



4th Winter School on Supramolecular Chemistry

Organised by the

International Research Training Group
“Generation of Supramolecular Functional Cavities -
Container Molecules, Macrocycles and Related Compounds”

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Galtür, Austria

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Dirk Brackemeyer F.E. Hahn (Münster)

Markus Schmidtendorf F.E. Hahn (Münster)

- **Session I** Monday, 28.2. 8.30 - 10.30
chair: Holger Kruse
 - Florian D. Henne
Carbene-stabilized Pnictogen(III)-centered Cations $LPnX_2$ and L_2PnX^{2+} ($Pn=P, As, Sb; X=Cl, N_3, CN$)
 - Federica Bertini
Preorganised Frustrated Lewis Pairs
 - Matthias Voß
Synthesis of Functionalized Macrocyclic Digallium-Compounds
- **Session II** Tuesday, 1.3. 8.30 - 10.30
chair: Steffi Roters
 - Verena Blase
Template Synthesis of PC^{NHC} and P_2C^{NHC} Ligands
 - Fabian Conrady
Stepwise assembly of metallosupramolecular architectures with di-NH,O-stabilized carbene building blocks
 - Frank Hengesbach
Synthesis of Al-C and Ga-C Condensation Products via Hydroalumination and Hydrogallation Reactions
- **Session III** Wednesday, 2.3. 8.30 - 10.30
chair: Matthias Voß
 - Carolin Dumke
New Linear Bidentate isocyanide Ligands: Suitable Building Blocks for Supramolecular Architectures?
 - Hester Zijstra
Dispersion-corrected DFT Study on Quadruplex Interactions in G-DNA Model Systems
 - Christian Appelt
Geminal Phosphorus/Aluminum-based Frustrated Lewis Pairs
- **Session IV** Thursday, 3.3. 8.30 - 10.30
chair: Carolin Dumke
 - Steffi Roters
Hydroalumination of Bis- and Tris(alkynyl)phosphines
 - Holger Kruse
Complexation of Small Molecules in Metal-Carben Cages
 - Dirk Brackemeyer
Synthesis and Coordination Chemistry of NH,HR-functionalized NHC-Ligands
- **Session V** Thursday, 4.3. 20.30 - 21.30
chair: Fabian Conrady
 - Nicole Megger
DNA-catalyzed Diels-Alder reaction
 - Jonas Moellmann
Application of the new DFT-D3 dispersion correction to periodic systems
- **Session VI** Friday, 4.3. 8.30 - 10.30
chair: Verena Blase
 - Markus Schmidtendorf
Synthesis of Supramolecular Structures by Metal-directed Self-assembly of N-heterocyclic Biscarbene Ligands
 - N. R. Shiju
Keynote: *Heterogeneous Catalysis: Concepts and Applications*

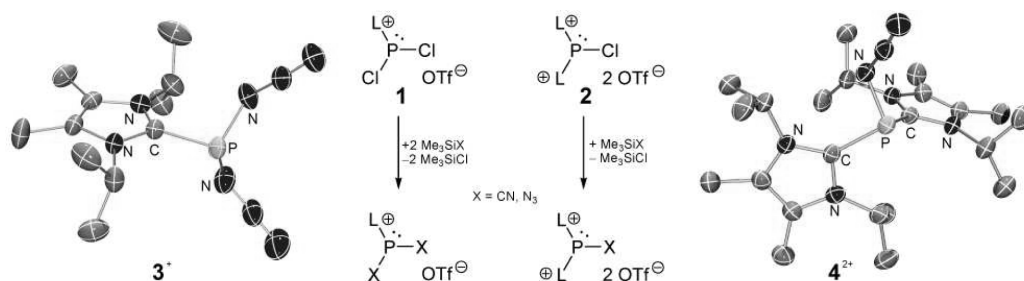
Carbene-stabilized Pnictogen(III)-centered Cations $LPnX_2^+$ and L_2PnX^{2+} (Pn = P, As, Sb; X = Cl, N₃, CN)

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Main group element-centered cations can possess unusual reactivity and are, therefore, promising reagents for new synthetic procedures. Several types of phosphorus-centered cations are known to date. Most of them require stabilization *via* adduct formation with Lewis bases. Multiply-charged phosphorus-centered cations which incorporate trivalent P(III)-atoms and are suitable for further functionalization are not readily accessible.

