2nd International Conference

MMM-II

INTERNATIONAL CONFERENCE ON MAIN-GROUP MOLECULES TO MATERIALS-II

DECEMBER 13-15, 2021

(VIRTUAL MODE)

Organised by the School of Chemical Sciences, NISER, Bhubaneswar

ABOUT

The chemistry of main-group elements has been thriving during recent years. While much of the research has been focused on unravelling the preparative methods, reactivity and structure of compounds where the main-group element is in a low-oxidation state or has a low coordination number, there has also been a shift in emphasis in examining the properties of such compounds in applications ranging from photophysical properties to catalysis. This diverse and rich chemistry has prompted us to organize a meeting dedicated to this theme. Fortuitously, many young researchers working in this theme have joined various Indian Institutes during recent years and have been contributing significantly.

It is appropriate that this second meeting (MMM-2020) is being held at the School of Chemical Sciences, National Institute of Science Education and Research, Bhubaneswar, where Organometallics, Catalysis, and Main group chemistry have had a synergistic influence on the growth of Chemistry in general and inorganic chemistry in particular. Some of the recent exciting developments and future challenges in the field will be highlighted in the three-day symposium through several invited lectures by senior and young faculty drawn from across the world. In addition, there will be a vibrant poster session involving young researchers.

COMMITTEE

Advisory Committee Members

- Prof. V. Chandrasekhar, Director, *TIFR-Hyderabad*
- Prof. T. K. Chandrashekar, *NISER-Bhubaneswar*
- Prof. M. Wagner, *Goethe-Universität Frankfurt am Main*
- Prof. R. Murugavel, *IIT-Bombay*
- Prof. H. B. Singh, *IIT Bombay*
- Prof. K. C. Kumaraswamy, *HCU*
- Prof. Anil J. Elias, *IIT-Delhi*
- Prof. M. S. Balakrishna, *IIT Bombay*
- Prof. V. R. Pedireddi, *IIT Bhubaneswar*
- Prof. V. G. Anand, *IISER-Pune*
- Prof. A. Srinivasan, *NISER-Bhubaneswar*
- Prof. G. Mugesh, *IISc*
- Prof. P. Thilagar,*IISc*
- Prof. Vinod K. Singh, *IIT-Kanpur*
- Prof. Lakshmi Kantam, *ICT-Mumbai*
- Prof. Jitendra Bera, *IIT-Kanpur*
- Prof. M. Ravikanth, *IIT-Bombay*

Local Organising Committee

Patron

Prof. Sudhakar Panda

Director, NISER Bhubaneswar

Convener

Dr. V. Krishnan, *NISER-Bhubaneswar*

Co-Convener

Dr. S. Nembenna, *NISER-Bhubaneswar*

Committee Members

All Faculty members of the School of Chemical Sciences,

NISER Bhubaneswar

Programme

13th December 2021

Time (**IST**)	
8:30–8:35	Welcome by Convener
8:35–8:40	Welcome Address by Director, NISER
8:40–8:50	Inagural Address by Prof. V. Chandrasekhar
8:50–9:00	**Break**
Session – I	**Chair: Prof. M. Ravikanth**
9:00–9:40	Prof. Cameron Jones (PL1)
9:40–10:10	Prof. Shabana Khan (IL-1)
10:10–10:40	Prof. Tarun Kanti Panda (IL-2)
10:40–11:00	**Break**
Session – II	**Chair: Prof. Jitendra K. Bera**
11:00–11:40	Prof. V. Chandrasekhar (PL2)
11:40–12:10	Prof. Sundargopal Ghosh (IL-3)
12:10–12:40	Prof. P. Thilagar (IL-4)
12:40-14.30	**Break & Poster presentation (PP1-PP12)**
Session – III	**Chair: Prof. A. Srinivasan**
14:30–15:10	Prof. Herbert W Roesky (PL3)
15:10–15:40	Prof. Shigeyoshi Inoue (IL-5)
15:40–16:10	Prof. Ganapathi Anantharaman (IL-6)
16:10–16:20	**Break**
Session – IV	**Chair: Prof. Moumita Majumdar**
16:20–17:00	Prof. Todd Marder (PL4)
17:00–17:30	Prof. Ajay Venugopal (IL-7)

14th December 2021

Time (**IST**)

Session – V	**Chair: Prof. V. R. Pedireddi**
8:30–9:10	Prof. Frieder Jäkle (PL5)
9:10–9:40	Prof. Eric Rivard (IL-8)
9:40–10:10	Prof. R. Boomi Shankar (IL-9)
10:10–10:20	**Break**
Session – VI	**Chair: Prof. Sharanappa Nembenna**
10:20–11:00	Prof. K. C. Kumara Swamy (PL6)
11:00–11:30	Prof. N. Dastagiri Reddy (IL-10)
11:30–12:00	Prof. Anukul Jana (IL-11)
12:00–12:15	Presentation by **Mr. Ershad Abubacker-RSC**
12:15–14:30	**Break & Poster presentation (PP13-PP29)**
Session –VII	**Chair: Prof. Anil J. Elias**
14:30–15:10	Prof. Dr. Matthias Wagner (PL7)
15:10–15:40	Prof. Rajendra S. Ghadwal (IL-12)
15:40–16:10	Prof. Sakya Sen (IL-13)
16:10–16:20	**Break**
Session – VIII	**Chair: Prof. Sujit Roy**
16:20–17:00	Prof. M. S. Balakrishna (PL8)
17:00–17:30	Prof. K. Muralidharan (IL-14)

15th December 2021

Time (**IST**)

Session – IX	**Chair: Prof. S. Nagendran/Co-Chair: Prof. Subrata Kundu**
8:30–9:10	Prof. François P. Gabbai (PL9)
9:10–9:40	Prof. Yang Qin (IL-15)
9:40–10:10	Prof. K. Geetharani (IL-16)
10:10–10:20	**Break**

Session – X	**Chair: Prof. S. Natarajan**
10:20–11:00	Prof. R. Murugavel (PL10)
11:00–11:30	Prof. Arnab Rit (IL-17)
11:30–12:00	Prof. G. Prabusankar (IL-18)
12:00–12:15	Presentation by **ACS representative**
12:15-14.30	**Break & Poster presentation (PP30-PP45)**

Session – XI	**Chair: Prof. J. Sankar**
14:30–15:10	Prof. Gilles Alcaraz (PL11)
15:10–15:40	Prof. Swadhin Mandal (IL-19)
15:40–16:10	Prof. Adinarayana Doddi (IL-20)
16:10–16:20	**Break**

Session – XII	**Chair: Prof. V. G. Anand**
16:20–17:00	Prof. G. Mugesh (PL12)
17:00–17:10	Winners of the Best Poster Presentation
17:10–17:15	Vote of thanks by co-convener

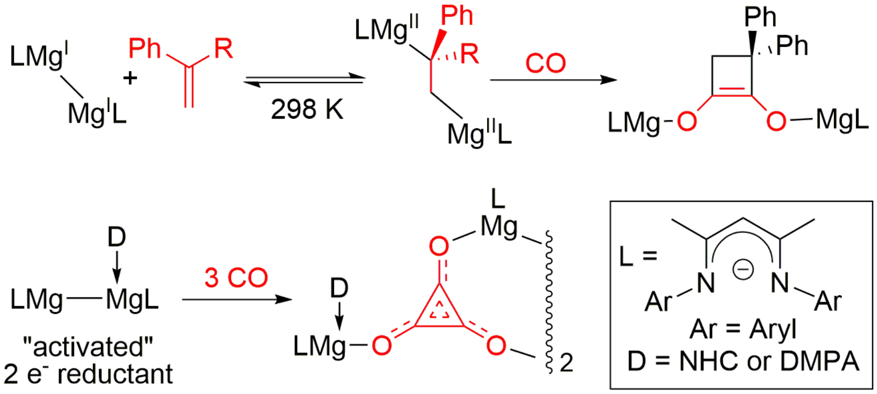
PL1

HIGHLY ACTIVATED MAGNESIUM(I) COMPOUNDS: POWERFUL REAGENTS FOR SMALL MOLECULE ACTIVATIONS

Cameron Jones[a*]
[a]School of Chemistry, Monash University, Melbourne, VIC, 3800, Australia
cameron.jones@monash.edu

ABSTRACT

Since the synthesis of the first stable magnesium(I) compounds was achieved in 2007, the unique properties these species possess has lent them to use as versatile reducing agents in both organic and inorganic synthetic protocols.[1] The products of such reactions are often inaccessible using more classical reducing agents. We have recently developed several classes of highly activated magnesium(I) and "masked" magnesium(I) systems, and have shown these to be markedly more reactive than their established counterparts.[2-4] In this lecture it will be shown that these compounds are powerful reagents for the "transition metal-like" activation of catalytically relevant small molecule substrates (e.g. CO, H_2, C_2H_4) (Figure 1). In several cases, small molecule activations are redox reversible under mild conditions, which gives hope for the eventual incorporation of magnesium(I) compounds into catalytic cycles.



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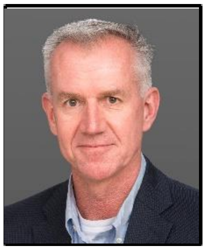
[3] Yuvaraj, K.; Douair, I.; Paparo, A.; Maron, L.; Jones, C. *J. Am. Chem. Soc.*, **2019**, *141*, 8764.

[4] Paparo, A.; Yuvaraj, K.; Matthews, A. J. R.; Douair, I.; Maron, L.; Jones, C., *Angew. Chem. Int.*, **2021**, *60*, 630

Bio-Sketch of Speaker



Cameron Jones

School of Chemistry, Monash University, Melbourne, VIC, 3800, Australia
cameron.jones@monash.edu

Cameron was born in Perth, Australia. He completed his BSc(Hons) degree at the University of Western Australia in 1984. From 1985-1987 he worked as a Research Officer at the University Department of Surgery, Royal Perth Hospital. His PhD degree was gained from Griffith University, Brisbane, under the supervision of Professor Colin L. Raston in 1992, for work on Group 13 metal hydrides. He then moved to a postdoctoral fellowship (1992-1994) at Sussex University under the supervision of Professor John F. Nixon FRS. From 1994 he held a lectureship at The University of Wales, Swansea before moving to a Readership in Inorganic Chemistry at Cardiff University (1998). There, he was promoted to a Personal Chair in Inorganic Chemistry in 2002. At Cardiff he founded (2004) and co-directed The Centre for Fundamental and Applied Main Group Chemistry. In 2007 he moved to Monash University, Melbourne, as an ARC Australian Professorial Fellow and Professor of Chemistry. He is currently the RL Martin Distinguished Professor of Chemistry at that institution, in addition to being the Director of the Monash Catalysis Initiative, which he co-founded in 2015. Cameron was elected as a Fellow of the Australian Academy of Science in 2017.

Selected Fellowships and Prizes

2019: Inaugural Thomas W. Powell Heep Foundation Hagler Institute Chair for Science at Texas A&M University.
2018: Fellow, The Hagler Institute of Advanced Study (HIAS) at Texas A&M University, USA.
2017: Return Senior Research Award of the Alexander von Humboldt Foundation.
2017: Elected Fellow of the Australian Academy of Science (AAS).
2017 - 2021: RL Martin Distinguished Chair of Chemistry.
2016: Royal Society of Chemistry (UK) Australasian Lectureship.
2014 - 2020: Honorary member of Magdalen College, Oxford.
2014: Frankland Award of the Royal Society of Chemistry, UK.
2013: HG Smith Memorial Medal of the Royal Australian Chemical Institute.
2013: Fellow Commoner, The Queen's College, Oxford.
2013: Visiting Fellow, Magdalen College, Oxford.
2012: Elected Fellow of the Royal Australian Chemical Institute.
2011: Burrows Award of the Royal Australian Chemical Institute.
2008: Senior Research Award of the Alexander von Humboldt Foundation.
2006: ARC Australian Professorial Research Fellowship (5 years).
2004: Royal Society of Chemistry's Prize and Medal for Main Group Element Chemistry.
2003: Elected Fellow of the Royal Society of Chemistry.

PL2

Reactivity of a NHC-coordinated Diphosphene and an Unsymmetrical N-P-N Ligand

Vadapalli Chandrasekhar[a,b]

[a] *Department of Chemistry, Indian Institute of Technology Kanpur, Kanpur-208 016, India*
[b] *Tata Institute of Fundamental Research Hyderabad, Gopanpally, Hyderabad- 500046*
vc@tifrh.res.in; vc@iitk.ac.in

ABSTRACT

The reactivity of a NHC-coordinated diphosphene will be discussed. Specifically, the stabilization of a Au(I) hydride and its reversible conversion to Au(I) formate upon reaction with CO_2 will be discussed (Figure 1).[1] We also will discuss the assembly of an unsymmetrical Imino─Phosphanamidinate (NPN) ligand and its reactivity with metal salts (Figure 1) .[2]

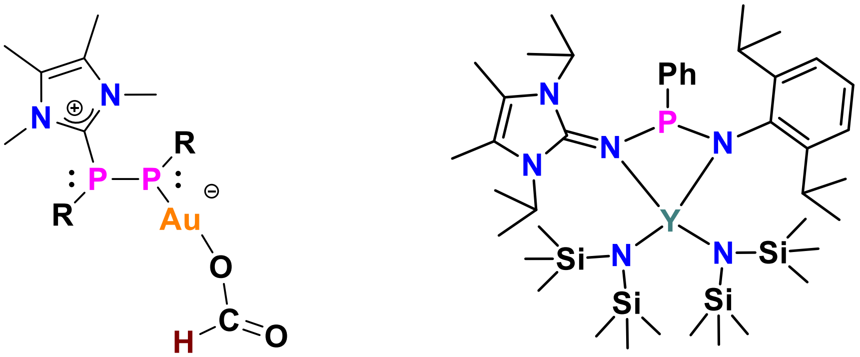


Figure 1

REFERENCES

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[2] Anga, S.; Acharya, J.; Chandrasekhar, V. *J. Org. Chem.* **2021**, *86*, 2224-2234.

Bio-Sketch of Speaker

Prof. V. Chandrasekhar

Tata Institute of Fundamental Research Hyderabad

Gopanpally, Hyderabad-500107, India

and

Department of Chemistry

Indian Institute of Technology Kanpur

Kanpur-208016, India

Email: vc@tifrh.res.in

Vadapalli Chandrasekhar obtained his PhD degree in 1982 from the Indian Institute of Science, Bangalore and postdoctoral work at the University of Massachusetts, Amherst, Massachusetts, USA. After briefly working at the Research and Development section of the Indian Petrochemicals Corporation at Vadodara, as a Senior Research Officer, he joined the Department of Chemistry at the Indian Institute of Technology Kanpur in 1987 where he has been a full professor since 1995. He served as the Head of the Department of Chemistry, IIT Kanpur (2008–10), and as the Dean of Faculty Affairs, IIT Kanpur (2011–12). He also worked at the Tata Institute of Fundamental Research, Centre for Interdisciplinary Sciences, Hyderabad, as a Senior Professor/Dean (2012–14) and Director (2014–17), National Institute of Science Education and Research (NISER), Bhubaneswar, India. Currently he is the Centre Director of the Tata Institute of Fundamental Research, Hyderabad. His research interests are in the area of molecular materials, inorganic rings and polymers, main-group organometallic chemistry and polynuclear metal assemblies. He has been a recipient of the S. S. Bhatnagar Award of the Council and Scientific Industrial Research, India, and the Friedrich-Wilhelm-Bessel Research Award of the Alexander von Humboldt Foundation, Germany (With Prof. H. W. Roesky at Goettingen 2003 Dec-2004 June).

