.V.; Kotbagi, T.V.; Dongare, M.K.; Umbarkar, S.B. *Tetrahedron Lett.* **2008**, *49*, 3616.

[3] Biradar, A.V.; Dongare, M.K.; Umbarkar, S.B. *Tetrahedron Lett.* **2009**, *50*, 2885.

P22

An Entry to Iron-modified Pincer Complexes: Bimetallic η^6, κ^1 POCOP-Pincer Iron Iridium Compounds

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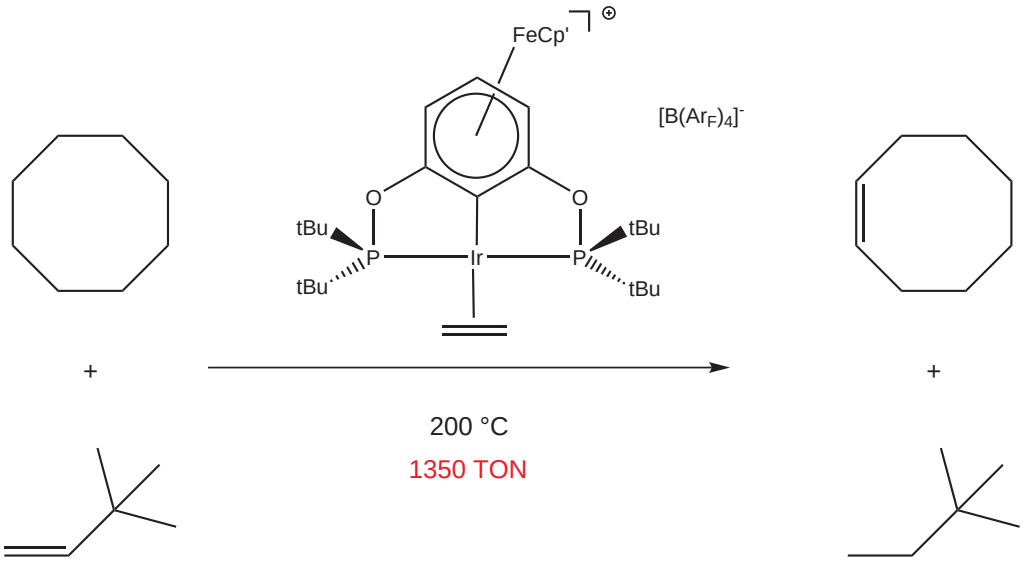
The $[(C_5H_2tBu_3)Fe]^+$, $[Cp'Fe]^+$, fragment was employed to functionalize POCOP (POCOP = C_6H_3-2,6-$(OP^tBu_2)_2$) iridium complexes by direct η^6-coordination of the $[Cp'Fe]^+$ fragment to the arene ring of κ^1-metallated POCOP-pincer ligands to give $\{[(C_5H_2tBu_3)Fe]$(POCOP)Ir(H)(I)$\}^+$, $[\mathbf{1}]^+$, and $\{[(C_5H_2tBu_3)Fe](POCOP)Ir(C_2H_4)\}^+$, $[\mathbf{2}]^+$. In these heterometallic complexes, the π- and σ-electrons of the POCOP-pincer phenyl anion are involved in η^6- and κ^1-coordination to iron(II) and iridium(III)/iridium(I), respectively. This binding mode leads to electron-poor Ir centers and imposes significant steric repulsions between the *t*Bu-groups on the cyclopentadienyl ring and the POCOP ligand framework as reflected in their solution NMR spectroscopic data and solid state structures. Preliminary catalytic studies show that the iron-modified cationic POCOP Ir complex ($[\mathbf{2}]^+$) is active in transfer dehydrogenation between cyclooctane (COA) and *tert*-butyl ethylene (TBE).