Since NHCs have been successfully used for the stabilization of unusual and highly reactive main group element species, we were recently able to synthesize and completely characterize the P(III) cations $[LPCl_2]^+$ (1^+) and $[L_2PCl]^{2+}$ (2^{2+}) (L = NHC). In addition, the subsequent transformations to unprecedented NHC stabilized cationic cyano and azidocomplexes $[LPX_2]^+$ and $[L_2PX]^{2+}$ (X = CN, N₃ (3^+ , 4^{2+})) are presented.^[1] Further investigations to extend this concept to the heavier pnictogen atoms As and Sb are also presented.



References:

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Preorganised Frustrated Lewis Pairs

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Since their discovery, frustrated Lewis pairs (FLPs) gained significant attention thanks to their ability to activate small molecules by splitting bonds heterolytically.^[1] This ability arises from the synergic effect of donor and acceptor sites which polarizes a chemical bond.^[2] We became interested in investigating on the reactivity of preorganised FLPs in which the donor and acceptor sites are situated in the same molecule and the active sites are ideally orientated for small molecule activation. In this context, we wish to present our experimental and computational work on the reactivity of methylene bridged P/B and P/Al based (F)LPs and their reactivity towards H₂ and CO₂, as well as the follow-up chemistry of the activated molecules towards useful products.



Figure 1: activation of small molecules (H₂ and CO₂) by methylene bridged P/B based FLP.

References:

[1] a) D.W. Stephan, G.Erker, *Angew. Chem.*, **2010**, 122, 50-81; *Angew. Chem. Int. Ed.*, **2010**, 49, 46-76; D. W. Stephan, *Dalton Trans.*, **2009**, 3129-3136; c) D.W. Stephan, *Org. Biomol. Chem.*, **2008**, 6, 1535-1539.

[2] a) S. Grimme, H. Kruse, L. Goerigk, G. Erker, *Angew. Chem. Int. Ed.*, **2010**, 49, 1402-1405.

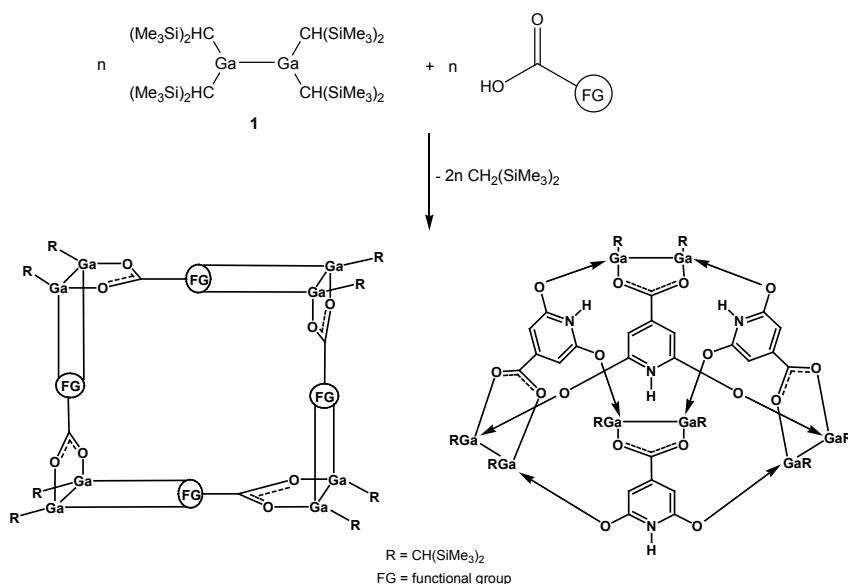
SYNTHESIS OF FUNCTIONALIZED MACROCYCLIC DIGALLIUM-COMPOUNDS

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Tetrakis[bis(trimethylsilyl)methyl]digallane(4) **1** is a facile starting material for the generation of unprecedented digallium-Compounds. The reactions with carboxylic acids afford interesting digallium dicarboxylates with two carboxylate ligands in the bridging position across the Ga-Ga-bond.^[1,2]

Here we report on recent results obtained with functionalized carboxylic acids. Novel, containing at least two further donor atoms in their organic backbone, macrocyclic and three-dimensional cage-like molecules could be isolated and characterized.



