XLI Reunión
Grupo Especializado de Química Organometálica
Alcalá de Henares, 20 de octubre de 2023

Presentación

La XLI Reunión del Grupo Especializado de Química Organometálica de la RSEQ (GEQO) toma en esta edición el formato de una jornada científica. Su objetivo es reunir a la comunidad científica española que trabaja en Química Organometálica, aglutinados en torno al GEQO, para conocer de primera mano los avances en este campo de investigación. Para ello intervendrán tanto investigadores consolidados de reconocido prestigio nacionales e internacionales, entre ellos los galardonados con los Premios GEQO 2023, así como algunos los miembros más jóvenes del Grupo que trabajan en nuestro país. En este espíritu, esta edición dedica parte de las sesiones a la intervención de investigadores en formación y a la discusión de sus trabajos. Al final de las sesiones de conferencias, tendrá lugar la entrega de los premios GEQO 2023.

Nuestro agradecimiento a la Universidad de Alcalá que nos acoge de nuevo en sus instalaciones.

Ana C. Albéniz
Presidenta del GEQO-RSEQ

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Programa

10:30h Acreditación/Café

11:00h Acto de Apertura

11:15h **Andrew Weller**
York University
Activating Alkanes using InCrystallo Organometallic Chemistry

12:00h **Julio Lloret-Fillol** Premio GEQO a la Excelencia Investigadora 2023
Instituto Catalán de Investigación Química
Photosynthesis as Inspiration for Reactivity of Low Valent Metal Complexes

12:30h Presentaciones Flash
FP1. **Carlos J. Carrasco.** Universidad de Sevilla
Water-soluble silver nanoparticles stabilized by N-heterocyclic carbenes derived from amino acids: synthesis, characterization and properties.
FP2. **Marcos López-Aguilar.** Universidad de Oviedo
Transformation of primary alcohols into chiral aldols by the one-pot hybrid tandem combination of Cu(II)- & organo-catalysis.

FP3. **David González-Liana.** Universidad de Rey Juan Carlos
Development of heterobimetallic Al-Mg complexes for the rapid ROP of lactides
FP4. **Elena Álvarez-Ruiz.** Universidad de Alcalá
Bonding modes and structural diversity of tantalum complexes supported by redox-active ligands.
FP5. **Diego Jaraba Cabrera.** Universidad de Alcalá
Exploring Trends in Salphen Based Group 13 Catalysts for Cyclic Carbonate Synthesis.
FP6. **Juan M. Delgado Collado.** IIQ-CSIC- Universidad de Sevilla
Neutral and cationic alkyl aluminium complexes supported by 2,6-bis(imino)pyridine-based ligand as Biomimetic Hydride Exchange Systems.

13:15h Comida

15:15h **Presentaciones Flash**
FP7. **Belinda Español-Sánchez.** ISQCH, Universidad de Zaragoza-CSIC
Unveiling Chemodivergent Faces of Janus-Type Rh_2NHC_2Uracilato Catalyst for Tandem Alkyne Dimerization-Hydrosilylation.
FP8. **Juan Pueyo.** ISQCH- Universidad de Zaragoza
Unprecedented Silver(III) Carbene Complexes.
FP9. **Víctor Esteban.** IU CINQUIMA- Universidad de Valladolid
Liquid crystals based on gold(I) complexes with an uncommon molecular structure.