P23

Electrochemical communication in mixed valent ruthenium-ferrocene moieties

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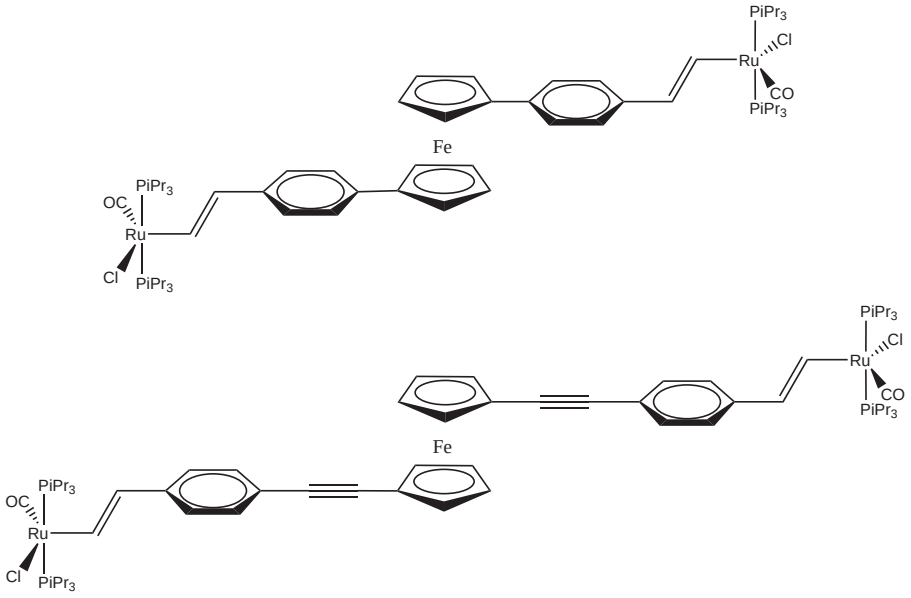
Part of our research deals with electrochemical/electronic communication in mixed-valent vinyl ruthenium complexes $\{RuCl(CO)(P^iPr_3)_2(vinyl)\}_nFc$ (n = 1, 2 and Fc = monosubstituted or 1,1'-disubstituted ferrocenes). These complexes were synthesized by insertion of the corresponding terminal alkyne into the Ru–H bond of $RuHCl(CO)(P^iPr_3)_2$. In their voltammograms, the complexes display two or three redox-waves. The mixed-valent radical cations and dications were electrogenerated inside a standard OTTLE cell, investigated by means of IR- and UV/Vis/NIR–spectroelectrochemistry and analyzed with respect to the electronic communication between the ruthenium moieties and the ferrocene nucleus and that between the two ruthenium vinyl moieties in the 1,1'-disubstituted derivatives. The corresponding mono-ruthenium ferrocene complexes served as reference for the identification of possible Intervalence Charge-Transfer (IVCT) bands in the diruthenium systems. The carbonyl ligands on the ruthenium atoms also provide a charge sensitive IR-label. Oxidation-induced IR band shifts help to identify the primary oxidation site and provide information about the level of electron delocalization between the individual constituents of these di- and trinuclear complexes.



P24

Immobilized Ferrocenyl Phosphine Palladium Complexes for the Heck-Mizoroki Reaction

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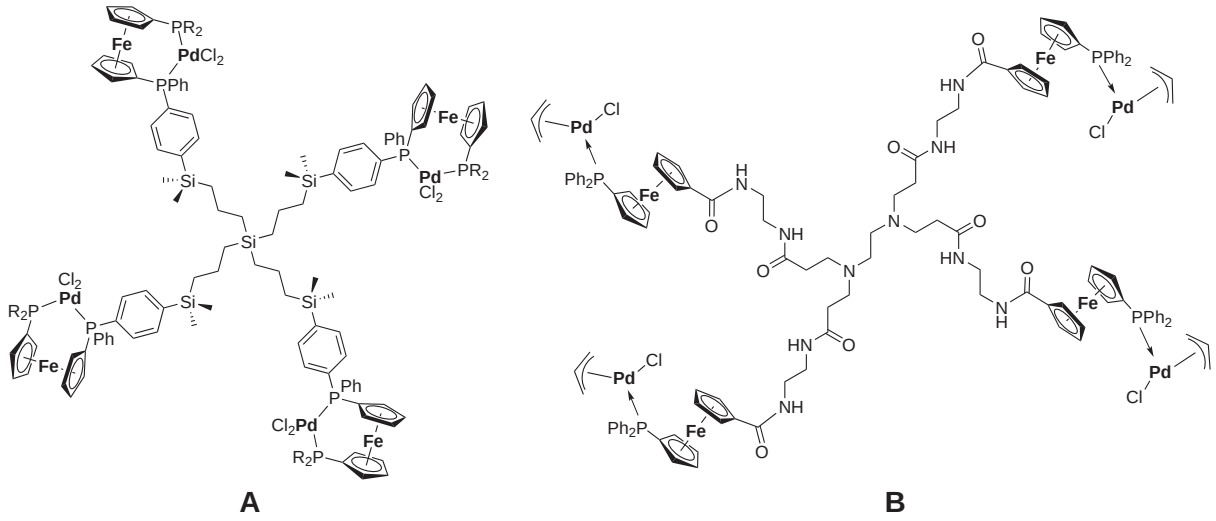
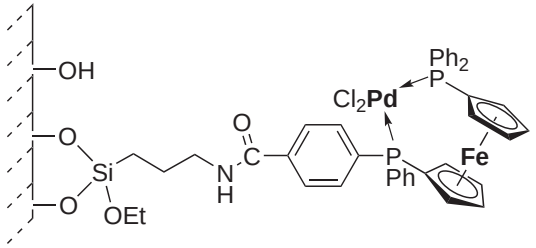
Metallodendrimers with carbosilane- (type **A** molecule) or polyamidoamine-scaffolds (type **B** molecule), accessible by applying a consecutive divergent synthesis methodology, were successfully applied as catalysts in the Heck-Mizoroki *C*,*C* cross-coupling reaction.