He is an elected Fellow of the Indian Academy of Sciences, Bangalore, the National Academy of Sciences, Allahabad, the Indian National Science Academy, New Delhi and the World Academy of Sciences, Trieste, Italy. He has been on the editorial board of several journals including, Organometallics. Currently he is on the editorial board of Dalton Transactions. His research work is documented in 400+ publications.

PL3

The chemistry of aluminum and silicon is an important subject for future developments

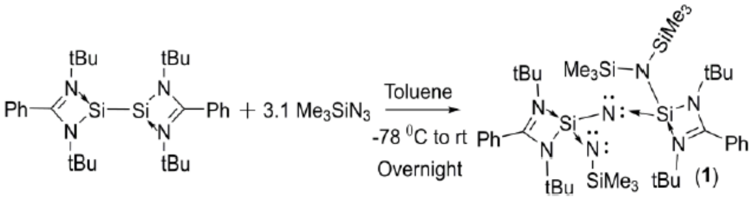
S. K. Sakar, M. Nazish, J. Li, Herbert W. Roesky,*

University of Göttingen, Tammannstrasse 4, 37077 Göttingen

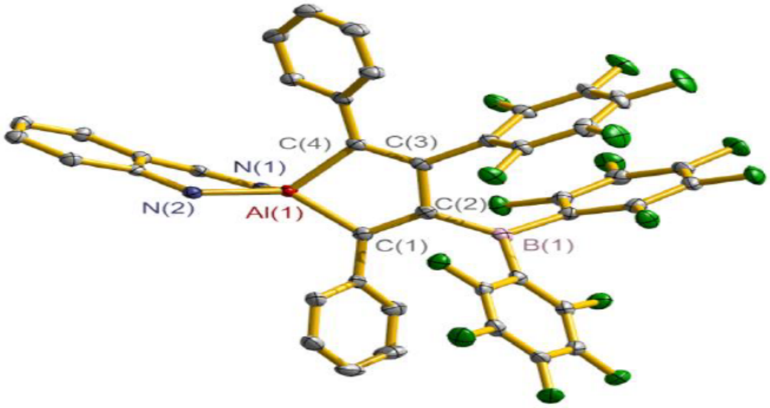
hroesky@chemie.uni-goettingen.de

ABSTRACT

The 1,2 benzene arrangement of silylene and phosphorus(III) substituents was investigated with various metals and non-metals to study their coordination behavior. The reduction of silylene with organo-boron dibromide resulted in an uncharged three-membered Si_2B 2 ∏ aromatic silaborirane. Moreover, we report on the first preparation of the mono and dication of disilabenzene species. The reactions of chlorosilylene with nitriles carrying electron-withdrawing substituents resulted in oxidative [1+2+1]-products with superelongated C–N σ-bonds. The reaction of TMSazide resulted in the formation of a nitrene without using any metal as a reducing agent.



An aluminum dialkine can be easy converted to an aluminum five-membered unsaturated ring in the presence of $B(C_6F_5)_3$. The mrchanism will be explained and the final structure is shown below.



Bio-Sketch of Speaker

Date of Birth 6.11.1935, Place of Birth Laukischken, 1963; Ph. D. Thesis:"Fluorination Reactions under High Pressure"; 1965 Postdoc with DuPont, Wilmington, Delaware, USA "Aluminum and Coordination Chemistry"; 1967 Habilitation Thesis "Chemistry of Substituted Phosphates"; 1971 – 1980 Professor of Inorganic Chemistry at the Johann-Wolfgang-Goethe-Universität,Frankfurt am Main; 1973 – 1976 Director of the Institute of Inorganic Chemistry at the J.-W.-G. Universität, Frankfurt am Main; 1980 – 2003 Director of the Institute of Inorganic Chemistry of the Georg-August-Universität Göttingen; 1985 – 1987 Dean of the Fachbereich Chemie, Georg- August-Universität Göttingen; Since 2003 Professor Emeritus

MAJOR AWARDS

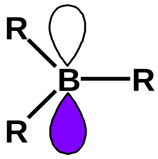
1960 Wöhler – Award; 1970 Dozenten - Award of the Fonds der Chemischen Industrie; 1985 Centenary Lecturer, Royal Society of Chemistry; 1985 Award of the Minister of Sciences in France ; 1986 French Alexander-von-Humboldt-Award; 1987 Leibniz-Award; 1990 Alfred-Stock-Memorial Award; 1994 Manfred and Wolfgang Flad Award; 1995 Literature Award of the Fonds der Chemischen Industrie; 1998 Carus Medal of Leopoldina; 1998 Carus Award of the City of Schweinfurt; 19 Grand Prix de la Fondation de la Maison de la Chimie ; 1998 Wilkinson Prize ; 1999 ACS Award for Creative Work in Fluorine Chemistry; 2004 CNR Rao Award of the Chemical Research Society of India; 2004 ACS Award in Inorganic Chemistry; 2005 Wittig-Grignard-Award, France; 2009 Prix International Henri Moissan, France ; 2012 Heinrich Rössler Preis, GDCh; 2013 Annual Award for Chemistry, Institute of Chemistry of Ireland; 2015 Blaise Pascal Medal, European Academy; 2018 Wacker Silicone Award; 2018 Silver Medal of the University Pardubice.

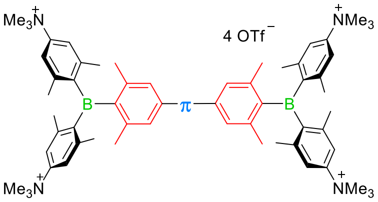
PL4

3-Coordinate Organoboron Compounds Light the Way: Synthesis, Optical Properties and Cell Imaging

Todd B. Marder[a,*]
[a]*Institute of Inorganic Chemistry, and Institute for Sustainable Chemistry & Catalysis with Boron, Julius-Maximilians-Universität Würzburg, Am Hubland, 97074 Würzburg, Germany*
todd.marder@uni-wuerzburg.de

ABSTRACT





Three-coordinate boron, with a vacant p_z-orbital and isoelectronic with a carbonium ion, can conjugate with organic π-systems as a strong π-acceptor in the excited state. Most 3-coordinate boron compounds are Lewis acidic, bind Lewis bases which disrupt this conjugation, and are sensitive to hydrolysis. Bulky substituents on B, such as mesityl (mes) groups, provide steric protection of the vacant p-orbital without disrupting the electronic communication with a π-system, resulting in compounds which are usually air and water stable. By suitable modification, they can also be made water soluble. We focus on the synthesis of dipolar, quadrupolar and octupolar compounds containing $B(Ar)_2$ groups, including those containing new π-acceptors considerably stronger than $B(mes)_2$, and their linear and nonlinear (2nd and 3rd order NLO, TPA and TPEF) optical properties, and their various applications which include OLEDs, cell imaging, and DNA/RNA/protein binding.

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[2] Wu, Z.; Nitsch, J.; Würthner, F.; Marian, C. M.; Ji, L.; Marder, T. B.; et al. *Angew. Chem. Int. Ed.* **2020**, *59*, 17137.
[3] Ban, Ž.; Griesbeck, S.; Marder, T. B.; Piantanida, I.; et al. *Chem. Eur. J.* **2020**, *26*, 2195.
[4] Griesbeck, S.; Lambert, C.; Yamaguchi, S.; Marder, T. B.; et al. *Chem. Sci.* **2019**, *10*, 5405.
[5] Merz, J.; Lambert, C.; Marder, T. B. et al. *Chem. Sci.* **2019**, *10*, 7516.
[6] Reviews: Berger, S. M.; Marder, T. B. *Mater. Horiz.*, **2021**, 8, DOI: 10.1039/D1MH00696G; Berger, S. M.; Ferger, M.; Marder, T. B. *Chem. Eur. J.* **2021**, *27*, 7043; He, J.; Rauch, F.; Finze, M.; Marder, T. B. *Chem. Sci.*, **2021**, *12*, 128; Ji, L.; Griesbeck, S.; Marder, T. B. *Chem. Sci.* **2017**, *8*, 846; Entwistle, C. D.; Marder, T. B. *Chem. Mater*. **2004,** *16*, 4574; Entwistle, C. D.; Marder, T. B. *Angew. Chem. Int. Ed. Engl*. **2002**, *41*, 2927.

Bio-Sketch of Speaker

Todd Marder received his B.Sc. from M.I.T. (1976) and Ph.D. from UCLA (1981), was a postdoc at the University of Bristol (UK), and a Visiting Research Scientist at DuPont Central Research. He joined the faculty at the University of Waterloo, Canada in 1985, was promoted to Associate Professor in 1989, and to Full Professor in 1993. He moved to Durham University (UK) in 1997 as Chair of Inorganic Chemistry, and to the University of Würzburg (Germany) in 2012 as Chair I of Inorganic Chemistry. He has published >400 papers (>26,800 citations, h-index = 91) and presented >400 invited lectures. He has held Visiting Professorships in the UK, France, Hong Kong, China, Japan, India, and Australia, and holds an Honorary Professorship at Durham University (UK), an Adjunct Professorship at the Hong Kong University of Science and Technology, a Guest Professorship at Shandong University (China), a Visiting Professorship at Northeast Normal University (China), and a Consultant Professorship at Northwestern Polytechnical University (China). He has served on the editorial boards of Organometallics, Inorganic Chemistry, Journal of Organometallic Chemistry, Polyhedron, Inorganica Chimica Acta, Applied Organometallic Chemistry, Canadian Journal of Chemistry, Chinese Journal of Chemistry, and Crystal Engineering.

Selected Honors and Awards

Fellow of the European Academy of Sciences
Fellow of the American Association for the Advancement of Science (AAAS)
Elected Member of the Bavarian Academy of Sciences
Fellow of the Royal Society of Chemistry
University of California Regents Intern Fellow (USA)
Royal Society of Canada Rutherford Memorial Medal for Chemistry (Canada)
RSC Awards in Main Group Element Chemistry and in Organometallic Chemistry (UK)
Royal Society Wolfson Research Merit Award (UK)
JSPS Invitation Fellowship (Japan)
Humboldt Research Award (Germany)
1000-Foreign Talents Award for Foreign Experts (China - declined)
Docteur Honoris Causa, Université de Rennes 1 (France)

Research Interests: Organometallic Chemistry; Conjugated organic, organoboron and organometallic materials for linear and nonlinear optics, bioimaging, and sensing; Homogeneous Catalysis; Synthesis of small organic molecules which trigger stem cell differentiation; Non-covalent Interactions: Crystal Engineering and Liquid Crystal Behavior; Flouroarene-arene interactions.

PL5

Borane Lewis Acids and B-N Lewis Pairs: From Molecules to Materials

Frieder Jäkle[a,*]
[a]*Department of Chemistry, Rutgers University Newark, Newark, NJ 07102*
fjaekle@newark.rutgers.edu

ABSTRACT

The incorporation of main group elements into conjugated materials is frequently exploited to achieve unusual properties and to enable new functions.[1] For instance, tricoordinate boron's participation in pi-delocalization can have a dramatic effect on the optical properties by selectively lowering the LUMO orbital levels. The electron-deficient character of boron also enables Lewis acid-base interactions, resulting in strong perturbations of the electronic structure. These materials have been studied for applications ranging from biological imaging, lasing, organic photovoltaics, to photochromic materials and molecular switches.

We have explored the incorporation of boron into conjugated oligomers, macrocycles, and polymers for optoelectronic applications.[2] We have also demonstrated that Lewis base-directed electrophilic aromatic C-H borylation provides an effective means to generate luminescent B-N containing conjugated materials that promote self-sensitized singlet oxygen generation.[3] Finally, we have found that "smart" dynamic materials can be achieved by embedding both Lewis acid and base sites into polymer networks.[4]

In this talk, I will discuss some of these discoveries and highlight their impact in diverse application fields ranging from organic electronics to fluorescence imaging, singlet oxygen sensitization, and the development of reprocessible elastomers.

References:

[1] (a) *Main Group Strategies towards Functional Hybrid Materials*, T. Baumgartner, F. Jäkle, Eds. John Wiley & Sons Ltd, Chichester, **2018**; (b) F. Vidal, F. Jäkle, *Angew. Chem. Int. Ed.* **2019**, *58*, 5846.

[2] (a) B. Meng, Y. Ren, J. Liu, F. Jäkle, L. Wan, *Angew. Chem. Int. Ed.* **2018**, *57*, 2183; (b) N. Baser-Kirazli, R. A. Lalancette, F. Jäkle, *Angew. Chem. Int. Ed.* **2020**, *59*, 8689.

[3] (a) K. Liu, R. A. Lalancette, F. Jäkle *J. Am. Chem. Soc.* **2017**, *139*, 18170; (b) K. Liu, R. A. Lalancette, F. Jäkle *J. Am. Chem. Soc.* **2019**, *141*, 7453; c) M. Vanga, R. A. Lalancette, F. Jäkle *Chem. Eur. J.* **2019**, *25*, 10133.

[4] (a) F. Vidal, H. Lin, C. Morales, F. Jäkle, *Molecules* **2018**, *23*, 405; (b) F. Vidal, J. Gomezcoello, R. A. Lalancette, F. Jäkle, *J. Am. Chem. Soc.* **2019**, *141*, 15963.