15:45h **Alba Collado** **Premio GEQO a Jóvenes Investigadores 2023**
Universidad Autónoma de Madrid
Design of Ir complexes for catalytic applications

16:15h **Miquel Costas** **Medalla Rafael Usón-2023**
Universitat de Girona
Minimalistic oxotransferases to address challenging functionalization reactions

17:00h Entrega de Premios GEQO 2023

17:15h Junta General del GEQO

18:15h Clausura

GEQO2023

Sede del congreso

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Conferencias

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28801 Alcalá de Henares

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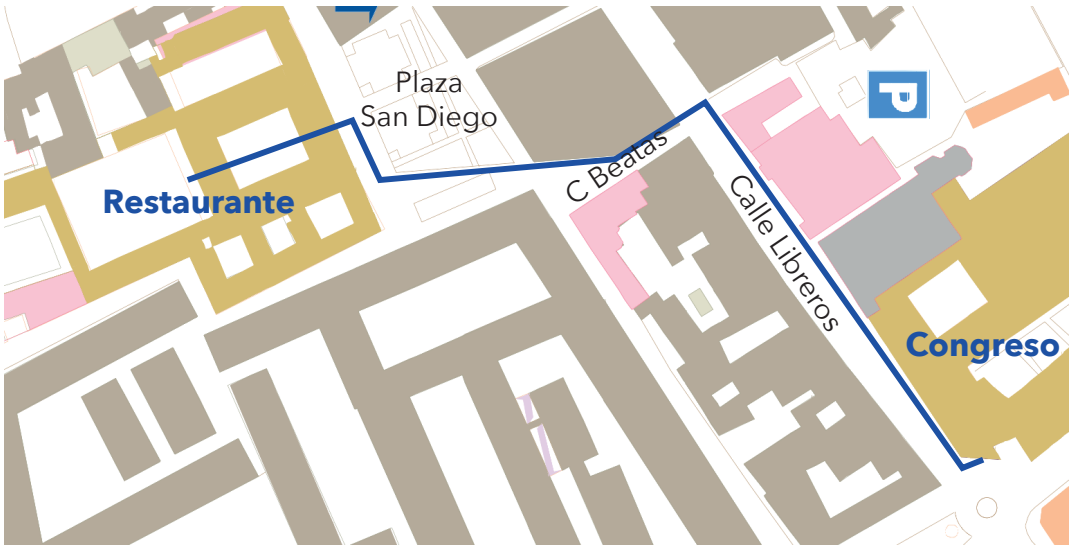

GEQO2023

XLI Reunión

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Alcalá de Henares, 20 de octubre de 2023

Resúmenes de las Presentaciones Flash

FP01

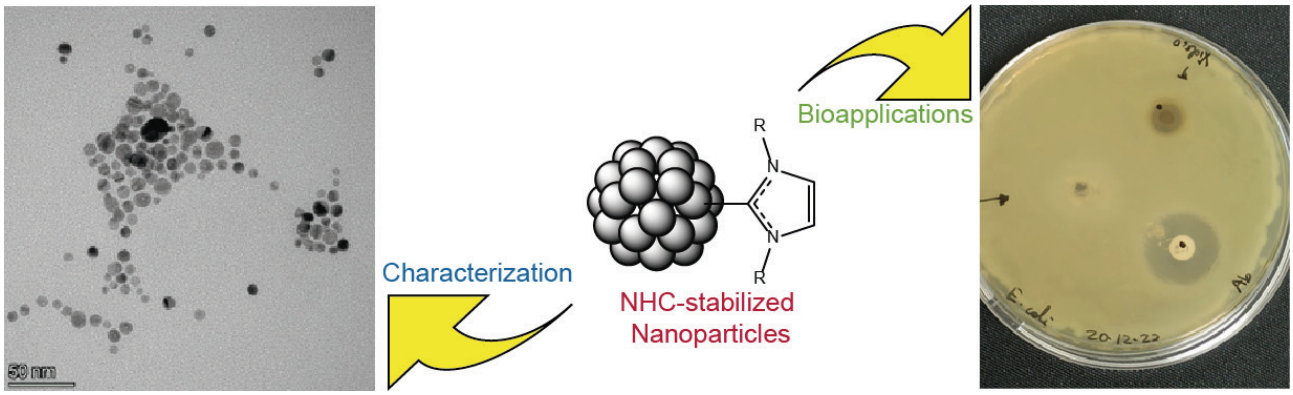
Water-soluble silver nanoparticles stabilized by *N*-heterocyclic carbenes derived from amino acids: synthesis, characterization and properties