A **B**

Based on these immobilization studies we heterogenized appropriate ferrocenyl phosphine palladium complexes on modified aerosil-300 (type **C** system). The synthesis, characterization and catalytic behavior will be presented.



C

[1] Dietrich, S.; Nicolai, A.; Lang, H. *J. Organomet. Chem.* **2011**, *696*, 739–747.

P25

Tetraferrocenyl Five-Membered Heterocycles — Electrochemistry in Multiredox Systems

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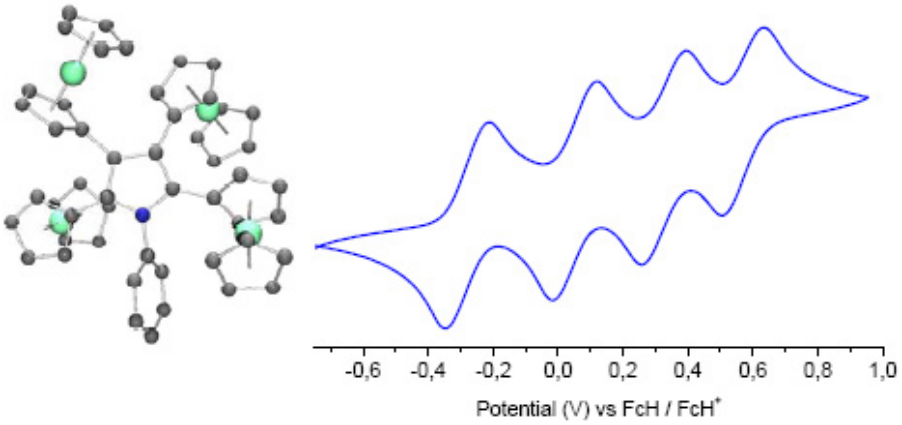
2,3,4,5-Tetraferrocenyl-substituted heterocycles such as thiophene, furan and pyrroles have successfully been synthesized using Negishi *C,C* cross-coupling reactions. Electrochemical studies including cyclic-, square wave-, and linear sweep voltammetry (CV, SWV, LSV) show the reversible behavior of each of the four oxidation steps independently, in all the heterocyclic systems. Spectro-electrochemical UV/Vis-NIR measurements confirm electronic communication as IVCT absorptions were found in the corresponding mono- and dicationic systems, except for the thiophene where the redox peak separation (CV, SWV) is mainly attributed to electrostatic effects.



These compounds show a linear relationship between the $\Delta E_{1/2}$ values and the oscillator strength f of the IVCT transitions as predicted by theoretical hypothesis for a series of molecules with similar geometries and hence, similar electrostatic properties.

[1] Hildebrandt, A.; Rüffer, T.; Erasmus, E.; Swarts, J.C.; Lang, H. *Organometallics* **2010**, *29*, 4900–4905.

[2] Hildebrandt, A.; Schaarschmidt, D.; Lang, H. *Organometallics* **2011**, *30*, 556–563.