Bio-Sketch of Speaker

Frieder Jäkle

Distinguished Professor
Department Chair and Graduate Program Director
Department of Chemistry, Rutgers University-Newark
73 Warren Street, Newark, NJ, 07102-1811
Ph: 973-353-5068 ; fjaekle@rutgers.edu ; http://react.rutgers.edu/~fjaekle/

Research Interests Lewis Acids, Supported Catalysts, Conjugated and Luminescent Materials for Optoelectronic, Sensing and Imaging, Supramolecular Polymers

Selected Academic Awards and Fellowships

- Fellow of the American Chemical Society (2019)
- *Angewandte Chemie* Author Profile (*ACIE* **2018**, *57*, 13378; DOI: 10.1002/anie.201805615)
- Rutgers University Board of Trustees Award for Excellence in Research (2017)
- ACS Akron Section Award (2012)
- Boron in the Americas Award (2012)
- *Friedrich Wilhelm Bessel Award* by the Alexander von Humboldt Foundation (2009-2010)
- *SEAM (Search for Electroactive Materials)* Award (2009)
- Alfred P. Sloan Foundation Research Fellowship (2006-2010)
- Rutgers University Newark *Hosford Award Lectureship* (2007)
- Rutgers University *Board of Trustees Research Fellowship* (2006)
- National Science Foundation *CAREER Award* (2004-2008)

Selected Recent Publications **(Google Scholar Link)**

1. D. Shimoyama, N. Baser-Kirazli, R. A. Lalancette, and F. Jäkle, *Angew. Chem. Int. Ed.* **2021**, *60*, 17942-17946.
2. F. Vidal, J. McQuade, R. A. Lalancette, and F. Jäkle, *J. Am. Chem. Soc.* **2020**, *142*, 14427-14431.
3. N. Baser-Kirazli, R. A. Lalancette, and F. Jäkle, *Angew. Chem. Int. Ed.* **2020**, *59*, 8689-8697.
4. M. Vanga, R. A. Lalancette, and F. Jäkle, *Chem. Eur. J.* **2020**, *25*, 10133-10140.
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PL6

Reactivity of Phosphonate and Sulfonate Based Systems: Some New Findings

K. C. Kumara Swamy,* A. Kalyani, Suraj, M. Shankar, and A. Srinivasarao
School of Chemistry, University of Hyderabad, Hyderabad-500046, Telangana, India.
kckssc@uohyd.ac.in; *kckssc@yahoo.com*

ABSTRACT

This talk will be mainly on the reactivity of phosphonate/phosphine oxide and sulfonate based systems. The precursors include phosphorus based allenes, allenoates, epoxy sulfonamides, ynamides and sulfonylimines. The products include a [Pd]-complex of allenylphosphine oxide, unusual dimer from allene, nucleobase appended phosphonate, a wide array of sulfonyl appended heterocycles including a spirocycle (Figure 1).[1]

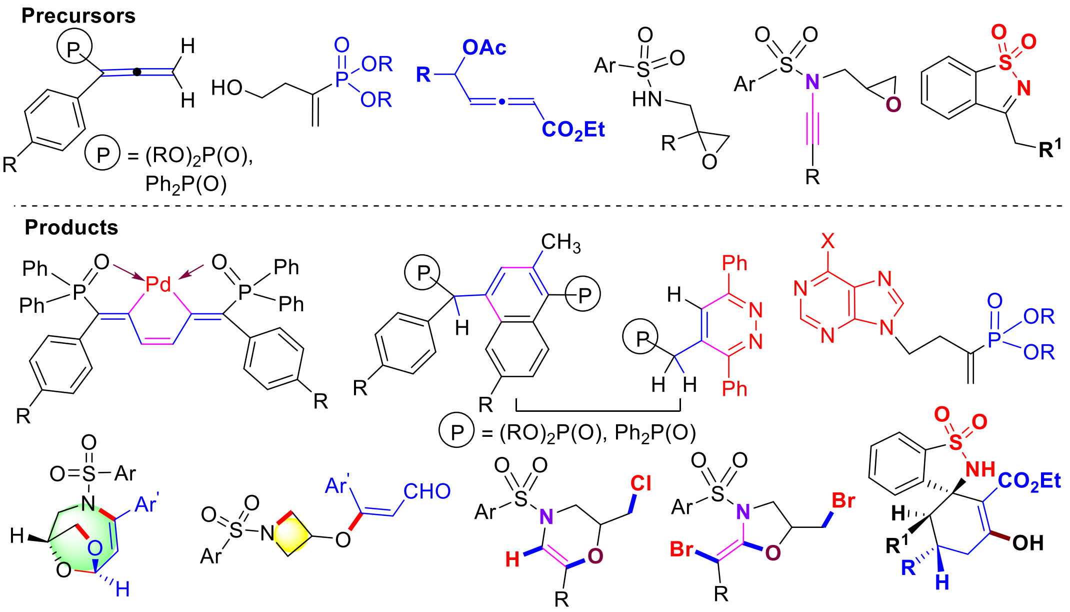

Figure 1: Illustrative precursors and products to be discussed in the talk.

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Bio-Sketch of Speaker

Name and designation: K C Kumara Swamy, Senior Professor

Address: School of Chemistry, University of Hyderabad, Hyderabad-500046, India

Email ID and Ph. No: kckssc@uohyd.ac.in; : 040-23134856 or 9849724004

**Fields of Research Interest : ** Main Group Chemistry, Organophosphorus chemistry, Allene chemistry, Ynamides/Sulfonamides

PhD supervision	: **25** (completed) + **8** (working)
Research grants completed/continuing	: **9** (completed) / **1** (ongoing)
Total peer-reviewed publications	: > **208**
Recognitions	: FASc, FNA

Three recent peer-reviewed publications:

- A. Siva Reddy and K. C. Kumara Swamy* (**2017**) Ethanol as a Hydrogenating Agent: Palladium-Catalyzed Stereoselective Hydrogenation of Ynamides to Give Enamides, *Angew. Chem. Int. Ed.* 56: 6984-6988.
- K. Selvaraj, S. Debnath and K. C. Kumara Swamy* (**2019**) Reaction of Indole Carboxylic Acid/Amide with Propargyl Alcohols: [4 + 3]-Annulation, Unexpected 3- to 2- Carboxylate/Amide Migration, and Decarboxylative Cyclization, *Org. Lett.* 21, 5447–5451.
- A. Sanjeeva Kumar, Sachin Chauhan, and K. C. Kumara Swamy* (**2021**) Contrasting Carboannulation Involving δ-Acetoxy Allenoate as a Four-Carbon Synthon Using DABCO and DMAP: Access to Spiro-carbocyclic and *m*-Teraryl Scaffolds, *Org. Lett.* 23, 1123–1129.

PhD: 1979-1984-Indian Institute of Science, Bangalore, India; (Advisors: Profs. S S Krishnamurthy and A R Vasudeva Murthy) on Cyclophosphazenes

PDF: 1986-1989-University of Massachusetts, Amherst, USA (Prof. Robert R Holmes) P, Si and Sn Chemistry

AvH Fellow: 1991, 1994, 2000, and 2014-University of Saarlandes/ Ludwig Maxmillian University- (Hosts: Prof. Michael Veith/ Prof. K. Karagisoff), Germany (Ga and P Chemistry)

University of Hyderabad: From 1989-till now, as a faculty member.

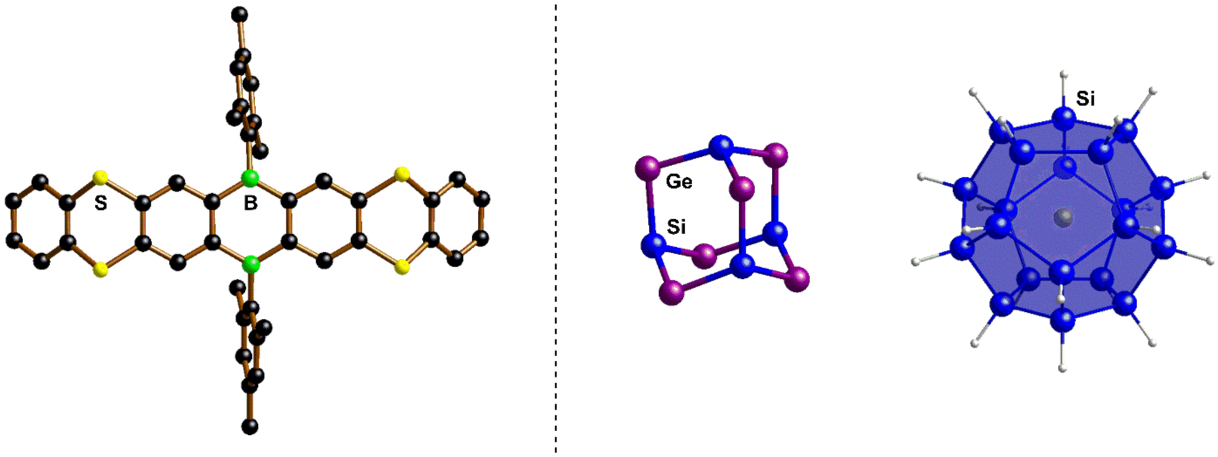
PL7

Boron-Doped Polycyclic Aromatic Hydrocarbons and Large Silicon Clusters

Marcel Bamberg[a], Tao Jin[a], Benedikt Köstler[a], Luigi Menduti[a], Matthias Wagner[a],*
[a]*Goethe-Universität Frankfurt, Campus Riedberg, 60438 Frankfurt am Main*
matthias.wagner@chemie.uni-frankfurt.de

ABSTRACT

The talk is divided in two parts dealing with compounds containing boron or silicon, both of which are key players in the chemistry of p-block materials. Part I is devoted to linear or helical B,S-doped polycyclic aromatic hydrocarbons that have ambipolar and charge-transfer properties; a fluorescence boost can be triggered by addition of Ag^+ cations. Part II deals with the straightforward and high-yield synthesis of Si,Ge-heteroadamantanes and siladodecahedranes ('silafulleranes'). This work paves the way to well-defined nanostructures of group IV elements.[1,2]



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Bio-Sketch of Speaker

Professor Matthias Wagner
Goethe University Frankfurt, Max-von-Laue-Strasse 7,
60438 Frankfurt/Main, Germany
https://www.uni-frankfurt.de/58708118/wagner

Education Experience

1992–1994	Oxford University, Postdoctor (advisor: Prof. M. L. H. Green)
1990–1992	LMU Munich, PhD (supervisor: Prof. H. Nöth)
1984–1990	LMU Munich, Diploma

Appointments

2000–present	Goethe University Frankfurt, Full Professor
1998–1999	Goethe University Frankfurt, Associate Professor
1994–1997	Technical University Munich, Habilitation (mentor: W. A. Herrmann)

Honors and Awards

2014	Member of the *Polytechnical Society Frankfurt*
1998	ˈHeisenberg awardˈ of the *German Science Foundation (DFG)*
1997	ˈKarl-Winnacker awardˈ of the *Hoechst AG*

Research Interests

B, Si, Ge chemistry, cluster chemistry, optoelectronic materials, homogeneous catalysis

Representative Publications

[1] Georg, I.; Bursch, M.; Endeward, B.; Bolte, M.; Lerner, H.-W.; Grimme, S.; Wagner, M. *Chem. Sci*., **2021**, *12*, 12419.
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PL8

Tertiary Phosphines with Functionalities: Synthesis, Transition Metal Chemistry and Catalytic Studies

Maravanji S. Balakrishna

Department of Chemistry, Phosphorus Laboratory,
Indian Institute of Technology Bombay, Powai, Mumbai 400076.
krishna@chem.iitb.ac.in

ABSTRACT

Ever growing interest in designing new phosphorus based ligands is mainly due to their adoptability to all types of metallic environments, and find applications in homogeneous catalysis.[1] In most of the reactions, although they display non-innocent behaviour, they do control the reactivity of the metal centre through both steric and electronic attributes.[2] However, there are instances wherein P—C bond cleavage has been observed and the same has been exploited in generating a variety of tertiary phosphines and also in alkylation and arylation reactions. In the present investigation, the reaction of amide bridged bisphosphine o-$Ph_2PC_6H_4C(O)N(H)C_6H_4PPh_2$-$o$ with palladium(II) salts induced an unexpected P—C bond cleavage of one of the P—Ph bonds, and formation of a new P—N bond resulting in a five membered cyclic 1,2-azaphospholene with the elimination of PhH. Similar reactions with platinum derivatives also resulted in 1,2-phospholene-phosphine complex, wherein the complex with a Pt—Ph bond was isolated and structurally characterized. Besides, several other complexes were also isolated including robust pincer complexes. The details will be presented.

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Bio-Sketch of Speaker

M S Balakrishna, Professor of Chemistry
Department of Chemistry
Indian Institute of Technology Bombay
Powai, Mumbai 400076

B.Sc., and M.Sc. from Mysore University
Ph.D from the Indian Institute of Science Bangalore
Postdoctoral Fellow at University of Alberta, Edmonton, Canada
Research Associate at Tulane University, New Orleans, USA

Joined the Chemistry Department at IIT Bombay as an Assistant Professor in 1996 and became Full Professor in 2005

Research Interest:
Main Group and Organometallic Chemistry
Organo-phosphorus chemistry
Homogeneous Catalysis and Anticancer studies

Published Research Papers: 210 + Five book chapters + Edited a book on Copper(I) Chemistry of Phosphorus ligands for Elsevier
Papers presented in conferences (Self and Group members): 160
Invited Lectures: 450+
Ph.D. Guided: 24
M.Sc. projects/res. associates/ Project staff/Postdoctoral Fellows guided: 38

PL9

Main group Lewis acids for applications in anion transport and catalysis

François P. Gabbaï

Department of Chemistry, Texas A&M University, College Station, Texas 77843-3255, United States of America

francois@tamu.edu

ABSTRACT

Research in the Gabbaï group has been dedicated to the synthesis and study of Lewis acidic main group compounds with the development of applications in molecular recognition and catalysis as the ultimate goals. This talk will highlight a series of recent results obtained in pursuit of these goals. The first part of the presentation will show how Lewis acidic boron-, antimony- and tellurium-based anion receptors can be deployed in aqueous media to effectively transport a range of anions across the phospholipid membrane of artificial vesicles and live cells.[1-4] The second part of the talk will show that the same type of main group Lewis acids can be used to engage both organic substrates and transition metal halides for application in organic and organometallic catalysis.[5]

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Bio-Sketch of Speaker

François Gabbaï was born in 1968 in Montpellier (France). Upon completion of his undergraduate chemistry studies at the Université de Bordeaux in 1990, he joined the graduate program at the University of Texas at Austin to work with Alan Cowley. After obtaining his Ph.D. in 1994, he was awarded an Alexander von Humboldt Fellowship and subsequently a Marie Curie Fellowship which allowed him to work with H. Schmidbaur at the Technische Universität München (Germany) as a postdoctoral fellow and later as an "Habilitand". In 1998, he joined Texas A&M University where he now holds the Arthur E. Martell Chair of Chemistry. François, who is a member of the advisory board of several international journals, has served as an associate editor for Organometallics between 2011 and 2019, and for Chemical Science since April 2019. He is a Fellow of the American Chemical Society (ACS), a Fellow of the Royal Society of Chemistry, and the recipient of the 2009 North American Dalton Lectureship. In 2016, he received the F. Albert Cotton Award in Synthetic Inorganic Chemistry from the ACS. His most recent recognitions include a 2019 Distinguished Achievement Research Award from the Texas A&M Association of Former Students and his promotion to the title of Distinguished Professor. His research interests revolve around the chemistry of p-block elements and late transition metals with applications in the domain of molecular recognition, anion sensing and transport, and catalysis.