Carlos J. Carrasco, Francisco Montilla, Agustín Galindo

Departamento de Química Inorgánica, Facultad de Química, Universidad de Sevilla, 41012 Sevilla.
E-mail: ccarrasco1@us.es

Metallic nanoparticles (MNPs) have attracted much interest in the last few decades in a wide range of applications in the fields of materials, catalysis, and medicine. In many cases, stabilization of MNPs is required to prevent agglomeration processes, which can be achieved by interaction with stabilizing substances such as polymers, dendrimers, surfactants or coordinated ligands. In recent years, the use of *N*-heterocyclic carbenes (NHCs) has become an alternative as stabilizing ligands for MNPs [1]. On the other hand, silver nanoparticles (AgNPs) have been extensively exploited in a variety of biological and biomedical applications due to their superior physicochemical properties, higher stability, and excellent biocompatibility [2].

Following our recent research on amino acid derived NHC metal complexes and their biological applications [3], we have selected imidazolium-based zwitterionic dicarboxylate to produce silver NHC-complexes soluble in aqueous media. These complexes have been used as precursors of new NHC-functionalized AgNPs, which have been characterized by using different techniques (DLS, TEM, etc). They were found to be stable in water, under air, remaining fully dispersed without agglomeration or Ag precipitation for a long time. Furthermore, these nanomaterials were found to have effective antimicrobial activity.



Financial support from Spanish Ministerio de Ciencia e Innovación (PGC2018-093443-B-I00) and Universidad de Sevilla (VII Plan Propio, V.1c) is gratefully acknowledged. C. J. C. thanks a research contract from PAIDI 2020, supported by the European Social Fund and the Junta de Andalucía.

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FP02

Transformation of primary alcohols into chiral aldols by the one-pot hybrid tandem combination of Cu(II)- & organo-catalysis

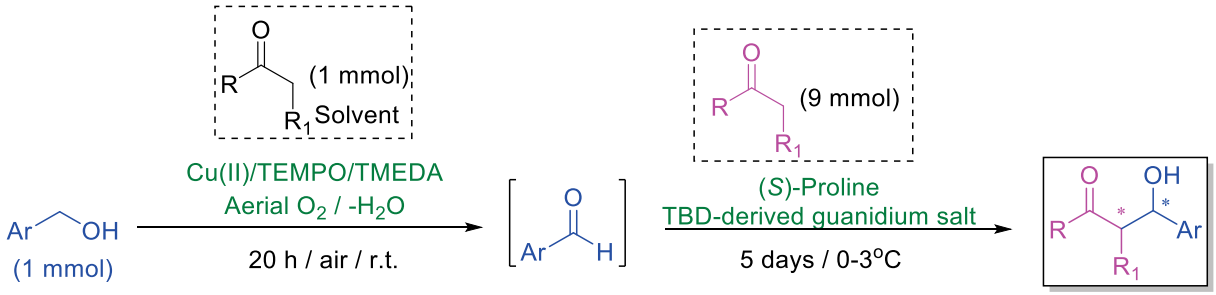
Marcos López-Aguilar[1], Marina Ramos-Martín[1], Joaquín García-Álvarez[1], Carmen Concellón[1], Vicente del Amo[1]

[1]Laboratorio de Química Sintética Sostenible (QuimSinSos). Departamento de Química Orgánica e Inorgánica (IUQOEM). Centro de Innovación en Química Avanzada (ORFEO-CINQA). Facultad de Química. Universidad de Oviedo. C/Julián Clavería 8, 33006, Oviedo (Spain)
e-mail: lopezamarcos@uniovi.es

Since the last decade and in the framework of organic synthesis, the design of one-pot tandem protocols is occupying a strategic place as new greener methodologies replacing standard and tedious stepwise synthetic processes[1]. In these one-pot tandem approaches, one of the most difficult challenges to solve is the design of hybrid protocols in which different synthetic organic tools are assembled in the same reaction media[2].