P26

Organometallic Chemistry With Emphasis On Electron Transfer Studies

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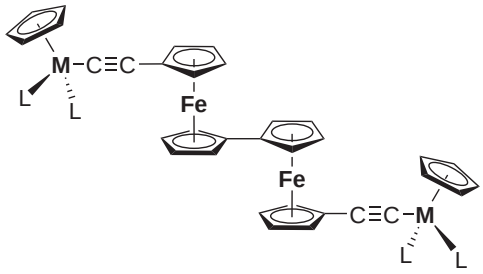
Complexes in which two redox-active transition-metal atoms are connected via carbon-rich (π-conjugated) organic bridging units have received increasing significance during the last years [1]. The use of an organometallic biferrocene-spacer have attracted much attention because it easily forms mixed-valent Fe(II)-Fe(III) species by electrochemical or chemical oxidation [2]. Molecules of type **A** are of interest, due to their robustness, electron richness and their rigid geometry. Bis(ethynyl)biferrocenes can be considered as bridging and redox-active units between transition metal fragments allowing communication through delocalized bonds in the respective array [1,3,4]. The spectroelectrochemistry of such molecules will be described including UV-Vis-NIR-, IR-, ESR-, Mößbauer-spectroscopy, cyclovoltammetry etc.



A

M = Ru, L_2 = 2 PPh_3; M = Ru, L_2 = dppf; M = Os, L_2 = 2 PPh_3; M = Fe, L_2 = dppe

[1] For example: (a) Long, N.J.; Williams, C.K. *Angew. Chem. Int. Ed.* **2003**, *42*, 2586; (b) Ceccon, A.; Santi, S.; Orian, L.; Bisello, A. *Coord. Chem. Rev.* **2004**, *248*, 683.

[2] (a) Meyer, T.J. et al. *Inorg. Chem.* **1975**, *14*, 506; (b) Mueller-Westerhoff, U.T. *Angew. Chem. Int. Ed. Engl.* **1986**, *25*, 702.

[3] For example: (a) Long, N.J. et al. *Organometallics* **1999**, *18*, 4261; (b) Colbert, M.C.B. et al. *Polyhedron* **1995**, *14*, 2759; (c) Dong, T.-Y. et al. *Organometallics* **2008**, *27*, 555.

[4] (a) Lohan, M.; Ecorchard, P.; Rüffer, T.; Justaud, F.; Lapinte, C.; Lang, H. *Organometallics* **2009**, *28*, 1878; (b) Lohan, M.; Justaud, F.; Roisnel, T.; Ecorchard, P.; Lapinte, C.; Lang, H. *Organometallics* **2009**, *28*, 1878.

P27

Metallocenyl-based Catalysts for C,C Coupling Reactions

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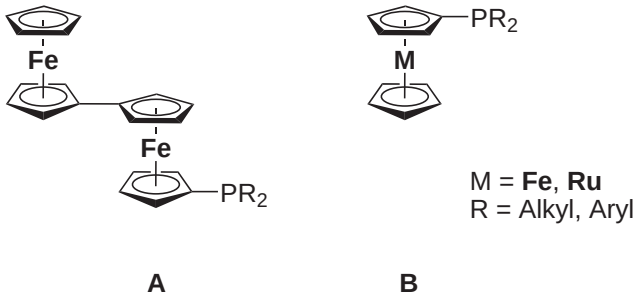
Metallocenyl phosphines have found versatile applications in homogeneous catalysis [1]. Especially electron rich and sterically hindered monodentate phosphines are of particular interest and were intensively studied in classic Suzuki- and Heck reactions [2]. However, less is known about the analogical biferrocenes (e.g. Type **A** molecules) and ruthenocenes (Type **B** molecules) [3].



In this contribution, we report the synthesis of a series of new ferrocenyl, biferrocenyl and ruthenocenyl phosphines. Furthermore, we were able to quantify the electronic properties of the different phosphino groups and compare them with the results of the catalytic investigations in the Suzuki and Heck reaction.

[1] (a) Stead, R.; Xiao, J. *Lett. Org. Chem.* **2004**, *1*, 148; (b) Gusev, O.V.; Peganova, T.A.; Kalsin, A.M.; Vologdin, N.V.; Petrovskii, P.V.; Lyssenko, K.A.; Tsvetkov, A.V.; Beletskaya, I.P. *Organometallics* **2006**, *25*, 2750.

[2] (a) Kataoka, N.; Shelby, Q.; Stambuli, J.P.; Hartwig, J.F. *J. Org. Chem.* **2002**, *67*, 5553.

[3] For example: Nettkoven, U.; Widhalm, M.; Kalchhauser, H.; Kamer, P.C.J.; van Leeuwen, P.W.N.M.; Lutz, M.; Spek, A. *J. Org. Chem.* **2001**, *66*, 759.