References:

- [1] W. Uhl, *Adv. Organomet. Chem.* **2004**, *51*, 53
 [2] W. Uhl, A.-C. Fick, T. Spies, G. Geiseler, K. Harms, *Organometallics* **2004**, *23*, 72

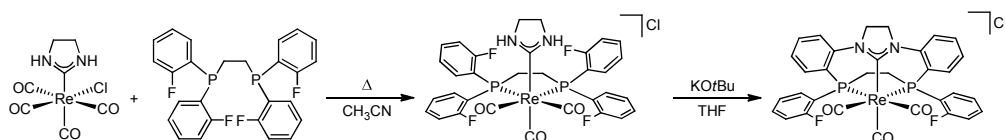
Template Synthesis of PC^{NHC} and P₂C^{NHC} Ligands

Verena Blase and F. Ekkehardt Hahn

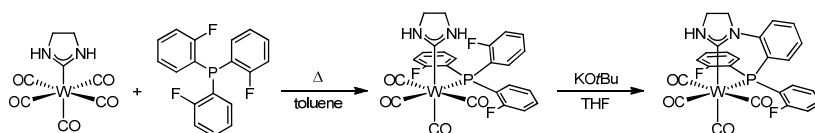
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N-Heterocyclic carbene complexes are well known and due to their diversity ubiquitous ligands in organometallic chemistry.^[1]

For the generation of a mixed carbene/phosphine macrocyclic ligand the coordination of a diphosphine as well as a carbene to a metal center is necessary. The NH,NH stabilized carbene undergoes, after deprotonation of the NH function, a nucleophilic attack at the fluorine substituted carbon atoms resulting in the formation of the macrocyclic ligand, for instance at the here shown rhenium(I) template.



In a tungsten pentacarbonyl carbene complex it is feasible to substitute one carbonyl ligand for a monophosphine. Thus, within this mixed carbene/phosphine tungsten complex, linking of the phosphine with the NHC generates a complex with a NR,NH stabilized carbene, which is a completely new method for the preparation of those complexes.



Reference

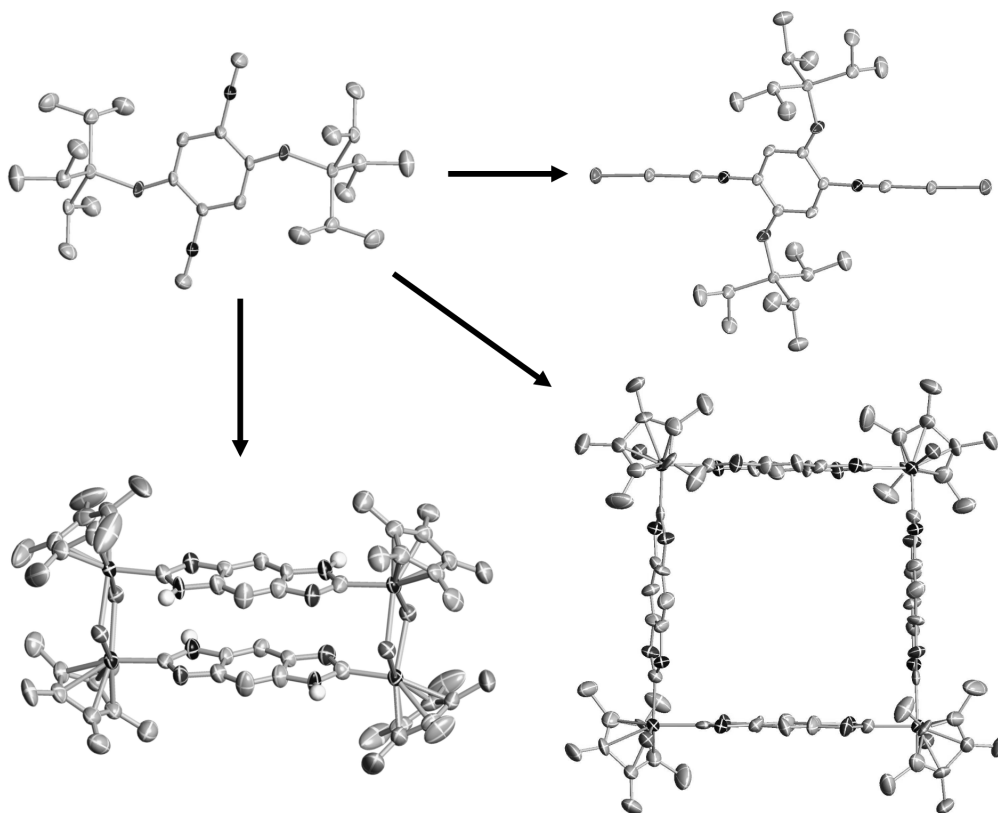
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Stepwise assembly of metallocupramolecular architectures with di-NH,O-stabilized carbene building blocks