In this sense, our group is developing an unprecedented methodology that combines the oxidation of primary alcohols into aldehydes by using a $CuCl_2$/TEMPO/TMEDA catalytic system [3] (note that the unwanted formation of acids is not observe and aerial O_2 is used as the oxidant), with the organocatalyzed [(S)-proline and a TBD-derived guanidium salt] and enantioselective aldol reaction of the in-situ generated aldehydes with different ketones[4].

Thus, our aim is to provide a simple but efficient, selective and straightforward methodology for the synthesis of chiral aldols (starting from raw materials) in which no isolation or purification of intermediates is needed.



Financial support. PA-22-BP21-088, PID2020-113473GB-I00.

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FP03

Development of heterobimetallic Al-Mg complexes for the rapid ROP of lactides

David González-Lizana,[1] Luis Fernando Sánchez-Barba,[1] Andrés Garcés,[1] Marta Navarro,[1] and Agustín Lara-Sánchez[2]

[1] Departamento de Biología y Geología, Física y Química Inorgánica, Universidad Rey Juan Carlos, Móstoles-28933-Madrid, Spain

[2] Universidad de Castilla-La Mancha, Departamento de Química Inorgánica, Orgánica y Bioquímica- Centro de Innovación en Química Avanzada (ORFEO-CINQA), Campus Universitario, 13071-Ciudad Real, Spain

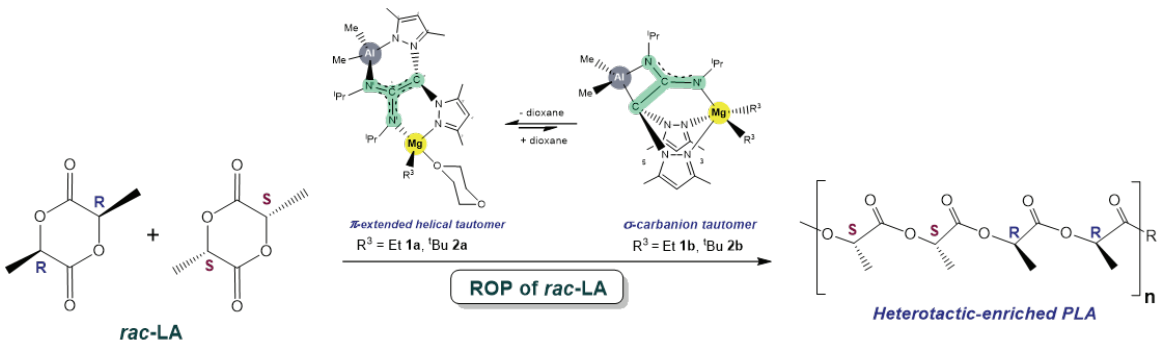
e-mail: david.gonzalezl@urjc.es

Keywords: Heterodinuclear scorpionate catalysts, synergic cooperation, rac-lactide

The successful architecture of active catalytic species with enhanced efficiencies is critical for the optimal exploitation of sustainable resources in industrially-demanded processes. In this work, we describe the preparation of novel helical heterobimetallic Al/Mg-based scorpionate complexes of the type [$AlMe_2$(pbpamd$^-$)MgR{κ^1-O-(OC_4H_8O)}] (R = Et **1a**, ^{t}Bu **2a**) as potential catalysts.