P28

A Convenient Way to Functionalized Phosphinoferrocenes and their Use in Carbon-Carbon Cross-Coupling Reactions

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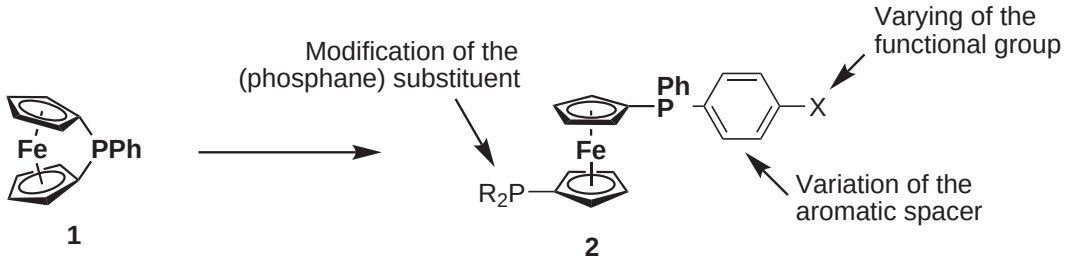
Ferrocenophane **1** was first described in the early 1980s [1]. To our surprise, it has gained only moderate attention since then. While its use for anionic polymerisation has been the topic of numerous reports [2], examples for employing **1** to prepare monomeric ferrocene compounds are rather scarce [3]. Virtually all corresponding synthesis methodologies rely on the ring-opening of **1** with an excess of phenyllithium [3].

Replacing phenyllithium by substituted lithioarenes allows the preparation of diverse type **2** molecules in a single reaction step.



Starting from **2** (X = Br) further modifications can be achieved either by halogen-metal-exchange and reaction of the thus prepared anion with suitable electrophiles or by carbon-carbon cross-coupling.

This methodology allows the synthesis of customized phosphinoferrocenes that can be applied in homogeneous catalysis, e. g. Heck olefination of aryl halides.

Within this contribution the synthesis and reaction chemistry of type **2** molecules as well as their application in carbon-carbon cross-coupling reactions will be reported.

[1] Seyferth, D.; Withers, H.P., Jr. *J. Organomet. Chem.* **1980**, *185*, C1.

[2] (a) Peckham, T.J.; Massey, J.; Honeyman, C.H.; Manners, I. *Macromolecules* **1999**, *32*, 2830; (b) Herbert, D.E.; Mayer, U.F.J.; Manners, I. *Angew. Chem.* **2007**, *119*, 5152.

[3] Podlaha, J.; Štěpnička, P.; Ludvík, J.; Císařová, I. *Organometallics* **1996**, *15*, 543.