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A range of *N,O*-heterocyclic carbene complexes based on benzoxazole are known in the literature.^[1] The use of 2-trimethylsiloxyphenyl isocyanide as a suitable starting material for these complexes has been also demonstrated.^[1] New disiloxy functionalized diisocyanide ligands were prepared and used for the stepwise assembly of tetranuclear iridium(III) and rhodium(III) molecular rectangles and squares with di-NH,O-stabilized carbene building blocks.



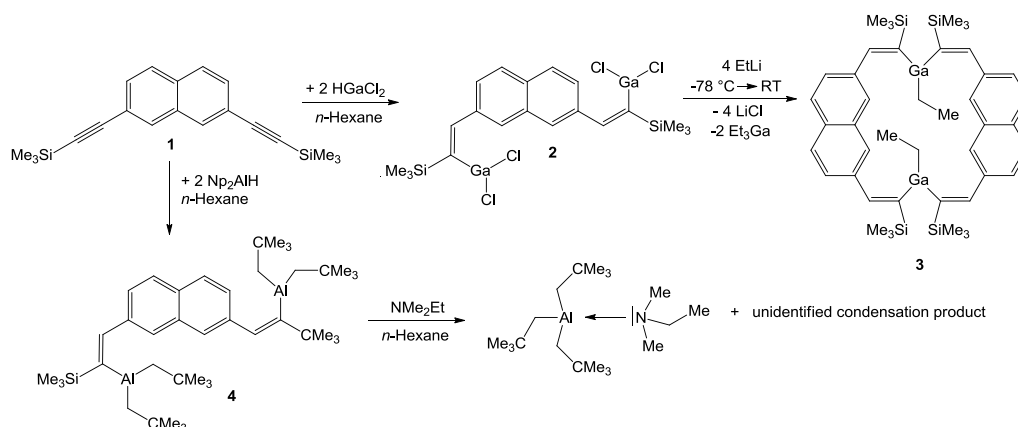
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Synthesis of Al-C and Ga-C Condensation Products via Hydroalumination and Hydrogallation Reactions

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Hydrometallation is a powerful method for the reduction of organic compounds containing homo- or heteronuclear double or triple bonds^[1] and leads to a broad variety of unusual oligoaluminium or –gallium compounds.^[2] Many reactions proceed by condensation under the release of the corresponding trialkylmetal derivatives and afford different types of clusters or cages. We hoped to synthesise novel cage compounds by the application of particularly preorganised bis(trimethylsilylethyne)s and therefore treated rigid aromatic alkynes with di(*tert*-butyl)- or dineopentylmetal hydrides.



Scheme 1. Hydrogallation of 2,7-bis(trimethylsilylethynyl)naphthalene **1** and alkylation of the product **2** leads to a macrocyclic inverse crown ether **3**. Hydroalumination of **1** and addition of a Lewis-basic amine yields an unidentified condensation product.