The design has been performed through the controlled sequential addition of the Al fragment to the ligand, followed by the Mg platform, resulting a planar π-C_2N_2(sp^2)–Al/Mg bridging core between metals. The new heterobimetallics have been unambiguously characterized by single-crystal X-ray analysis. NOESY, DOSY and EXSY NMR studies as well as DFT calculations corroborate both a rearrangement in solution into complexes containing an unprecedented apical carbanion with a direct σ-C(sp^3)–Al covalent bond named [{Mg(R)(pbpamd$^-$)Al($Me)_2$}] (R = Et **1b**, tBu **2b**) and the interconversion equilibrium between both isomers.[1]

We verified their utility and high efficiency as catalysts in the well-controlled Ring-Opening Polymerization of the bio-renewable L- and rac-lactide at 23 ºC, reaching an unprecedented TOF value near to 25 000 h^{-1} for rac-LA at this temperature, and exerting an unexpected level of heteroselectivity up to Pr = 0.80. Very interestingly, kinetics experiments allowed to demonstrate apparent first-order with respect to catalyst and lactide, which supports a synergic intramolecular cooperation between centers with electronic communication among them, which is the responsible to outperform the activity of their Al/Mg mono- and even their homodi-nuclears constituents.



Scheme 1: Ring opening polymerization of rac-LA with heterobimetallic Al-Mg catalysts.

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FP04

Bonding modes and structural diversity of tantalum complexes supported by redox-active ligands

Elena Álvarez-Ruiz,[1] Alberto Hernán-Gómez, [1] Avelino Martín, [1]
Miguel Mena[1] and Cristina Santamaría.[1]

[1] *Departamento de Química Orgánica y Química Inorgánica. Instituto de Investigación Química "Andrés M. del Río" (IQAR), Universidad de Alcalá, Campus Universitario, E-28805 Alcalá de Henares, Madrid, Spain.*
e-mail: elena.alvarezr@uah.es

Developing new metal-ligand interactions is essential for applied organometallic chemistry as it dictates the reactivity of the generated compounds.[1] This has been notably relevant for compounds of group 5 elements in maximum oxidation state, in which the incorporation of redox-active ligands has made them capable of mediating multielectron processes.[2] In this regard, ortho-phenylendiamido (*o*-PDA) ligands display flexibility in their coordination modes and the possibility of undergoing one or two electron redox processes. Nevertheless, the combination of these ligands with early transition metals has been less investigated.[3]

Herein, we report our studies on the combination of different *o*-PDA ligands and the fragment $[TaCl_{5-n}(\eta^5\text{-}C_5H_4SiMe_3)_n]$ (n = 0, 1). Through a systematic study, we have achieved control over the binding mode of the *o*-PDA ligands, which can coordinate through the nitrogen atoms or the central phenylene ring, adopting different electronic structures.

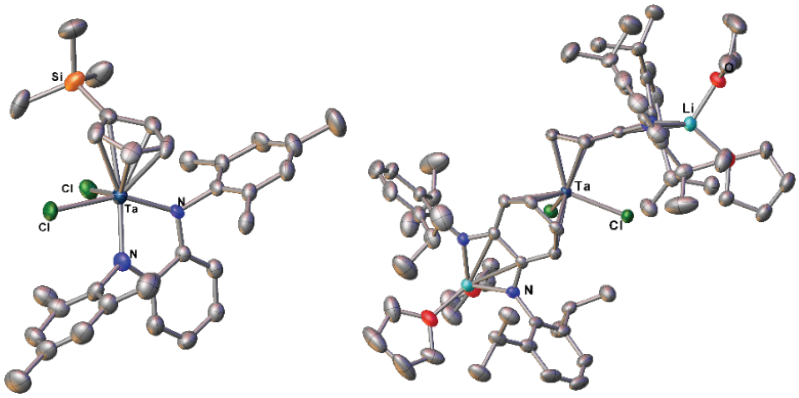

Figure 1. Solid state structures of o-PDA-Ta compounds with two different coordination modes.

Financial support. Financial support for this work was provided by the Ministerio de Ciencia, Innovación y Universidades (PGC2018-094007-B-I00), Comunidad de Madrid (Programa Atracción de Talento, 2018-T1/AMB-11478), and Universidad de Alcalá (Programa Estímulo a la Investigación de Jovenes investigadores CM/JIN/2019-030, CM/JIN/2021-031).