PL10

Enhancing lanthanide single-ion magnetism through phosphorus based ligands: Role of symmetry and axiality

Ramaswamy Murugavel

Department of Chemistry, Indian Institute of Technology Bombay,
Mumbai-400 076, India. rmv@chem.iitb.ac.in

ABSTRACT

The current rush in the field of SMMs is driven by better understanding of the effects of crystal field (CF) and molecular symmetry on the magnetic properties, especially in the case of mononuclear paramagnetic complexes. This has led to the advent of highly anisotropic air-stable single-ion magnets (SIMs) with magnetic blocking temperatures and anisotropic energy barriers. This talk would summarize our recent research in the light of the emergence of the importance of CF and symmetry in 4f ion based single-ion magnets (SIMs), especially in the context of SIMs with D5h symmetry, apart from commenting on the synthetic efforts adopted to place these metal ions in unusual coordination geometries.

Bio-Sketch of Speaker

Professor R. Muragavel
Department of Chemistry
Indian Institute of Technology Bombay
Powai, Mumbai 400076

Ramaswamy Murugavel received his B.Sc. and M.Sc. degrees from University of Madras and Ph.D. from IISc. He carried out postdoctoral work at the University of Göttingen and joined the chemistry faculty of IIT Bombay in December 1997, where he is currently Biswas Palepu Distinguished Chair Professor and J C Bose National Fellow. He is a fellow of the Indian Academy of Sciences, the Indian National Science Academy, and the Royal Society of Chemistry. He has been conferred with J. C. Bose National Fellowship, Swarnajayanti Fellowship, Alexander von Humboldt Fellowship, DAE-SRC Outstanding Investigator Award, DFG Mercator Professorship, C. N. R. Rao National Prize in Chemical Sciences, S. C. Bhattacharya Award for Excellence in Research in Basic Sciences, SASTRA-CNR Rao Prize, DAE Young Scientist Award, CRSI Bronze Medal, MRSI Medal, and J. C. Ghosh Medal. His research work has been published in the form of 200+ publications. His current research interests include transition metal organophosphate chemistry, molecular magnetism in lanthanide complexes, metal phosphate materials and covalent organic frameworks for energy applications.

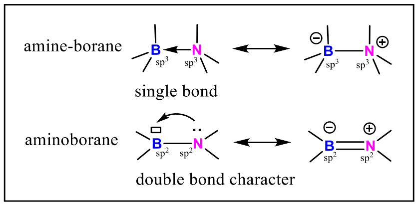
PL11

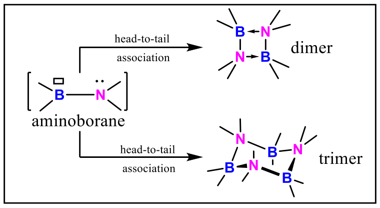
B-N bonds engineering: from B-H bond activation to polyaminoboranes

Gilles Alcaraz[a],* Marc Devillard[a]
[a]*Université de Rennes, CNRS, ISCR–UMR 6226, Rennes F-35000, France.*
gilles.alcaraz@univ-rennes1.fr

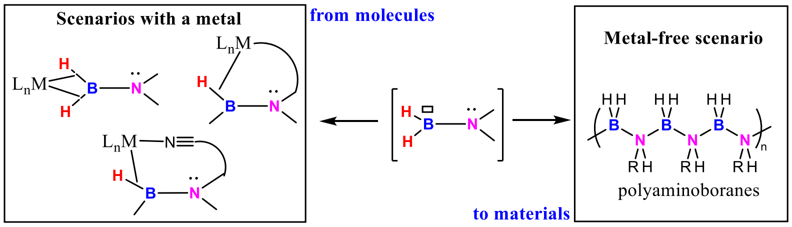
ABSTRACT

Aminoborane chemistry and B-N bond engineering offer many opportunities to better understand the synthesis and properties of a variety of molecules and materials incorporating this motif. The character of the B-N bond can be varied from single to double depending on the substitution pattern of the B-N unit and the respective hydridization of the atoms. In the case of aminoboranes that are the inorganic analogues of alkenes, these molecules can be obtained in their monomeric form otherwise they stabilize by self-association into dimers or trimers.





This situation is strongly dependent on the way of generating and stabilizing them. In this regard, metal induced B-H activation processes have proven to be efficient for both, even enabling their polymerization and thus offering an access to the corresponding aminoboranes. To make this discussion more concrete we will go from the molecule to the material via different B-H activation scenarios around the aminoborane chemistry[1] to finish by a metal-free polymerization process for the preparation of a variety of polyaminoboranes including functionalized one.[2]



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Bio-Sketch of Gilles Alcaraz

Université de Rennes, CNRS, ISCR–UMR 6226, Rennes F-35000, France.

gilles.alcaraz@univ-rennes1.fr

- In 1995, Gilles Alcaraz got his Ph.D from the Université de Toulouse 3 under the supervision of Dr. Antoine Baceiredo and Dr. Guy Bertrand: "Electron deficient species and P-containing constrained cycles".

- In 1997, after a post-doctoral position in ETH-Zürich (CH) with Pr. Dr. Hansjörg Grützmacher on phosphiranes chemistry, he was hired as CNRS fellow at the University of Rennes 1 in Dr. Michel Vaultier's group. His research activities focused on solid-supported boron chemistry involving Suzuki-Miyaura coupling and multicomponent reactions. Then he started to develop the chemistry of diisopropylaminoborane in palladium-catalyzed borylation reactions exploiting B-H bond activation.

- In 2006, he moved to the Laboratoire de Chimie de Coordination (LCC) in Toulouse to collaborate with S. Sabo-Etienne and Mary Grellier within the newly created team "Organometallic Architecture and Catalysis". In this framework, he developed an organometallic boron chemistry focusing on the activation of B-H bonds and involving unconventional (monosubstituted and polyfunctional) boranes mostly derived from the chemistry of aminoboranes and amine-boranes. In 2011, he was promoted CNRS research director.

- In 2016, he moved back to the University of Rennes 1 and joined the Institute of Chemical Sciences (ISCR). His interest is still in the organic and organometallic chemistry of boron. A particular focus is on aminoboranes chemistry and B-N bonds engineering in close connection with molecules displaying optical properties and polymers.

PL12

The Main Group Elements of Life

Govindasamy Mugesh

Department of Inorganic and Physical Chemistry, Indian Institute of Science, Bangalore 560 012

mugesh@iisc.ac.in

ABSTRACT

More than 60 chemical elements have been detected in human body. However, only 28 of them are known to participate in biological processes. These include 11 bulk biological elements, 12 essential trace elements and 5 elements possibly essential for bacteria, plants and/or animals. Interestingly, most of the biological processes involve main group elements. While the lighter elements such as C, H, O, N, S and P constitute more than 98% of the human body in the form of proteins, nucleic acids, carbohydrates, hormones, and vitamins, some of the heavier main group elements also play crucial roles in the life processes. In this talk, two such main group elements - selenium and iodine - in biological chemical reactions will be discussed.

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Bio-Sketch of Speaker

Govindasamy Mugesh
Department of Inorganic and Physical Chemistry
Indian Institute of Science
Bangalore 560012, INDIA
Email: mugesh@iisc.ac.in
WWW: http://ipc.iisc.ac.in/gm.php

G. Mugesh received his B.Sc. (1990) and M.Sc. (1993) degrees from the University of Madras and Bharathidasan University, respectively. He obtained his Ph.D. (1998) at the Indian Institute of Technology, Bombay, under the supervision of Prof. H. B. Singh. In 2000, he moved to Germany as an Alexander von Humboldt Fellow at the Technical University, Braunschweig, to work with Prof. Wolf-Walther du Mont. In 2001-2002, he worked with Prof. K. C. Nicolaou at the Scripps Research Institute, as a Skaggs postdoctoral fellow. The research in Mugesh's laboratory ranges from fundamental chemical synthesis and reaction mechanism at the molecular level to practical biomedical applications.

Mugesh is a recipient of IIT Bombay Distinguished Alumnus Award (2021); SASTRA-CNR Rao Award in Chemistry & Materials Science (2021); Dr. Ghanshyam Srivastava Memorial Award, Indian Chemical Society (2020); Infosys Prize in Physical Sciences (2019); CRSI Silver Medal (2019); National Prize for Research on Interfaces of Chemistry and Biology (2017); Rajib Goyal Prize in Chemical Science (2017); Bhagyatara Award (2017); ISCB Award for Excellence (2016); J. C. Bose National Fellowship (2015); Shanti Swarup Bhatnagar Prize (2012); AstraZeneca Excellence in Chemistry Award (2012); CDRI Award for Excellence in Drug Research (2010); Swarnajayanti Fellowship (2006-07); Ramanna Fellowship, DST (2006).

He is a fellow of the National Academy of Sciences, India (2012), Indian Academy of Sciences (2012) and Indian National Science Academy (2016). He currently serves as a Vice-President of the Chemical Research Society of India (CRSI), President of the Asian Chemical Editorial Society (ACES). He also serves in the Editorial or Editorial Advisory Boards of Chemistry – A European Journal (ChemPubSoc, Europe), Organic and Biomolecular Chemistry (RSC), ACS Omega (ACS); Bioorganic Chemistry (Elsevier) and Biological Chemistry (De Gruyter, Germany).

IL1

Access to CAAC Stabilized Stable Gold Nanoparticles

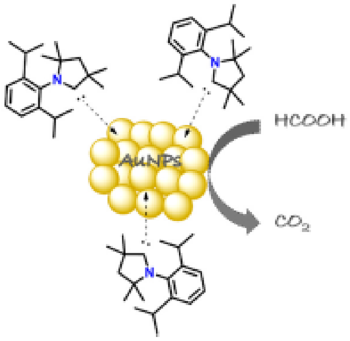
Shabana Khan[a*]

[a]*Department of Chemistry, Indian Institute of Science Education and Research Pune, Dr. Homi Bhabha Road, Pune- 411008, India*

Email: shabana@iiserpune.ac.in

ABSTRACT

The N-heterocyclic carbenes (NHCs) have gained significant popularity as coordinating ligands due to their ability to make stable complexes with transition metals. Recently, N-heterocyclic carbenes (NHCs) have attracted increasing attention as alternative ligands for coating Au, and other nanocolloids as their steric and electronic properties can easily be tuned.[1] Nonetheless, the use of most nucleophilic carbene analogue, cyclic (alkyl)(amino)carbenes (CAAC), in nanoparticle synthesis is still minimal. There are only two examples of CAAC being utilized as a ligand to stabilize metal nanoparticles.[2-3] Herein, we present CAAC-supported gold nanoparticles' synthesis, characterization, and catalytic application.



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Bio-Sketch of Speaker

Name: Dr. Shabana Khan (Associate Professor)

Address: Indian Institute of Science Education and Research (IISER) Pune, India; Dr. Homi Bhabha Road, Pune-411008, Maharashtra, India

E-mail: shabana@iiserpune.ac.in

Research Area: Main group chemistry, Organometallic chemistry, Catalysis

Shabana Khan obtained her Ph.D. degree from the Indian Institute of Technology, Delhi, in 2008. Subsequently, she received Deutscher Akademischer Austausch Dienst (DAAD) postdoctoral fellowship to work with Prof. Herbert W. Roesky at the University of Goettingen, followed by a second postdoc with Prof. Manuel Alcarazo at the Max Planck Institute for Coal Research. She joined IISER Pune as an assistant professor in 2013 and presently working as an associate professor.

Research interests:

Her research interest includes the synthesis of low-valent compounds, their reactivity, and their application in catalysis.

Awards and Recognitions:

1. International advisory board member of *European Journal of Inorganic Chemistry* (EJIC) and *Chemistry- An Asian Journal* (2022- onwards).
2. Received SERB-POWER fellowship award 2021.
3. Alexander von Humboldt Fellowship for an experienced researcher (2020-2022).
4. International advisory board member of *Organometallics* (2018 - 2021).
5. Received Young Scientist Award in Chemical Frontiers Conference, Goa-2018.

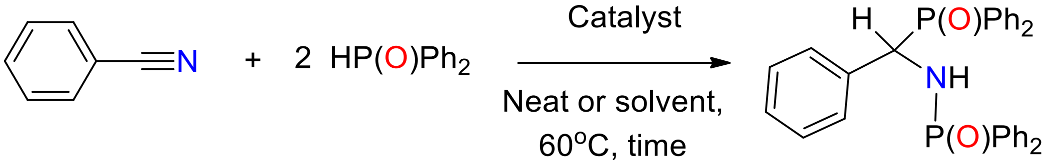
IL2

Synthesis of Organophosphorus Compounds Mediated by Main Group Metal Catalysts

Tarun K. Panda*
Department of Chemistry, Indian Institute of Technology Hyderabad, Kandi, 502284,
Sangareddy, Telangana, India, (tpanda@chy.iith.ac.in)

ABSTRACT

Organophosphorus compounds, such as α-aminophosphonates and related derivatives, considered as the structural analogs of α-amino acids, have significant importance as ligands in synthetic organic chemistry and mainly in medicinal,[1] pharmacological and agricultural chemistry[4] due to their potential biological activity as enzyme inhibitors, antibiotics, antihypertensives, antitumor, antibacterial, and enzyme-inhibitors.[2] Due to this, more efforts have been made in catalysis research to develop an efficient method for the synthesis of α-aminophosphine oxides over the last few years.[3] In our recent work we have explored the use of various *s* and *p* block metals as pre-catalysts in the hydroboration[4] and hydrophosphorylation[5] of nitriles and alkynes for the facile synthesis of amines and organophosphorus compounds respectively. Easy availability, nontoxicity, and economic viability of main group metal complexes have encouraged us to explore their feasibility as pre-catalysts in double hydrophosphorylation of nitriles as well terminal alkynes with diphenylphosphane oxide. We also explored an efficient and convenient procedure for the synthesis of α-aminophosphonates by the one-pot three-component reaction of aldehyde, amine, and diphenylphosphine oxide, or diethyl phosphite catalyzed by β-ketoiminato indium complexes under solvent-free conditions.[6]



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Bio-Sketch of Speaker

Tarun Kanti Panda
Professor
Department of Chemistry
Indian Institute of Technology Hyderabad,
Kandi, Sangareddy, Telangana, India
Contact Number: +91-40-23016254
E-Mail: tpanda@chy.iith.ac.in, tpanda@iith.ac.in
Homepage: https://sites.google.com/site/tkpandagroup/home

Tarun K. Panda obtained his Master of Science in Chemistry from IIT, Kanpur in 2002 and received his Dr. rer. nat from Freie Universität Berlin, Germany in 2005 under the supervision of Prof. Dr. Peter W. Roesky in the area of Organometallic Chemistry. Dr. Panda joined the working group of Prof. Dr. Matthias Tamm at TU Braunschweig, Germany as a postdoctoral fellow in 2006. He was awarded the Japan Society for the Promotion of Science (JSPS) postdoctoral fellowship in 2008 to work with Prof. Kazushi Mashima in the Graduate School of Engineering, Osaka University, Japan. In 2010, he returned to India to join the Department of Chemistry, Indian Institute of Technology Hyderabad (IITH) India as Assistant Professor. He was promoted to Associate Professor in 2015 and Professor in 2019 at the same Institute. He has been awarded the CRSI Bronze medal 2021 for his significant contribution to main group metal chemistry. His principal research interests include the development and understanding of the mechanistic insights of well-defined earth-abundant, non-toxic, and environmentally benign metal complexes using various amido and amidophosphine ligands and their utilization in catalytic hydroboration, hydroamination, hydrophosphorylation reaction, and ring-opening polymerization under ambient reaction conditions.