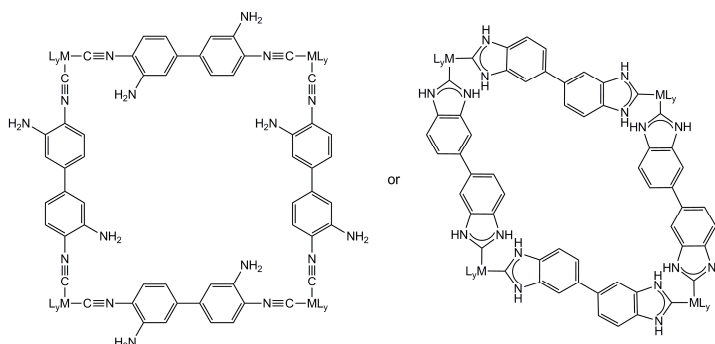
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New Linear Bidentate Isocyanide Ligands: Suitable Building Blocks for Supramolecular Architectures?

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4,4'-Diisocyanobiphenyl is already presented in the literature as a suitable ligand to connect two metal centers. Our interest is focused on the assembly of four metal complex fragments, in a square planar fashion, as it has already been described for other bidentate linear ligands. A further substitution of the biphenyl spacer enables a change of the size of the supramolecular ring by a switch from isocyanide to carbene. The desired ligand is 3,3'-diamino-4,4'-diisocyanobiphenyl. Depending on the electron density at the metal center, the isocyanide bond is either deactivated for a nucleophilic attack, or an intramolecular ring closure occurs, yielding the bridging dicarbene ligand.



Acknowledgements and References

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Dispersion-corrected DFT Study on Quadruplex Interactions in G-DNA Model Systems

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At the termini of chromosomes in basically all vertebrates a distinctive DNA pattern has been observed, termed ‘G-quadruplexes’ [1]. In short, these structures consist of DNA quartets stacked on top of each other with the quartets themselves consisting of four DNA bases positioned in one plane. Usually, the bases involved in such quartets are guanine bases. In this study we have computationally investigated if we can expect diversity of quartet structures in these quadruplexes. We have accomplished this by defining an environment of two guanine quartets, such that a third quartet can be positioned in between, which then can take on different character. Our investigation is based on a state-of-the-art density functional theoretical (DFT) approach (BLYP-D/TZ2P) as implemented in the ADF program [2]. What we found is that indeed a guanine quartet shows the most favorable interaction with its environment. Nevertheless, the interaction of other quartets with the model environment is quite similar to that of a guanine quartet and so purely based on our data we can expect diversity of the quartets in the quadruplex structures. Furthermore, we have investigated the effect of sodium ions positioned between the quartets, which are known for their ability to stabilize guanine quadruplex structures.

References:

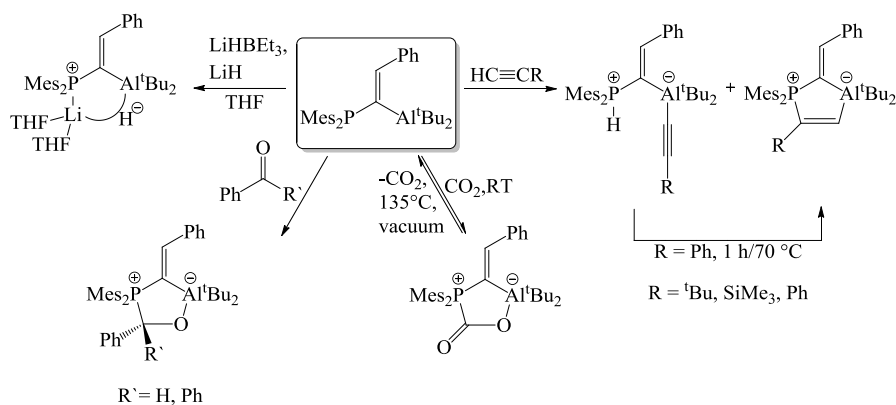
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Geminal Phosphorus/Aluminum-based Frustrated Lewis Pairs

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Frustrated Lewis-pairs bearing donor and acceptor sites in close proximity are of considerable interest for the dipolar activation of small molecules. So far, phosphines, amines, thioethers and carbenes have been applied as Lewis base, while polyfluorinated boranes are the common Lewis acid in FLP chemistry. Alanes, as the better Lewis acids, circumvent the need for electron-withdrawing substituents due to the relatively high positive charge at the metal center. The simple one-step synthesis of these P/Al-based FLPs proceeds via the hydroalumination of alkynylphosphines. Their unique structural motif has shown to be suitable for the activation of terminal alkynes^[1], carbonyl compounds including carbon dioxide^[1], as well as alkali metal hydrides and borohydrides.