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FP05

Exploring Trends in Salphen Based Group 13 Catalysts for Cyclic Carbonate Synthesis

Diego Jaraba Cabrera[1], Carlos Díez-Poza[1], Ryan Lewis[2], Lucía Álvarez-Miguel[1], Alex Hamilton[2], Marta E. G. Mosquera[1] and Christopher J. Whiteoak[1]

[1] Universidad de Alcalá, Grupo SOSCATCOM, Departamento de Química Orgánica y Química Inorgánica, Facultad de Farmacia and Instituto de Investigación Química Andrés M. del Río (IQAR), Campus Universitario, Ctra. Madrid-Barcelona Km. 33,600, 28871 Alcalá de Henares, Madrid, Spain.
[2] Sheffield Hallam University, Biomolecular Sciences Research Centre and Department of Biosciences and Chemistry, College of Health, Wellbeing and Life Sciences, Howard Street, Sheffield, UK.
Email: diego.jaraba@uah.es

The synthesis of cyclic carbonates through the atom efficient coupling of epoxides to carbon dioxide (CO_2) presents an interesting application of CO_2 as a C_1 source in high oxidation state. Over recent years, a large number of catalysts have been studied, focusing on readily prepared ligands, such as salphens[1] and aminotrisphenols.[2] Regarding group 13 metals, it is notable that most reports have focused on the use of aluminium-based compounds likely because of the well-established Lewis acidity and its natural abundance. However, little attention has been paid to the heavier group 13 elements (gallium and indium).

This work presents the synthesis of aluminium, gallium and indium salphen compounds (Figure 1) with variation of the halide ligand and studies their application as catalysts for the synthesis of cyclic carbonates. The effects of changing the metal centre and halogen in catalysis shows unexpected trends which are discussed and fully supported through a complete DFT study.

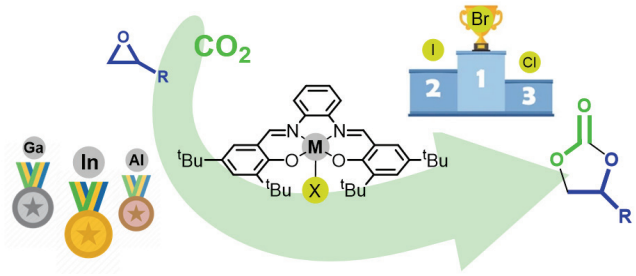

Figure 1

Financial support. CJW would like to thank the Comunidad de Madrid (Spain) for funding (Programa de Atracción de Talento 2019: Modalidad 1; Award number 2019-T1/AMB-13037, and CM/JIN/2021-018). All authors would like to acknowledge funding from the Spanish Government (RTI2018-094840-BC31 and PID2020-113046RA-I00/AEI/10.13039/501100011033) and the Universidad de Alcalá (UAH-AE-2017-2). DJC thanks the Comunidad de Madrid (Spain) and European Union for funding a contract under the Programa INVESTIGO (47-UAH-INV).