Publications:

1. Bhattacharjee, J.; Sarkar, A.; Panda, T. K.; *Current Opinion in Green and Sustainable Chemistry*, **2021**, *31*, 100545.
2. Rej, S; Das, A.; Panda, T. K.; *Advanced Synthesis & Catalysis*, **2021**, *363*, 4818-4840
3. Banerjee, I.; Panda, T. K.; *Org. Biomol. Chem.*, **2021**, *19*, 6571-6587.
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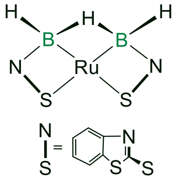
IL3

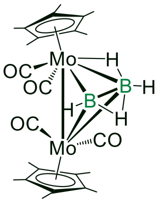
Structural Paradigms in Metallaborane Chemistry

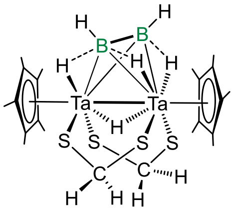
Sundargopal Ghosh
Department of Chemistry, Indian Institute of Technology Madras, Chennai 600 036, India
Email: sghosh@iitm.ac.in

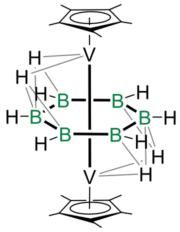
ABSTRACT

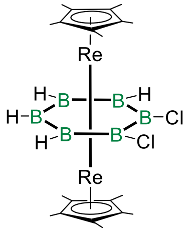
The fascinating aspect of metallaborane chemistry is that several classic organometallic complexes that defined fundamental structural and bonding paradigms are mimicked by many isoelectronic metallaborane analogues.[1] In this connection, diborane compounds not only mimics several classic organometallic compounds but also they have been extensively explored for the broad understanding of the chemical bonding and catalysis.[2] For example, we have recently synthesized and structurally characterized a bimetallic diborane(4) which mimics the Cotton dimolybdenum–alkyne complex $[\{CpMo(CO)_2\}_2C_2H_2]$.[3] Also, we have isolated the first classical diborane(5) $[B_2H_5]^-$, in which the *sp*^{2}-B center is stabilized by the electron donation from tantalum.[4] The isolation of boron analogue of benzene, i.e., planar B_6H_6 is a long-time dream of any boron chemist. Theoretical calculations suggested that the formation of triple-decker sandwich complex may led to the isolation of planar B_6H_6.[5,6] Indeed, for the first time, we are able to isolate a planar B_6H_6 by making triple-decker sandwich complex with two {VCp*} or {TiCp*} fragments. The key results of this work will be presented.











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Bio-Sketch of Speaker

Sundargopal Ghosh

Professor
Department of Chemistry, Office 317
Indian Institute of Technology Madras
Chennai 6000 36
Phone (o): 91 44 2257 4230; Phone (res): 91 44 22576230
Fax: 91 44 2257 4202; Mobile 9884432944
WEBPAGE: http://chem.iitm.ac.in/Faculty/ghosh/

Title of the talk: Structural Paradigms in Metallaborane Chemistry

Biography:

Prof. Sundargopal Ghosh obtained his B.Sc. and M.Sc. from University of Calcutta. He then received his PhD from Indian Institute of Technology Bombay in 1998. Following a postdoctoral fellowship with Professor Thomas P. Fehlner at the University of Notre Dame, USA he joined the Department of Chemistry at Indian Institute of Technology Madras in 2005 where he is currently a Professor. His research interests lie in the area of transition metal-boron compounds and their application in catalysis and small molecule activation. He has 238 scientific publications in internationally acclaimed journals. For his contribution in chemical science, Chemical Research Society of India (CRSI) in 2013 conferred him with Bronze Medal and he was awarded Institute Research & Development Awards (IRDA) in 2014 by IIT Madras. He is an elected fellow of Indian Academy of Sciences (FASc) and Fellow of the National Academy of Sciences (FNASc). He is awarded Professor Priyadaranjan Ray Memorial Award in 2019. He has supervised 26 PhD students; most of them hold positions in well-known academic institutions.

Selected Contributions

1. K. Saha, D. K. Roy, R. D. Dewhurst, S. Ghosh and H. Braunschweig, *Acc. Chem. Res.*, **2021**, *54*, 1260.
2. S. Kar and S. Ghosh, Borane Polyhedra beyond Icosahedron. in: *Structure and Bonding.* Ed. D. M. P. Mingos, Springer, Berlin, Heidelberg, **2021**, https://doi.org/10.1007/430_2021_85
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IL4

Extending BN/C=C Isosterism for Developing Novel Functional Materials

Thilagar P*

aDepartment of Inorganic and Physical Chemistry, IISc Bangalore-560012

Email: thilagar@iisc.ac.in

ABSTRACT

There has been a great deal of resurgence in boron chemistry in recent years. Substitution of isoelectronic B–N units for C=C units produce molecules with structural similarities to the all-carbon frameworks but with fundamentally altered electronic and optical properties. Ever since the revolutionary work of Dewar nearly sixty years ago, the liaison between B–N and C–C has attracted attention of organic, inorganic, materials, and computational chemists equally, in recent years. New applications and novel molecular scaffolds resulted from these studies. Recently, our group pioneered the concept of controlling the optical characteristics of luminescent compounds by constraining the molecular conformations. As a result of systematic investigations, very significant advances have been made in our understanding of the solid-state optical properties of several BN-compounds. In this talk, some quite interesting aspects of delayed fluorescence of BN compounds will be presented.

Bio-Sketch of Speaker

P. Thilagar obtained his B.Sc. from Tagore Arts College and M.Sc from Pondicherry Central University. He received his Ph.D. in 2007 working with Prof. V. Chandrasekhar at the Indian Institute of Technology Kanpur (IIT-K) and has postdoctoral experience from working at the University of Rutgers with Prof. Frieder Jakle. In 2009, he joined the Indian Institute of Science as a faculty member in the Department of Inorganic and Physical Chemistry. In 2009 he was elected as Young Associate of the Indian Academy of Sciences and was the recipient of the CRSI (Chemical Research Society of India) Bronz medal in Chemistry (2017). He serves in the Editorial Advisory Board of Organometallics journal published by the American Chemical Society. He also serves in the International Editorial Board of Aggregates and Chemphotochem, the journals published by the Wiley vch. He served as guest editor for the special issues on “Main-Group Molecules to Materials” in the Journal of Organometallic Chemistry. He has also served as guest editor for the special issues on “Recent Advances in Stimuli-responsive Photoluminescence Switching of Purely Organic Compounds” in the Journal Frontiers in Chemistry. He has organized two international and three national-level conferences. He has written popular articles on boron chemistry for the general science audience. His research work has received international media attention and has been featured in Science Translational Medicine Chemical News, Chemical Engineering News, and Atlas of Science. His current research interests concentrate on the development and possible applications of various classes of main group elements containing luminescent dyes and the medicinal aspects of boron-containing peptides.

Aluminium Complexes with NHCs and NHIs in Bond Activations and Catalysis

Shigeyoshi Inoue*

Department of Chemistry, Institute of Silicon Chemistry and Catalysis Research Center,
Technical University of Munich, Lichtenbergstraße 4, 85748 Garching bei München, Germany

E-mail:s.inoue@tum.de

ABSTRACT

As the third most abundant element in the Earth's crust, aluminium with its favorable environmental and toxicological properties is a very promising and desirable candidate for use in bond activations and catalysis. Low-oxidation state aluminium compounds have presented a particular challenge for synthetic chemists, with a noticeable dearth of such compounds in the literature compared to those based on neighbouring elements. Recently, several research groups have shown that these aluminium complexes undergo facile oxidative addition with a series of strong σ bonds and can also act as catalysts. In this presentation, synthesis, isolation and reactivity of selected aluminium compounds using N-heterocyclic carbenes (NHCs) and N-heterocyclic imines (NHIs) will be delivered. Particularly, unique small molecule activations and homogenous catalysis by using these aluminium complexes will be presented.

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[10] Xu, H.; Weetman, C.; Hanusch, F.; Inoue, S. *submitted.*

Bio-Sketch of Speaker

Shigeyoshi Inoue

Address: Department of Chemistry, Institute of Silicon Chemistry & Catalysis Research Center, Technical University of Munich, Lichtenbergstraße 4, 85748 Garching bei München, Germany

Homepage: https://www.department.ch.tum.de/si/home/

Tel: +49-89-289-13834 **E-mail**: s.inoue@tum.de

Employment

Since 2020	Professor of Silicon Chemistry (W3), Technical University of Munich
2015-2020	Professor of Silicon Chemistry (W2), Technical University of Munich
2010-2015	*Sofja Kovalevskaja* Professor, Technical University of Berlin
2009-2010	*JSPS Postdoc Fellow*, Technical University of Berlin with Prof. M. Driess
2008	*Humboldt Postdoc Fellow*, Technical University of Berlin with Prof. M. Driess

Education

2008	Ph.D.	University of Tsukuba with Prof. A. Sekiguchi
2005	M.Sc.	University of Tsukuba with Prof. A. Sekiguchi
2003	B.Sc.	University of Tsukuba

Research Field

Main Group Chemistry, Silicon Chemistry, Organometallic Chemistry, Catalysis.

Awards and Recognition

Eugen und Ilse Seibold Prize from *German Research Foundation* (2020), ERC Consolidator Grant (2020), NISTEP Award from *Ministry of Education, Culture, Sports, Science and Technology, Japan* (2018), Carl Duisberg Memorial Prize from *German Chemical Society* (2017), The Chemical Society of Japan Award for Young Chemists (2015), ERC Starting Grant (2014), AUDC Prize from *German Chemical Society* (2012), Sofja Kovalevskaja Award from *Alexander von Humboldt Foundation* (2010).

IL6

Multifunctional MOFs for Docking/Sensing and Catalysis

Sharad Kumar Sachan, Sarita Tripathi, Namita Singh, Renganathan Srirambalaji and Ganapathi Anantharaman*
Department of Chemistry, Indian Institute of Technology (IIT) Kanpur, Kanpur -208016
garaman@iitk.ac.in

ABSTRACT

Porous materials such as zeolites have a significant impact both industrially and day-to-day applications in life. The structural rigidity due to primary $[SiO_4]^{4-}$ and $[AlO_4]^{3-}$ units in the zeolites renders framework stability which are found to be one of the prime criteria for its vast applications. At times, the lack of functional properties, and the nuances of the synthetic procedure limit these materials' growth.[1] Alternatively, coordination polymers (CPs) or metal-organic frameworks (MOFs) have gained enormous attention due to their simplicity in preparation, structural diversity, and the applications in gas-adsorption, separation of small molecules, catalysis, sensing of small molecules to hazardous materials, drug delivery, nonlinear optics, proton conductivity, and biological systems. The robustness of the MOFs against hydro- and thermal stability under different pH solutions without losing the crystallinity and their porosity is an essential criterion for the above potential applications.[1-3] In this talk, the imidazole-carboxylic acid-based robust CPs/MOFs and their applications towards the areas of gas adsorption, luminescence-based sensing/remediation of hazardous materials, and catalysis will be presented.[4]

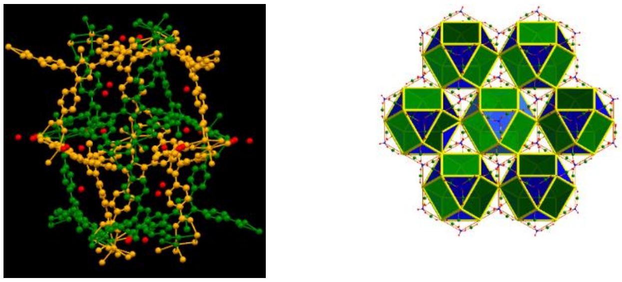

Figure: Cuboctahedral 3D- MOFs of cadmium and indium

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Bio-Sketch of Speaker

Name: **Dr. G. Anantharaman**
Academic degree:
PhD (2003) Univ. of Göttingen, Germany (Professor H. W. Roesky)
MSc (1999) IIT Bombay
Year of joining: 2004
Current designation: Associate Professor
Previous designations held:
Lecturer (2004-2007)
Assistant Professor (2007-2016)
Specialization: Main Group Chemistry, Organometallics, Coordination Chemistry

publications: Over 45
of PhD graduated: 12
# of MSc project/thesis guided: 16

Recognitions:

- **Indian Chemical Society Research Excellence Award** for Oral presentation at INTERNATIONAL SEMINAR on "Recent Advances in Chemistry & Material Sciences (2020) Month-long Program for August 2020, In Commemoration of the 159th Birth Anniversary of Acharya Prafulla Chandra Ray
- Commendation letters from Director, IIT Kanpur for teaching courses in Advanced main group chemistry, Inorganic Chemistry Laboratory Experiments, and Application of Modern Instrumental Methods
- Obtained a DFG fellowship for the year 2003-2004 during my Ph.D.
- IIT Bombay Research Paper Awards for the years 2007 and 2011

Contributions outside institute level activities

- Subject expert for appointment of "Guest/permanent Faculty" at Invertis University, Bareilly- UP, India and M. M. M. University of Technology, Gorakhpur
- Member and expert committee for M. Sc syllabus, Department of Chemistry & Environmental Science, M. M. M. University of Technology, Gorakhpur
- Member Board of studies, M. M. University of Technology, Gorakhpur from 2017-2020
- Member, Research Degree Committee (RDC) of Chemistry/Applied Chemistry discipline, Dr. A.P.J. Abdul Kalam Technical University, Lucknow
- Member, The Chemical Research Society of India (CRSI) from 2004

IL7

Antimony and Bismuth Lewis Acids: Catalytic Hydrosilylation

Ajay Venugopal

School of Chemistry, Indian Institute of Science Education and Research Thiruvananthapuram

venugopal@iisertvm.ac.in

ABSTRACT

Salts of heavier pnictogens (Pn), antimony, and bismuth in +3 oxidation state are employed as Lewis acids in organic synthesis.[1] Common examples of these salts include chlorides, carboxylates, and trifluoromethanesulfonate. A qualitative model for the origin of Lewis acidity in Sb(III) and Bi(III) compounds was proposed by Norman in 1994.[2] According to this model, a polarized Pn–X bond has a corresponding low lying antibonding σ*-orbital that can accept a pair of electrons. The Pn–X bonds constitute the primary bonds, while the interaction between antibonding orbitals and Lewis bases constitutes the secondary bonding. The energy levels of the antibonding orbitals and the Lewis acidity of PnX_3 depend on the extent of polarization in primary bonds. Ligand choice determines the tuning of the σ* orbital energy providing a tool to control the Lewis acidity in antimony and bismuth Lewis acids. Based on our recent findings, this presentation will provide insights on the ligand effects as a design parameter to access new antimony and bismuth Lewis acids.[3] Catalytic hydrosilylation is demonstrated as proof of our concept.