Scheme 1. Activation of C=O, C-H, B-H bonds and splitting of Lithiumhydride.

References:

- [1] C.Appelt, H. Westenberg, F. Bertini, A. W. Ehlers, J. C. Slootweg, K. Lammertsma, W. Uhl, *Angew. Chem. Int. Ed.* **2011**, *accepted*.

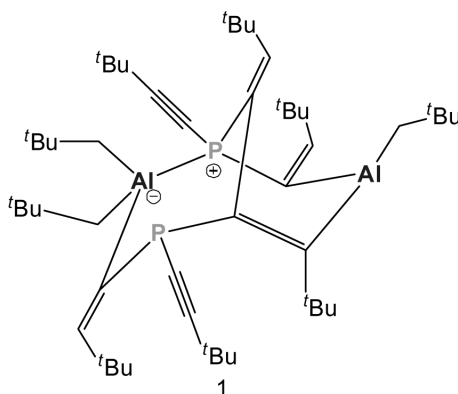
Hydroalumination of Bis- and Tris(alkynyl)phosphines

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Hydroalumination reactions are well-known procedures for the reduction of unsaturated organic compounds^[1]. Treatment of alkynylphosphines with equimolar quantities of dialkylaluminium hydrides leads to the formation of the phosphinoalanes with basic donor (P) and acidic acceptor (Al) sites in close proximity that are able to activate small molecules.^[2] The investigations of the influence of a second or a third alkyne moiety on the course of the hydroalumination reactions show that unprecedented secondary processes take place.^[3] Our recent results show that the treatment of tris(*tert*-butylethynyl)phosphine with di(*neo*-pentyl)aluminium hydride in the molar ratio of two to three leads to the heterocyclic, zwitterionic compound **1**.



References:

- [1] W. Uhl, *Coord. Chem. Rev.* **2008**, 252, 1540.
- [2] C. Appelt, H. Westenberg, F. Bertini, A. W. Ehlers, J. C. Slootweg, K. Lammertsma, W. Uhl, *Angew. Chem. Int. Ed.* **2011**, *accepted*.
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Complexation of Small Molecules in Metal-Carben Cages

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A density functional theory (DFT) investigation of the structures and energetics of a recently published tetra-silver metallosupramolecular container build up from NHC units [1] is presented. To properly account for *London* dispersion interactions our latest atom pair-wise dispersion correction DFT-D3 [2] is used to calculate binding energies of small molecules (among others CH₄, CO, CS, H₂, N₂) within the silver-NHC cage. An illustrative example for the inclusion of a small molecule is the non-covalent complexation of H₂ in the cage center which yields a relatively large binding energy of about 3 kcal/mol at the TPSS-D3/def2-TZVPP level of theory. Possible metallophilic interactions within the cage are shortly discussed along with a simple MO analysis of the metal-carben bond which reveals sigma-bonding character.

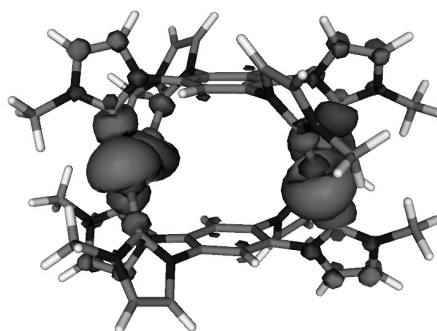


Figure 1: Isosurface plot showing a sigma-bonding type molecular orbitals (HOMO)

References:

- [1] A. Rit, T. Pape and F.E. Hahn *J. Am. Chem. Soc.*, 2010, *132*, 4572-4573.
- [2] S. Grimme, et. al. *J. Chem. Phys.* **2010**, *132*, 154104