References

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FP06

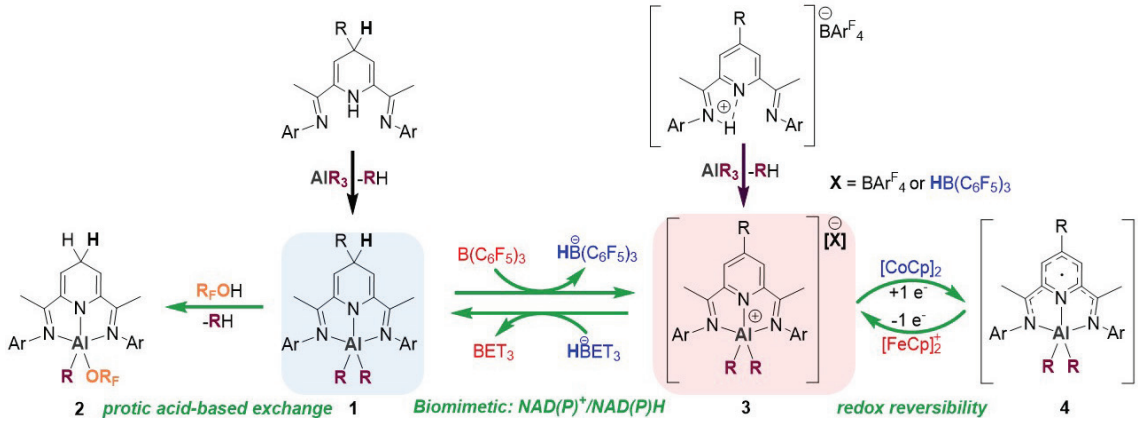
Neutral and cationic alkyl aluminium complexes supported by 2,6-bis(imino)pyridine-based ligand as Biomimetic Hydride Exchange Systems

Juan Manuel Delgado Collado, Juan Cámpora Pérez, Antonio Rodríguez Delgado

Instituto de Investigaciones Químicas (IIQ) Universidad de Sevilla-CSIC.
C/ Américo Vespucio, 49, 41092, Sevilla, Spain.
juanma.delgado@iiq.csic.es

2,6-bis(imino)pyridines (BIP) are a versatile family of ligands with many applications in coordination chemistry and catalysis.[1] The redox non-innocent nature makes them difficult to be studied, however, there are some exceptional cases that allow the properties of these compounds to be explored.[2]

In this work, we are reporting the synthesis of a series of alkyl aluminium complexes from the reaction of dihydropyridine with an alkyl metal (1). We found that compound (**1**) reacted with a perfluoroalcohol, similarly to its zinc analogue,[3] selectively affording the mixed alkyl/alkoxide dihydropyridinate complex (**2**). Furthermore, the addition of a strong Lewis acid to this system (**1**) led to the formation of cationic aluminium complex (**3**), in analogous way to reported zinc species.[4] Alternatively, we developed a synthesis route of these systems (**3**) from the cationic BIP ligand and AlR_3. Once the cationic complex is formed (**3**), we can return to the dihydropyridinate system (**1**) by adding a strong reducing agent. These reactions suggest that BIP-based ligands can act as biomimetic hydride reductants, similar to the redox exchangers of pyridine-based coenzymes (e.g., NAD(P)H/NAD(P)$^+$) in biological systems. In addition, the cationic compound (**3**) also behaves as a redox-reversible systems (**4**), allowing ligand-centred one-electron redox reactions with one-electron redox reagents.



Scheme 1.

Financial support. This work was supported by Spanish Research Agency (AEI), and Junta de Andalucía through the European Union (Feder Funds) projects PGC2018-095768-B-100 and PY20_0104 respectively.

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FP07

Unveiling Chemodivergent Faces of Janus-Type Rh_2NHC_2Uracilato Catalyst for Tandem Alkyne Dimerization-Hydrosilylation

Belinda Español-Sánchez, Jesús J. Pérez-Torrente, Ricardo Castarlenas

bespanol@unizar.es

Tandem catalysis involves subsequent transformations which entails distinct reaction mechanisms [1]. Most examples contain heterodinuclear systems, in which the presence of two different metals facilitates divergent reaction mechanisms [2]. In contrast, involvement of homodinuclear complexes in tandem catalysis are limited. The identical chemical environment around the metal center hampers their efficiency in conducting mechanistically distinct reactions [3]. In this context, homodimetallic Janus-type rhodium complexes [(IPr)(coe)Rh(κ²*O,N*-U-κ²*O',N'*)Rh'(coe')(IPr')] have been prepared using uracil as the binding ligand. This species has been revealed as efficient catalyst for tandem alkyne dimerization-hydrosilylation. Furthermore, its monometallic analogues [(IPr)(coe)Rh(κ²*O²,N¹*-Uracil)] and [(IPr)(coe)Rh(κ²-*O⁴,N³*-Uracil)] have been synthesized, and we are able to demonstrate that each rhodium center proceeds by a different mechanism, depending solely on the coordinated atoms of the nitrogenous base. Thus, Rh(κ²*O²,N¹*-Uracil) is efficient in dimerization of terminal akynes [4], while Rh(κ²*O⁴,N³*-Uracil) in hydrosylilation of alkynes. Hence, Rh(κ²-O,N-U-κ²-O',N')Rh', are able to couple both reactions, hydrosilylating the enyne generated in the dimerizationof the alkyne (Figure 1).