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Bio-Sketch of Speaker

Ajay Venugopal is an associate professor at the Indian Institute of Science Education and Research Thiruvananthapuram and works in main group chemistry. In 2016, he established a state-of-art laboratory in the scenic new campus. The primary focus of his research is on understanding the structure and bonding in reactive main group compounds, stabilization of unusual coordinate modes, activation of inert chemical bonds, and Lewis acid catalysis. Curiosity-driven research in the isolation of reactive main group cations comprising magnesium, zinc, aluminum, antimony, and bismuth has led his group to explore their potential as Lewis acids in catalytic hydrosilylation.

IL8

Unlocking the Potent Donor Ability of Anionic *N*-Heterocyclic Olefins

Eric Rivard[a,*]

[a]*Department of Chemistry, University of Alberta, 11227 Saskatchewan Dr., Edmonton, Alberta, CANADA*

erivard@ualberta.ca

ABSTRACT

Over the past decade, our group has studied a class of carbon-based ylide donor that we have termed as *N*-heterocyclic olefins (NHOs).[1] These ligands have the general framework, NHC=CR_2, where NHC = *N*-heterocyclic carbene unit, and are sufficiently Lewis basic to stabilize unusual main group entities, such as Sn(II) hydrides.[2] In this presentation I will be discussing the chemistry of a deprotonated *anionic* NHO and its use to access low-coordinate main group species,[3] including the first acyclic diorganosilylene.[4] More recent directions involve the development of an easy-to-handle Zn(II) aNHO source[5] and access to an In(I)-aNHO tetramer.

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Bio-Sketch of Speaker

Prof. Eric Rivard, University of Alberta

Prof. Eric Rivard completed his Ph.D. at the University of Toronto under the supervision of Professor Ian Manners. After NSERC sponsored postdoctoral work with Professors Jonas Peters (Caltech) and Philip Power (University of California, Davis), and a brief research stay with Professor Cameron Jones (Monash University), he joined the University of Alberta in 2008, where he is now a Full Professor. He has given > 150 invited lectures worldwide and was recently an Alexander von Humboldt Experienced Researcher Fellow in Germany. He was also a Japanese Society for the Promotion of Science (JSPS) Long-term Visitation Fellow in 2015, an RCMS Visiting Professor at Nagoya University in 2016, was the inaugural 2016 Michael Lappert Lecturer (Royal Society of Chemistry, UK), and won the 2018 Strem Chemicals Award for Pure and Applied Inorganic Chemistry (Canadian Society for Chemistry). He is currently on the Editorial Advisory Boards for *Chemical Society Reviews*, *Inorganic Chemistry*, and *Dalton Transactions*. The Rivard group studies fundamental low-coordinate and main group hydride chemistry, catalysis, semiconducting nanomaterial synthesis, and the development of phosphorescent materials and conjugated polymers based on main group elements.

Selected review articles from the Rivard group:

[1] Main Group Metal Hydrides: Roy, M. M. D.; Omaña, A. A.; Wilson, A. S. S.; Hill, M. S.; Aldridge, S.; Rivard, E. *Chem. Rev.* **2021**, *121*, 12784.

[2] Main Group π-Conjugated Materials: Parke, S. M.; Boone, M. P.; Rivard, E. *Chem. Commun.* **2016**, *52*, 9485.

[3] Inorganic Hydrocarbons: Rivard, E. *Chem. Soc. Rev.* **2016**, *45*, 989.

IL9

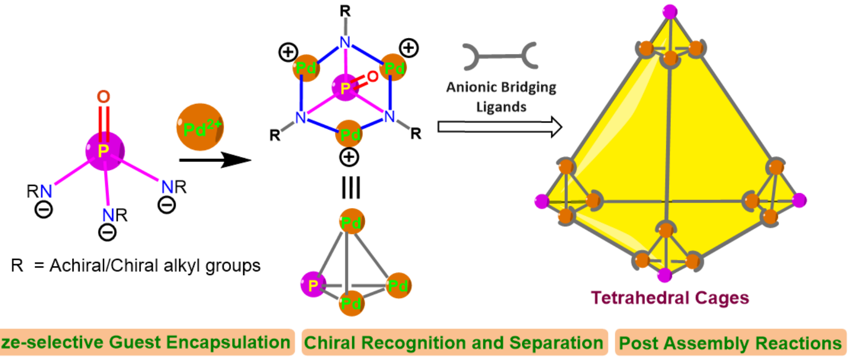
Neutral Polyhedral Pd(II) Cages Supported by Tris(imido)phosphate Trianions

Ramamoorthy Boomishankar[a,*]

[a] *Chemistry Division, Indian Institute of Science Education and Research, Dr. Homi Bhabha Road, Pune - 411008, India*
boomi@iiserpune.ac.in

ABSTRACT

Polyhedral cages derived from metal-ligand coordination bonds are an important class of materials in supramolecular chemistry. Our group has developed a facile route for preparing neutral polyhedral Pd(II) cages in tetrahedral and cubic topologies supported by the elusive tris(imido)phosphate trianions, $[(RN)_3PO]^{3-}$ $((X)^{3-})$, analogous to PO_4^{3-} ion as the cis-protecting units. These cages consist of the $(Pd_3X)^{3+}$ clusters as the corners and wide-angle chelating ligands such as oxalate dianions, pyrazine dicarboxylate anions and anilate anions as linkers. All the obtained cage assemblies offer excellent platforms for studying host-guest chemistry in solution as well as in the solid-state and post-assembly reactions.[1,2] Further, by employing PBUs containing chiral imido(phosphate) trianions, enatiopure cages have been prepared that show chiral recognition and separation.[4,5]



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[4] Yadav, A.; Sarkar, M.; Subrahmanyam, S.; Chaudhary, A.; Hey-Hawkins, E.; Boomishankar R. *Chem. Eur. J.* **2020,** *26,* 4209-4213.

Bio-Sketch of Speaker

Profile: Prof. Boomi Shankar obtained his B.Sc. (1996) and M.Sc. (1998) in Chemistry from Madura College affiliated to Madurai Kamaraj University, Madurai, India. He then obtained his Ph.D. from the Indian Institute of Technology, Kanpur, India in 2004 under the supervision of Prof. V. Chandrasekhar. Soon after obtaining his Ph.D. degree in January 2004, he took a short-term postdoctoral position at the University of Illinois at Urban-Champaign, USA. He then worked at the University of Liverpool as a Senior Research Associate for about three years between November 2004 and December 2007. In April 2008, he joined as an Assistant Professor at IIT, Guwahati and later moved to IISER Pune in December 2010. He became an Associate Professor in December 2014 and a full Professor in December 2019.

Research Interests: The research focus of his group falls in the broad interface of inorganic and materials chemistry with emphasis to synthesis, structure, physical properties and energy applications. At present, his research group is mainly working on two major topics. The first one deals with the chemistry of polyhedral and chiral cages derived from rigid and flexible phosphoramide scaffolds, especially on the development of neutral Pd(II) cages supported by cis-blocking tris(imido)phosphate trianions, and their utility in host-guest chemistry, chiral separation and catalysis. The second major area addresses on the new-design of organophosphorus scaffolds for obtaining organic, hybrid organic-inorganic and metal-organic ferroelectric materials and their utility in piezoelectric energy harvesting.

Awards: He has received the Bronze medal of the Chemical Research Society of India for the year 2022 and recently the Science and Technology Award for Research (STAR) from the Science and Engineering Research Board (SERB), India.

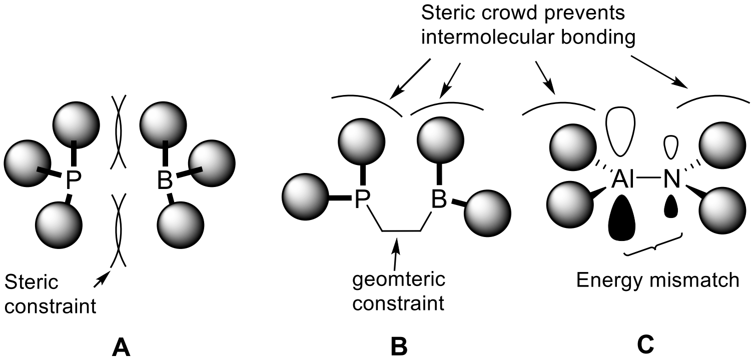
IL10

Intramolecular C-H Activation in Imidoalanes: Involvement of Al–N Frustrated Lewis Pairs

by N. Dastagiri Reddy, Dept. of Chemistry, Pondicherry University, Pondicherry – 605014

In the past decade the concept of Frustrated Lewis Pairs (FLPs) has created a great interest especially among the main-group researchers. “An FLP is a combination of a Lewis acid and base that exhibits FLP chemistry” is a broader definition of an FLP. FLP chemistry involves the concerted action of a Lewis acid and base segregated at the transition state on a substrate molecule.[1] The most common FLP systems contain phosphorous based species as Lewis base and boron based species as Lewis acid.

An FLP system may contain a simple mixture of a Lewis acid and a Lewis base (Figure1, **A**) or a single molecule in which a Lewis pair is incorporated (Figure1, **B**). In the former case, the formation of the Lewis adduct is restricted by the steric crowd around the acid and the base. The latter systems are designed in such a way that the formation of the adduct is restricted geometrically and sterically. However, it is also possible even the directly bonded donor and acceptor atoms can still act as active Lewis pairs purely due to the poor π-overlap of the orbitals (Figure1, **C**). This is due to energy mismatch of the orbitals on the donor and the acceptor atoms. Though the first two types of FLPs (**A** and **B**) have been thoroughly explored and several hundreds of articles appeared in the literature, studies on the third type (**C**) are limited to only one article.[2] Calculations on the inorganic ring systems, which have been reported in the literature, suggest that the π-overlap of orbitals of N and Al in alumazene (Al_3N_3 ring) is almost nil.[3] This was supported by the great tendency of three coordinate Al–N compounds to form dimers, trimers or tetramers to complete the fourth coordination *via* σ-bond. In order to explore the FLP chemistry of three coordinate Al–N compounds, a few reactions have been carried out in our research laboratory and the results will be discussed in detail during the presentation.



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Bio-Sketch of Speaker

Dr. N. Dastagiri Reddy
Associate Professor
Dept. of Chemistry
Pondicherry University
Date of Birth: 10th of May, 1967
M.Sc., Sri Krishnadevaraya University, Anantapur, 1993
Ph.D., IIT Kanpur, 1999

Postdoctoral research:

1. Purdue University, USA, 1999 – 2000. (Prof. RA Walton)
2. Universität Göttingen, Germany (Alexander von Humboldt Fellow), 2000 – 2002. (Prof. HW Roesky)
3. University of Calgary, Canada, 2002 – 2003. (Prof. WE Piers)
4. Lehigh University, USA, 2003 – 2004. (Prof. Li Jia)

Professional Appointments

Assistant Professor, Dept. of Chemistry, Pondicherry University from 2005 to 2013

Associate Professor, Dept. of Chemistry, Pondicherry University since 2013

Awards/Honours

Alexander von Humboldt Fellowship

Visited Goettingen University and Karshruhe Institute of Technology, Germany 6 times for doing summer research after joining Pondicherry University under AvH follow-up programs

Research Publications

38 research publications

Research Areas

- Main-group metal based homogeneous catalysis: Production of bio-degradable polymers like polycaprolactone, polylactide, polycarbonates etc.
- Organometallic chemistry of main-group elements, especially, B, Al, Ga, Si and Ge.
- Design and synthesis of transition metal based homogenous catalysts for Suzuki-Miyaura cross coupling reactions in neat water and polymerization of polar olefins.

Projects and Students

Completed two DST projects and one CSIR project. Currently one SERB (DST) project is being carried out.
5 research scholars have been awarded PhD degree
Guided 5 MPhil students

IL11

Redox Processes in Low-Valent Low-Coordinate Main-Group Compounds

Anukul Jana

Tata Institute of Fundamental Research Hyderabad, Gopanpally, Hyderabad 500046, Telangana, India
Email: ajana@tifrh.res.in

ABSTRACT

The The synthesis of unprecedented class of compounds are always important for the development of new chemistry. Last three-four decades there has been tremendous progress in the chemistry of low-valent low-coordinate main group compounds and it is possible due to the successful isolation of this class of compounds which were once thought to be an elusive: such as singlet carbene, compounds having multiple bond between two heavier elements (e.g. disilene and diphosphene), boryl lithium, borylene, and phosphinidene.

With our 7-8 years efforts we were able to developed convenient synthetic route for the syntheses of low-valent low-coordinate main-group compounds such as organic radicals,[1] diradicals,[2] (π-conjugated) radical-cations,[3] (poly) cations,[4] NHC-coordinated diphosphene/phosphinidene/phosphinidene oxide,[5] electronically/geometrically modified alkenes/imines[6] and π-conjugated molecule with electron deficient atom.[7] In my presentation I will showcase how we are employing these low-valent low-coordinate main-group compounds as a synthons and reagents by means of redox (reduction/oxidation) processes.

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(7) Maiti *et al., J. Am. Chem. Soc.* **2021**, *143*, 3687–3692.

Bio-Sketch of Speaker

Anukul Jana

Associate Professor-G

Tata Institute of Fundamental Research Hyderabad
Gopanpally, Hyderabad-500107, Telangana, India
Tel: +91-40-2020-3088
Contact Number: +91 7674092333
E-mail: ajana@tifrh.res.in

Homepage: http://www.tifrh.res.in/tcis/faculty/anukul-jana

Dr. Anukul Jana obtained his Ph.D. in 2009 from University of Göttingen, Germany under the guidance of Professor Herbert W. Roesky. His doctoral thesis focused on the chemistry of compounds with low-valent Group 14 elements. He did his first postdoctoral research work as an Alexander von Humboldt fellow in the group of Professor Paul Knochel, Ludwig-Maximilians-Universität, Germany. Later on, he moved to pursue his second post-doctoral research in the group of Professor David Scheschkewitz, Universität des Saarlandes, Germany. In March 2014, Dr. Anukul Jana started his independent career at TIFR Hyderabad. His current research interest is in the chemistry of low-valent low-coordinate Group 13-15 elements.