Synthesis and Coordination Chemistry of *NH,NR*-functionalized NHC-Ligands

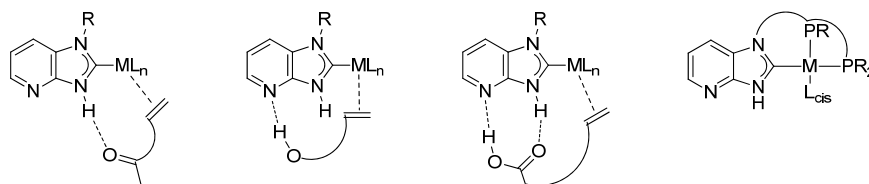
Dirk Brackemeyer, F. Ekkehardt Hahn

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For almost three decades N-heterocyclic carbenes have been highly investigated and have established their important role in transition metal catalysis.^[1] *NH,NR*-stabilized NHCs are less reviewed and studies show, that these ligands do not only affect the catalytic active metal but in fact are able to afford a regio and substrate specific reaction due to their H-donor-function.^[2]

By introducing a nitrogen atom to the benzimidazole backbone in close proximity to the *NH*-function and thereby another possibility for hydrogen bonding we hope to extend its substrate specific potential. Furthermore, as an H-acceptor it leads to a reversal of the substrate recognition unit.

Our aim is the synthesis of *NH,NR*-stabilized NHC ligands based on 4-azabenzimidazole at low-valent electron-rich transition metal complexes. In addition the imidazole should be functionalized to gain a tridentate ligand containing two phosphorus donors besides the carbene and hence improve substrate selectivity *via* precoordination in *cis*-position to the carbene.



References:

- [1] F. E. Hahn, M. C. Jahnke, *Angew. Chem. Int. Ed.* **2008**, *47*, 3122–3172.
- [2] N. Meier, F. E. Hahn, T. Pape, C. Siering, S. R. Waldvogel, *Eur. J. Inorg. Chem.* **2007**, 1210–1214.

DNA-catalyzed *Diels-Alder* reaction

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The synthesis of enantiopure compounds is highly desirable. As metal- and biocatalysts often have a limited scope, a new class of catalysts was created, combining the best characteristics of both catalytic systems. Therefore, a catalytically active transition metal complex was attached to a biopolymer

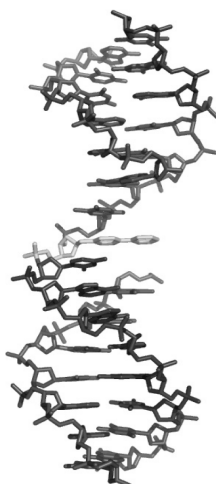


Figure 1: Model of a B-DNA containing the artificial bipyridine nucleotide.

scaffold, e.g. a protein or a polynucleotide, resulting in a so-called hybrid catalyst. The use of DNA as a chiral hybrid catalyst has been reported previously, with high enantioselectivities, e.g. for Cu(II) mediated *Diels-Alder* reactions. In those reports, a 2,2'-bipyridine derivative was used as the Cu(II)-binding ligand, either intercalated into the DNA^[1] or attached to its 3'- or 5'-phosphate moieties^[2].

We report here the first DNA-based catalysis using an artificial 2,2'-bipyridine nucleotide incorporated directly into a regular DNA double helix (Figure 1). The results of a Cu(II)-catalyzed *Diels-Alder* reaction, performed in the presence of different oligonucleotides, will be presented.

References

- [1] a) G. Roelfes, B.L. Feringa, *Angew. Chem. Int. Ed.* **2005**, *44*, 3230-3232; b) G. Roelfes, A. J. Boersma, B. L. Feringa, *Chem. Commun.* **2006**, 635-637; c) A. J. Boersma, B. L. Feringa, G. Roelfes, *Org. Lett.* **2007**, *9*, 3647-3650; d) A. J. Boersma, J. E. Klijn, B. L. Feringa, G. Roelfes, *J. Am. Chem. Soc.* **2008**, *130*, 11783-11790; e) F. Rosati, A. J. Boersma, J. E. Klijn, A. Meetsma, B. L. Feringa, G. Roelfes, *Chem. Eur. J.* **2009**, *15*, 9596-9605.
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Application of the new DFT-D3 dispersion correction to periodic systems

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Density functional theory (DFT) is the most commonly used method for applied quantum chemistry. One of its flaws is the inability to accurately predict van-der-Waals interactions. One alternative to account for the missing dispersion interaction is a post-DFT dispersion correction term.