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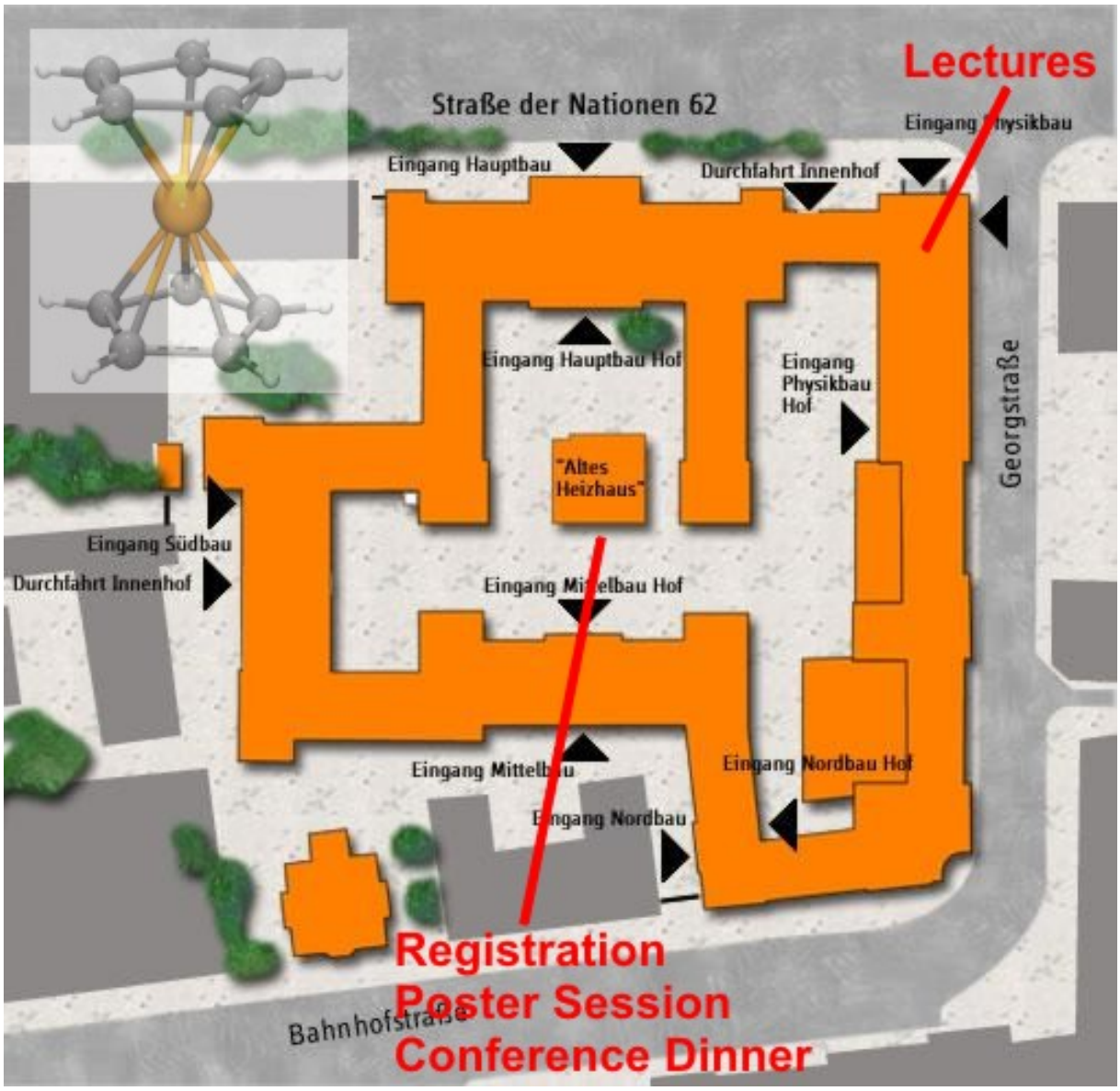
Notes

Notes

Site Plan



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Schedule								
Monday, February 14			**Tuesday, February 15**			**Wednesday, February 16**		
			09:00–09:50	G. Erker	**I2**	09:00–09:50	I. Manners	**I4**
			09:50–10:10	D. Schaarschmidt	**O7**	09:50–10:10	G. Lackner	**O19**
			10:10–10:30	L. Taghizadeh Ghoochany	**O8**	10:10–10:30	A. Glöckner	**O20**
			10:30–11:00	**Coffee Break**		**10:30–11:00**	**Coffee Break**	
			11:00–11:20	K. Kowalski	**O9**	11:00–11:20	A. Korotvička	**O21**
			11:20–11:40	K. Kaleta	**O10**	11:20–11:40	M. Braun	**O22**
			11:40–12:00	C. Thoms	**O11**	11:40–12:00	D. Weismann	**O23**
			12:00–12:20	A.C. Tagne Kuate	**O12**	12:00–12:30	Closing Remarks, Prizes	
10:00–13:00	**Arrival and Registration**		**12:20–14:00**	**Lunch Break**		**12:30**	**Departure**	
13:00–13:20	Opening Remarks							
13:20–14:10	C. Lapinte	**I1**	14:00–14:50	I. Butler	**I3**			
14:10–14:30	A. Hildebrandt	**O1**	14:50–15:10	B. Hildebrandt	**O13**			
14:30–14:50	C. Herfurth	**O2**	15:10–15:30	C. Färber	**O14**			
14:50–15:20	**Coffee Break**		**15:30–16:00**	**Coffee Break**				
15:20–15:40	R.F. Winter	**O3**	16:00–16:20	K. Rademann	**O15**			
15:40–16:00	D. Siebler	**O4**	16:20–16:40	S. Pandey	**O16**			
16:00–16:20	R. Breuer	**O5**	16:40–17:00	M. Gawron	**O17**			
16:20–16:40	C. Gers	**O6**	17:00–17:20	A.D. Russell	**O18**			
17:00–19:00	**Poster Session**		**18:00**	**Conference Dinner (BBQ)**				