IL12

Stable Main-Group Radicals and Diradicals Based on Carbon-Donor Ligands

Mahendra K. Sharma, Dennis Rottschäfer Falk Ebeler, Rajendra S. Ghadwal*

Molecular Inorganic Chemistry and Catalysis, Center for Molecular Materials, Faculty of Chemistry, University of Bielefeld, Germany
rghadwal@uni-bielefeld.de; www.ghadwalgroup.de

ABSTRACT

Stable radicals and diradicals are appealing candidates as building-blocks for advanced functional materials, which are pivotal for addressing the current issues related to sustainability and energy.[1] This is because of the promising optical, magnetic, and electronic properties of these open-shell species.[2] Moreover, synthetic access to thermally stable radicals for their detailed investigation is crucial to enhance our understanding about chemical bonding as well as to exploit their potential in synthesis and catalysis. The central focus of our research endeavors is the isolation and exploration of stable main-group radicals and diradicals[3] supported by unconventional carbon-donor ligands (CDLs). Therefore, the development (as well as assessment of the stereoelectronic properties) of a fundamentally new class of CDLs is an important topic of our research program.[4]

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Bio-Sketch of Speaker

Rajendra Ghadwal, University of Bielefeld, GERMANY

Research interests:

Low-valent (open-shell in particular) main-group chemistry: Stable radicals and diradicals, π-conjugated systems, electronic structure and photo-physical properties.
Organometallic Catalysis: Ligand design, stereoelectronic properties, mesoionic carbenes (MICs), redox-active carbenes, transition metal (Ni and Cu) catalysis, MIC-Cu-emitters.

Recognition:

Heisenberg Research Fellow of the German Research Foundation (DFG)
Feodor Lynen Research Fellowships for experienced researchers (AvH Foundation)

Selected publication:

[1] M. K. Sharma, F. Ebeler, T. Glodde, B. Neumann, H.-G. Stammler, R. S. Ghadwal, *J. Am. Chem. Soc.* **2021**, *143*, 121–125.
[2] M. K. Sharma, D. Rottschäfer, T. Glodde, B. Neumann, H. G. Stammler, R. S. Ghadwal, *Angew. Chem. Int. Ed.* **2021**, *60*, 6414–6418.
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[5] M. K. Sharma, S. Blomeyer, T. Glodde, B. Neumann, H.-G. Stammler, A. Hinz, M. van Gastel, R. S. Ghadwal, *Chem. Sci.* **2020**, *11*, 1975–1984.
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IL13

Amidinatohypersilylsilylene: A New Synthon in Silicon Chemistry

Sakya S. Sen

Inorganic Chemistry and Catalysis Division, CSIR-National Chemical Laboratory, Pune, India

ss.sen@ncl.res.in

ABSTRACT

At the "10th International Symposium on Organosilicon chemistry" in Poland in 1993, Nils Wiberg termed tris(trimethylsilyl) moiety as "hypersilyl" moiety (hereinafter we shall follow Wiberg's nomenclature) to distinguish it from the very related tri(tert-butyl)silyl group, which he named "supersilyl" group. The advantages of the hypersilyl group are not only the good σ-donation or pronounced steric bulk, but the commercial availability of the precursors and possibility of further functionalization due to the presence of the $SiMe_3$ moieties. In our part, we have prepared a new silylene connected with a hypersilyl moiety1 and studied its reactivity towards small molecules.[1,2,3] Functionalization of the TTSS moiety led to the formation of unsymmetric disilenes.[4] The chemistry was subsequently extended to germanium and tin.[5]

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5. Bisai, M. K.; Ajithkumar, V. S.; Gonnade, R. G.; Sen, S. S. *Organometallics* **2021**, *40*, 2651–2657.

Bio-Sketch of Speaker

Dr. Sen received his Ph.D. in 2010 at the University of Göttingen, Germany. Postdoctoral work followed (2011-2013), working with Prof. Holger Braunschweig at the University of Würzburg, Germany, supported by the AvH Foundation. In 2014, he was appointed as a senior scientist at CSIR-NCL, Pune, where he is currently serving as a Principal Scientist since 2018. Dr. Sen is the recipient of CSIR-Young scientist award in 2017, INSA medal for Young Scientist in 2018, Merck Young Scientist Award, 2019, Swarnajaynti fellowship in 2021. He has been selected as a ChemComm Emerging Investigator 2018 and Early Career Advisory Board Member of ACS Catalysis (2019-2021).

IL14

Materials of main-group elements: Complications, solution and property enhancement

Krishnamurthi Muralidharan*, Billakanti Srinivas, and M. Hanumantha Rao
School of Chemistry and Advanced Centre of Research in High Energy Materials, University of Hyderabad, Hyderabad, 500046. India
murali@uohyd.ac.in

ABSTRACT

Many materials produced using main-group elements find application in various fields such as environmental remediation, energy harvesting devices, catalysis, and high propellant science and technology. The synthetic procedures used to produce materials decide the purity, which will influence the property of materials. For example, long-chain organic molecules are used during the synthesis of metal chalcogenide-based semiconductors as stabilizing agents. Those molecules surround the nano/micro particles. But these surfactant molecules are not contributing much towards the targeted applications but sometimes become a hindrance to the proposed applications. On the other hand, the oxidative stability of metals nanoparticles can be enhanced by either organic surfactant molecules or by coating with polymers.

We have identified a few shortcomings of materials property and tried to solve these complications through adopting new synthetic protocols. In this lecture, the problems of Al and B - based materials concerning theirs use as the propellant and how we could circumvent those problems will be discussed. Similarly, how the electron movement is hindered by organic surfactant molecules surrounding the metals chalcogenides nano/micro particles and how to evade this issue through a new synthetic method will also be discussed. The enhancement of materials property of Al, B, Sulphides and their application in the various field will be covered briefly.

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Bio-Sketch of Speaker

Dr. K. MURALIDHARAN

Professor
School of Chemistry
University of Hyderabad
Gachibowli, Hyderabad 500 019
Email: murali@uohyd.ac.in;
Tel: + 91 40 2313 4819 (Office); + 91 40 2313 4919

EDUCATION

Ph. D Chemistry (2003) Indian Institute of Technology (IIT) Kanpur

M.Sc Applied Chemistry (1997) Anna University, Chennai

PG Diploma in Applied Chemistry (1994), Loyola College, Chennai)

B.Sc Chemistry (1993) A. A. Arts College, (Affiliated to Madras University), Villupuram, Tamilnadu.

FELLOWSHIP

- Centenary Postdoctoral Fellow, Indian Institute of Science (2007)
- Postdoctoral Fellow, Southern Methodist University, Dallas, Texas, USA (2005 to 2006)
- Postdoctoral Fellow, University of Idaho, Moscow, Idaho, USA (2003 to 2005)

POSITIONS

- Professor, School of Chemistry, University of Hyderabad (from 2016)
- Associate Professor, School of Chemistry, University of Hyderabad (2013 to 2016)
- Assistant Professor, School of Chemistry, University of Hyderabad (2007 to 2013)
- Scientist, APL Research Centre, Aurobindo Pharma, Hyderabad (2006 to 2007)

RECOGNIZATION

- Editorial Board Member of the journal “Energetic Materials Frontiers” (from 2019)
- Elected member of The National Academy of Sciences, Allahabad (from 2016)
- Associate member of AP Akedemi of Sciences (from 2015)

RESEARCH INTEREST

Inorganic chemistry/Materials/Polymers/Energy materials

OTHER DETAILS

No of research papers published: **57**

No of PhDs completed: **11**. No of PhDs working: **6**

No of research projects completed: **5**. No of ongoing research projects: **2**

IL15

Cross-Conjugated Poly(chalcogenylene vinylene)s

Yang Qin

Department of Chemical & Biomolecular Engineering, Institute of Materials Science, University of Connecticut, Storrs, CT 06250, USA

yang.qin@uconn.edu

ABSTRACT

We describe our synthetic methodologies, through combination of acyclic diene metathesis (ADMET) and post-polymerization modification (PPM) reactions, for the preparation of poly(thienylene vinylene)s (PTVs) and poly(selenylene vinylene)s (PSVs) with systematically varied structures. First, we prepared PTVs, PSVs and their random copolyemrs (PSV-co-PTV).[1] By replacing sulfur atoms with selenium, PSVs were found to possess reduced crystallinity and a smaller bandgap of ca. 1.6 eV, while PSV-co-PTV shows physical/electronic properties between those of the corresponding homopolymers. Secondly, we successfully prepared a series of novel PTVs and PSVs functionalized with F, Cl, Br and I atoms at the 4-positions of thiophene rings.[2] Such halogenation not only displays capabilities of fine-tuning polymer properties but also provides opportunities for further functionalization through PPM reactions, which enabled us to introduce several thiophene and benzene-based conjugated side chains on the polymer backbone.[3] Interestingly, the obtained PTV and PSV derivatives with strongly electron-withdrawing side-chains displayed rarely observed fluorescence, suggesting changes in excited state structure and dynamics. We further extended this methodology to the synthesis of regio-regular cross-conjugated PTVs[4] as well as the first examples of stable poly(furylene vinylene) (PFV) polymers. Our methodologies provide a facile means to systematically study the structure-property relationships of poly(chalcogenylene vinylene)s, which can enhance our basic understanding in CPs and potentially lead to new materials for emerging electronic applications.

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[4] Y. M. Katba-Bader, L. Meng, C. Guan, Y. Qin, *Polymer* **2021**, *231*, 124150.

Bio-Sketch of Speaker

Dr. Yang Qin was born and grew up in Sichuan province, located in the southwest region of China and famous for spicy foods and giant pandas. He obtained his B.S. degree in chemistry from Peking University in 2000 and Ph.D. degree, under Prof. Frieder Jäkle, from Rutgers University in 2006. After two postdoctoral appointments with Prof. Marc Hillmyer at University of Minnesota and with Prof. Barney Grubbs at Brookhaven National Laboratory, Dr. Qin joined the Department of Chemistry & Chemical Biology at University of New Mexico as an assistant professor in the fall of 2010 and was promoted to the rank of associate professor in 2017. He moved his research group to the University of Connecticut in August 2020. Research in Dr. Qin's group is focused on design and synthesis of conjugated organic and polymeric materials, organic/inorganic hybrid materials, and their applications in energy and environment. He has published over sixty peer-reviewed papers and received several awards including the UNM Research Allocation Award, UNM Office of Vice President for Research Equipment Award, Sandia National Lab-UNM Alliance Award, NSF CAREER Award, and the NIH NM-INBRE Award.

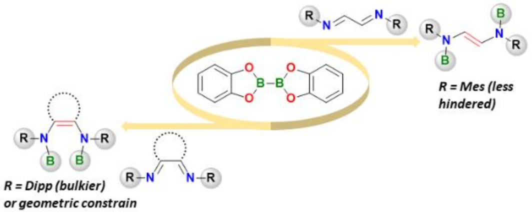
IL16

Homolytic Cleavage of Diboron Compounds by Diazabutadiene Derivatives

Piyush K Verma[a], Naresh K Meher[b], K. Geetharani[a,*]
[a]*Department of Inorganic and Physical Chemistry, Indian Institute of Science Bangalore*
Email: geetharani@iisc.ac.in

ABSTRACT

Homolytic cleavage of diboron compounds and their addition over unsaturated bonds had been explored since mid of the 20th century. Starting from the uncatalyzed addition of diboron tetrahalides over C═C and C≡C bonds, the field has witnessed a critical milestone with the discovery of transition metal (TM) catalyzed diboration reactions where the TM complexes cleaves the B-B bond either directly by oxidative addition or by transmetallation reaction in the presence of base.[1] Another very important development in the area of diboron activation have been achieved in the recent past where two nucleophilic moieties can coordinate to both boron atom of the diboron and results in the homolytic cleavage of B-B bond.[2] In this line we have found a class of compound, diazabutadiene (DAB) derivatives, capable of cleaving the B-B bond of diboron homolytically.[3] The diazabutadiene molecule coordinates to the boron atoms of diboron through its nitrogen atom and results in a homolytic cleavage of the B-B bond along with the formation of a new π bond between the carbon atoms of its backbone. The product's geometry was found to be influenced by the substituents of the DAB unit. Reaction of 2,6-diisopropylphenyl substituted diazabutadiene (DippDAB) with bis(catecholato)diboron (B_2cat_2) produced the product having *cis* geometry whereas mesityl substituted diazabutadiene (MesDAB) results in *trans* geometry across the newly formed C=C bond. Preliminary mechanistic investigation suggests the absence of any radical intermediate in the homolytic cleavage of B-B bond by DABs, as, in the presence of the radical scavengers like TEMPO and 9,10-dihydroanthracene, the reaction between DABs and B_2cat_2 proceeds with no drop in efficacy. Furthermore, crossover experiments suggest a concerted reaction pathway for this cleavage.[4]



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Bio-Sketch of Speaker

Dr. K. GEETHARANI
Assistant Professor
Department of Inorganic & Physical Chemistry
Indian Institute of Science
Bangalore 560012, INDIA

Research Interests

- Development of Base Metal Catalysts for Borylation Reactions.
- Main Group Catalyst for New Reaction Chemistry
- Boronic Acids for Biological Applications
- Catalytic Transformation of Molecular Nitrogen into Ammonia
- New Methodologies for Trifluoromethylation Reactions

Recognition

- **2020:** SERB- Women Excellence Award (Presented by the President of India)
- **2019:** NASI-Young Scientist Platinum Jubilee Award.
- **2019:** Young Scientist Medal, Indian National Science Academy (INSA).
- **2018:** Young Associate, Indian Academy of Sciences.
- **2015**: DST Inspire Faculty Award.
- **2013**: Alexander von Humboldt postdoctoral fellowship, Germany.
- **2013**: "Werner prize"- Best Ph.D. thesis in Inorganic and Analytical Chemistry, Indian Institute of Technology Madras, India.

Selected Publications

- Verma, P. K.; Meher, N. K.; Geetharani, K.* Homolytic Cleavage of Diboron(4) Compounds by Diazabutadienes ***Chem Commun.,*** 2021, 57, 7886 – 7889. *Highlighted on the Cover Page of the Article*
- Siddiqui, S.; Bhawar, R.; Geetharani, K.* Iron-Based Catalyst for Efficient Borylation of Unactivated Alkyl Halides. ***J. Org. Chem***., 2021, 86, 1948-1954.
- Verma, P. K.; K. Sujit Prasad.; D. Varghese.; Geetharani, K.* Cobalt(I)-Catalyzed Borylation of Unactivated Alkyl Bromides and Chlorides. ***Org. Lett.,*** 2020, 22, 1431-1436.
- Verma, P. K.; Setulekshmi, A. S.; Geetharani, K.* Markovnikov-Selective Co(I)-Catalyzed Hydroboration of Vinylarenes and Carbonyl Compounds. ***Org. Lett.,*** 2018, 20, 7840-7845.
- Verma, P. K.; Souvik, M.; Geetharani, K.,* Efficient Synthesis of Aryl Boronates via Cobalt-Catalyzed Borylation of Aryl Chlorides and Bromides. ***ACS Catal.,*** 2018, *8*, 4049-4054. **(**Highlighted in Synfacts 2018, 14(07), 0746).