A less empiric and more accurate method of this dispersion correction has been developed (DFT-D3)[1]. It uses a new concept of fractional coordination numbers to calculate atom-pairwise specific dispersion coefficients. Additionally to the asymptotically important C_6/R^6 dispersion term, a scaled C_8/R^8 contribution and a non-additive three-body term are included. This method has been extended to periodic systems [2].

With this new periodic approach, adsorption processes of organic molecules on noble metal surfaces are investigated. The adsorption energy and structure of benzene and PTCDA on Ag(111) and Au(111) surfaces are calculated with PBE-D3. The new dispersion correction predicts adsorption energies and substrate-surface distances in good agreement with experimental data; thus strongly improves on the old DFT-D2 version.

References:

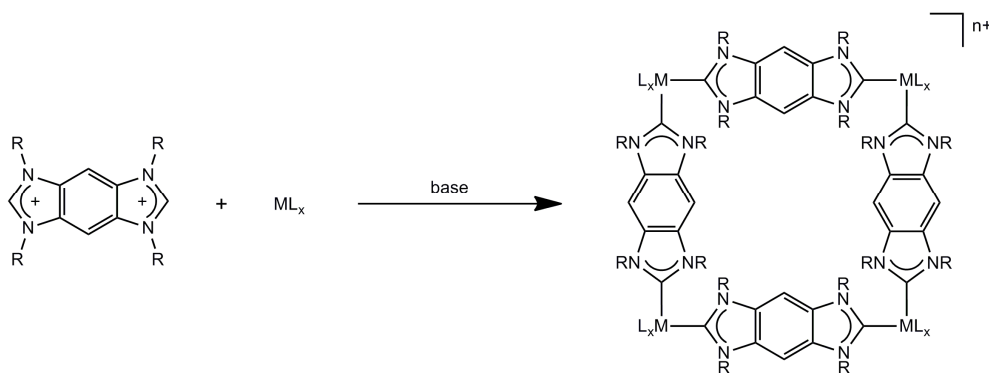
- [1] Stefan Grimme, et. al. *J. Chem. Phys.* **2010**, 132, 154104
- [2] Jonas Moellmann, Stefan Grimme, *Phys. Chem. Chem. Phys.* **2010**, 12, 8500

Synthesis of Supramolecular Structures by Metal-directed Self-assembly of N-heterocyclic Biscarbene Ligands

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Metal-directed self-assembly has become an important tool in supramolecular chemistry since J.-M. Lehn first demonstrated the spontaneous formation of a double-stranded helical complex from bipyridine and Cu(I) ions.^[1] Subsequently, a large number of metal-helicates and other three-dimensional supramolecular structures have been described. However, only a few examples are known which incorporate carbene ligands in a self-assembly process. Encouraged by the first successful metal-directed self-assemblies of a carbene-bridged rectangle and square, we became interested in the synthesis of supramolecular structures employing biscarbene ligands.^[2]



References:

- [1] J.-M. Lehn, A. Rigault, J. Siegel, J. Harrowfield, B. Chevrier, D. Moras, *Proc. Natl. Acad. Sci. U.S.A.* **1987**, *84*, 2565–2569.
- [2] (a) F. E. Hahn, C. Radloff, T. Pape, A. Hepp, *Organometallics* **2008**, *27*, 6408–6410.
(b) F. Conrady, F. E. Hahn *unpublished results*.

Heterogeneous Catalysis: Concepts and Applications

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In this talk, I will first describe the fundamental concepts of catalysis in general and heterogeneous catalysis in particular. I will then present some examples of our recent work on clean, heterogeneously catalysed routes for the production of valuable chemicals. These include catalytic routes to caprolactam and acrylonitrile which are monomers of widely used synthetic polymers.

References:

[1] <http://home.medewerker.uva.nl/n.r.shiju/>