IL17

Impact of the Ancillary NHC Ligands in the Catalytic Performances of Their Transition Metal Complexes

Arnab Rit[*a]

[a]Department of Chemistry, Indian Institute of Technology Madras
Chennai – 600036; arnabrit@iitm.ac.in

ABSTRACT

Ancillary ligands are known to play crucial roles in the catalytic activity of any metal complexes and their stereoelectronic parameters are normally considered as important factors to tweak their properties including catalytic activity. Over the past few decades, *N*-Heterocyclic carbenes (NHCs) have established themselves as an important class of ligands in various fields including homogeneous catalysis.[1] Although extensively utilized in catalysis, detailed study on the combined steric and electronic influence of the ancillary NHC ligand in transition metal catalyzed various (de)hydrogenation processes are rather limited.[2] Detailed understanding of this type would definitely provide useful information for future catalyst developments. To study such effects, we have synthesized a series of Ru^{II}-complexes with either orthometalated C_{NHC}^C_{phenyl}-bidentate NHC ligands or unsymmetrical chelating ligands where an imidazolylidene (ImNHC) is coupled to a pendant triazolylidene (tzNHC)/N-donor (Fig. 1). To understand the influence of such ligand variations, all these complexes were applied in hydrogenation as well as borrowing hydrogen (BH) reactions which revealed that substantial tailoring of catalytic activity is possible by altering their steric and electronic profiles.[3] Further, the change of the bridging unit from CH_2 to phenyl group allows access to diverse heterobometallic complexes, *via* selective and controlled metalation, for application in tandem catalytic transformations.

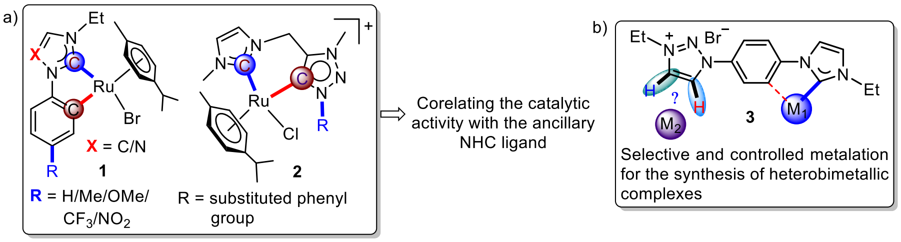

Figure 1. (a) Ru^{II}-NHC complexes used in this study and (b) ligand design for the synthesis of heterobimetallic complexes.

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Bio-Sketch of Speaker

Name: ARNAB RIT

Department of Chemistry
IIT Madras
Contact Number: 044-2257-4205
Email: arnabrit@iitm.ac.in
Homepage: http://chem.iitm.ac.in/faculty/arnab/

After graduating from IIT Kharagpur in 2007, Dr. Rit has earned his doctorate degree in organometallic chemistry in 2011 from WWU Muenster, Germany. After that he was a post-doctoral researcher at RWTH Aachen, Germany and Marie-Curie post-doctoral fellow for one and half year at the University of Oxford. In December, 2015 he joined IIT Madras as an Assistant Professor and currently working on the synthesis and catalytic application of various metal-NHC complexes.

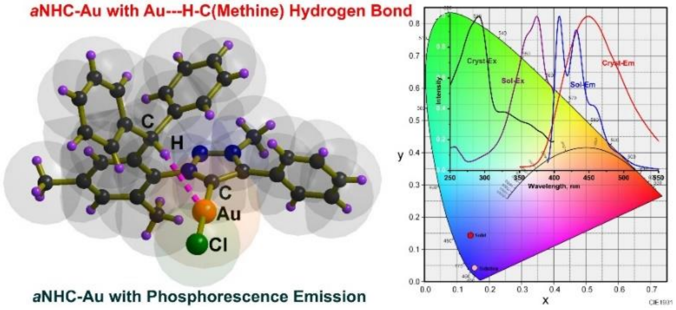
IL18

Elusive Gold-Hydrogen Bond in Gold-Carbenes

Moulali Vaddamanu[a], Mannem Adinarayana[a], Osamu Tsutsumi [b], Ganesan Prabusankar[a,*]
[a]*Department of Chemistry, Indian Institute of Technology Hyderabad*
India-502 285; [b]Department of Applied Chemistry, Ritsumeikan University, Japan-525-8577
Email: prabu@chy.iith.ac.in

ABSTRACT

The dubiety over the interaction between gold and hydrogen has intrigued chemists since 2014. The interaction between gold and hydrogen is crucial in understanding the mechanistic aspects of catalysis research, such as C–H activation reactions. However, gold with the highest electronegativity, electron affinity, nobility along with the lowest possible coordination number has a unique contribution in the Au····H–C interactions. The nature of the interaction between gold and hydrogen leads to the unresolved question. Thus the mononuclear gold(I)-*N*-heterocyclic carbene molecules have been synthesized and characterized to understand the interactions between gold and hydrogen. Their single-crystal X-ray analysis reveals the influence of the *n*-alkyl groups on solid-state packing. These mononuclear gold(I)-carbene molecules exhibit rare intramolecular gold hydrogen-bonding and luminescence features.[1-3] The paradigm emission shift arises from a short-chain *n*-alkyl substituted carbene gold complex to a long *n*-alkyl chain substituted carbene gold complex in the crystalline state due to the carbon-carbon rotation of the *n*-alkyl group, which tends to promote unusual solid packing. Hence *n*-alkyl group adds a novel emission property in the crystalline state. The relationship between the *n*-alkyl group with intramolecular gold hydrogen-bonding as well as the luminescence properties in the crystalline state will also be addressed.



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Bio-Sketch of Speaker

Prof. Ganesan Prabu Sankar, PhD., (IIT Bombay)
Department of Chemistry
Indian Institute of Technology Hyderabad, INDIA-502 285
Phone : +91 94 94 06 07 32; +91 40 23 01 62 56
E-Mail: prabu@iith.ac.in; Web: http://www.iith.ac.in/~prabu/

Research Field

General Field:
Organometallic Chemistry

Specific Fields:
Organometallic Synthesis | Late Transition Metal Chemistry | Main Group P-Block Chemistry | Molecular Activation | Molecules to Materials | Molecules for Medicines

Awards and Fellowships

2021	Fellow of Royal Society of Chemistry, UK
2020	DUO-ASEM Professor Fellowship, Germany
2020	Best Teaching Award, IIT Hyderabad, India
2013	Alexander von Humboldt Fellowship, Germany
2013	IIT Bombay Research Paper Award, India
2008	Alexander von Humboldt Fellowship, Germany

Selected Publications

1) ACS Applied Polymer Materials, 2020, 2(3), 1388-1397.
2) Organometallics, 2020, 39(12), 2202-2206.
3) Dalton Transactions, 2020, **49**, 17331-17340.
4) International Journal of Biological Macromolecules, 2020, 147, 117-130.
5) Chemistry An Asian Journal, 2021, 16(5), 521-529.
6) Chemistry An Asian Journal, 2021, 16(13), 1767-1772.
7) Dalton Transactions, 2020, In Press.

IL19

From CO_2 activation to catalytic reduction: a metal-free approach

Swadhin K Mandal

Indian Institute of Science Education and Research Kolkata

Mohanpur -741246

Email: swadhin.mandal@iiserkol.ac.in

ABSTRACT

Ever increasing emission of CO_2 into our atmosphere because of over exploitation of natural resources, it is imperative that the world looks towards a portfolio of carbon mitigation solutions, rather than a single strategy. Not surprisingly, continuous efforts are required to find solutions to address the issue of excessive CO_2 emission and its potential effects on climate change. In this regard, the use of CO_2 as a C1 source is considered as an attractive strategy as CO_2 has the potential to be a great asset for the industrial sector. With particular emphasis, the reduction of CO_2 offers an alternative to fossil fuels for various organic industrial feedstocks and fuels. As a result, efficient approaches for the reduction of CO_2 into products such as methanol can generate value out of its emissions. Accordingly, in recent years, metal-free catalysis has emerged as a sustainable approach because of the mild reaction conditions by which CO_2 can be reduced and functionalized to various value-added products. The metal-free catalytic reduction of CO_2 offers an alternative opportunity for the development of chemical processes with low cost, earth-abundant, non-toxic reagents, and low carbon footprint.

In this talk, I will brief about our recent efforts in developing metal-free catalysts for catalytic reduction and reductive functionalization of CO_2.[1-6]

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[3] S. C. Sau, P. K. Hota, S. K. Mandal, M. Soleilhavoup, G. Bertrand *Chem. Soc. Rev.* **2020**, *49*, 1233-1252

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[6] S. C. Sau, R. Bhattacharjee, P. K. Vardhanapu, G. Vijaykumar, A. Datta, S. K. Mandal *Angew. Chem. Int. Ed.* **2016***, 55,* 15147 –15151

Bio-Sketch of Speaker

Dr. Swadhin K. Mandal
Professor, Department of Chemical Sciences,
Indian Institute of Science Education and Research-Kolkata
Mohanpur Campus, Mohanpur
PO- BCKV, Pin-741246, Dist- Nadia, West Bengal
e-mail: swadhin.mandal@iiserkol.ac.in
***Web:* http://swadhin-mandal.weebly.com/**

Academic and Professional Career:

- Current Position: Professor (since 2018 October), Department of Chemical Sciences, IISER Kolkata
- Head of the Department of Chemical Sciences, IISER Kolkata, March 2018- August 2021
- Alexander von Humboldt Postdoctoral Fellow (2006-2007) with Prof Herbert W Roesky: University of Goettingen, Germany.
- Postdoctoral Fellow (2002- 2006) with Prof. Robert C Haddon: University of California, Riverside, USA.
- Ph.D. (1996-2002): Department of Inorganic and Physical Chemistry, Indian Institute of Science, Bangalore, India. Supervisor: Prof. S S Krishnamurthy
- M.Sc. (Chemistry, 1994-1996): University of Kalyani, Kalyani, India. (Secured 1st rank in the University)

Awards and Professional Recognition:

- Fellow, Indian Academy of Sciences, 2021
- Awarded with the Friedrich Wilhelm Bessel Research Award, 2020 by Alexander von Humboldt Foundation
- Shanti Swarup Bhatnagar Prize in Chemical Sciences for 2018
- Invited as Editorial Advisory Board member of 'Chemical Science' published as the flagship journal by Royal Society of Chemistry during 2020-2022
- Invited as the Visiting Professor at IIT Mumbai during 2020-2022
- Editorial Advisory Board member of Chemical Science, Organometallics, Inorganic Chemistry and J. Chemical Science
- Fellow of Royal Society of Chemistry (FRSC) under the "Leaders in the Field" category.
- Awarded with SERB Distinguished Investigator Award.
- CRSI bronze medal, 2018
- YIM-Young Scientist Award -2012 by YIM-Boston held during 6-8th October, 2012 at MIT, Boston, USA.
- Alexander von Humboldt fellowship (2006).

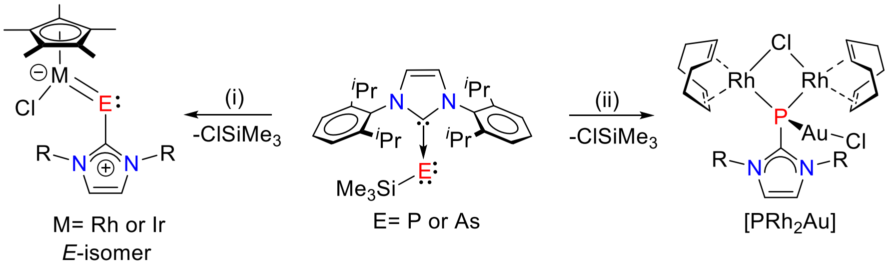
IL20

NHCs Supported Main Group Adducts: Novel Ligands for Stabilization of Reactive Organometallic Fragments

Adinarayana Doddi[a*] Dirk Bockfeld,[b] and Matthias Tamm[b]
[a]*Department of Chemical Sciences, Indian Institute of Science Education and Research, Berhampur*
[b]*Technical University Braunschweig, Germany*
E-mail: *adoddi@iiserbpr.ac.in*

ABSTRACT

*P*nictinidenes (:ER) are highly reactive low valent element (I) compounds, and are considered as analogs of carbenes ($:CR_2$). Due to their gas phase and low temperature stability, they have limited access for further studies. Isolation of such species was achieved by Arduengo type N-heterocyclic carbenes in the form of (NHC)→Pnictinidene adducts.[1,2] Recently, we have developed a different high yielding method for the isolation of NHC supported new pnictinidene adducts [(NHC)$ESiMe_3$ and (NHC)EH, E = P, As)] and the later adducts were introduced as synthons for the preparation of terminal carbene–phosphinidenide and arsenidenide metal complexes of the type [(NHC=E)ML_n] (ML_n= (cymene)RuCl and (η^5-C_5Me_5)RhCl) (Scheme).[2,3] Their spectroscopic and structural characteristics showed their similarities with aryl-phosphinidene counterparts.[3-5] The monoanionic "(NHC)E" moiety forms highly covalent M–P double bonds and is also capable of bridging two or three metal atoms.[2,5] In this presentation, isolation of different reactive (NHC)G-15 adducts and their use in the stabilization of reative, and unusual organometallic fragments will be discussed.



Scheme: Metal-Phosphinidenide complexes; i) [(Cp*)MCl_2]$_2$ and ii) [Rh(COD)Cl]$_2$ and AuCl.

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[2] (a) A. Doddi, D. Bockfeld, T. Bannenberg, P. G. Jones, M. Tamm. *Angew. Chem. Int. Ed.* **2014**, *53*, 13568; b) M. Peters, A. Doddi, T. Bannenburg, M. Freytag, P. G. Jones and M. Tamm. *Inorg. Chem*. **2017**, *56*, 10785.

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Bio-Sketch of Speaker

Dr. Adinarayana Doddi

MSc.: Indian Institute of Technology Madras

Doctoral Studies (PhD)(2013) Ruhr University Bochum, Germany
Supervisor; Prof. Roland A Fischer

Postdoctoral Work
Technical University Braunschweig, Germany
Supervisor: Prof. Dr. Matthias Tamm

Subgroup Leader/Postdoctoral Associate
Technical University Braunschweig, Germany
Supervisor: Prof. Dr. Matthias Tamm

Ramanujan Faculty (2019)
Department of Chemical Sciences, IISER Berhampur

Assistant Professor (2019)
Department of Chemical Sciences, IISER Berhampur

Awards

- Ramanujan Fellowship-2019 by SERB, Department of Science and Technology, Government of India
- Two times secured a travel fellowship by the DAAD to attend the National and International Conferences, For example, “ICOMC-2018, held in Florence, Italy from 15–20th July 2018
- Secured a travel fellowship (by the DAAD to attend International Conference “ICOMC-2014, Sapporo in Japan held on 13–18th July 2014
- Postdoctoral research grant by DFG, Technical University Braunschweig
- Doctoral fellowship by the Graduate Scholl of Chemistry and Biochemistry (GSCB), Faculty of Chemistry and Biochemistry, Ruhr University Bochum

Research Interests

Organometallics, Activation of Small Molecules, and Homogeneous Catalysis

Selected Publications

[1] A. Doddi, D. Bockfeld, T. Bannenberg, P. G. Jones, M. Tamm. *Angew. Chem. Int. Ed*. **2014**, *53*, 13568

[2] A. Doddi, D. Bockfeld, A. Nasr, T. Bannenberg, P. G. Jones, M. Tamm. *Chem. Eur. J*. **2015**, *21*, 16178.

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