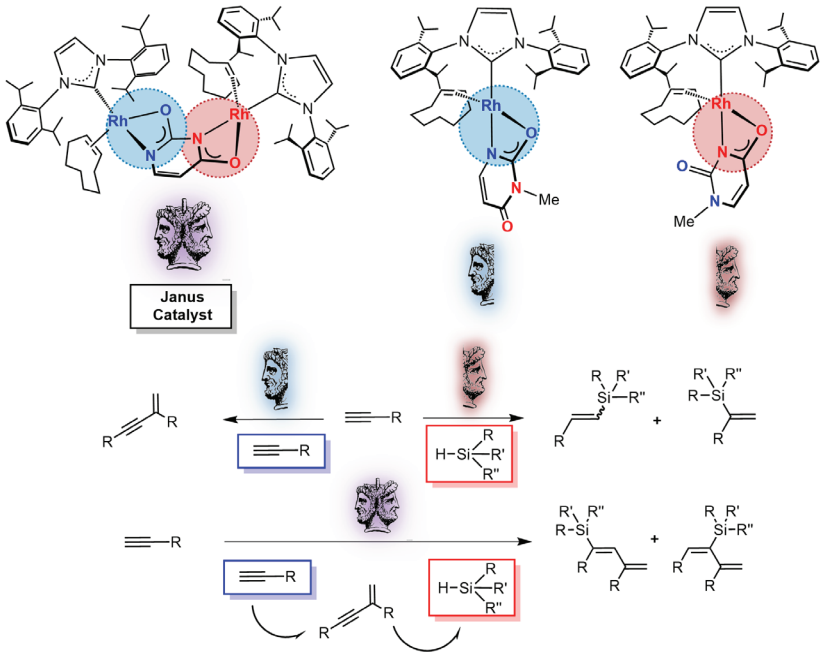

Figure 1. Tandem Alkyne Dimerization-Hydrosilylation.

References

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FP08

Unprecedented Silver(III) Carbene Complexes

Juan Pueyo, Daniel Joven-Sancho, Antonio Martín, Babil Menjón, Miguel Baya.

Instituto de Síntesis Química y Catálisis Homogénea, Departamento de Química Inorgánica. Universidad de Zaragoza, C/ Pedro Cerbuna 12 50009 Zaragoza.

Email: juanpueyo7@gmail.com

High valent transition metal (TM) carbene complexes have achieved enormous relevance, in connection to their application as methatesis, carbene transfer or oxidation catalysts. Whereas for early TM both homocarbene and N-heterocyclic carbene high valent derivatives are well-known, for late TM this family is largely composed of M-NHC compounds.

Focusing on group 11, high valent metal carbene complexes of the lighter elements, copper and silver, constitute chemical oddities. Indeed, whereas hardly a couple of Cu^{III} examples are known, using tetra(NHC)[1] or bis(NHC)-bis(pyridine) ligands,[2] no Ag^{III}-carbene compound has been reported so far.

In this communication we wish to present the synthesis and characterization of a series of unprecedented Ag^{III}-NHC compounds, obtained by a novel strategy using an unconventional Ag^{III} fluoride derivative as precursor.[3] These complexes show Inverse Ligand Field electronic structures together with unexpected thermodynamic stabilities.

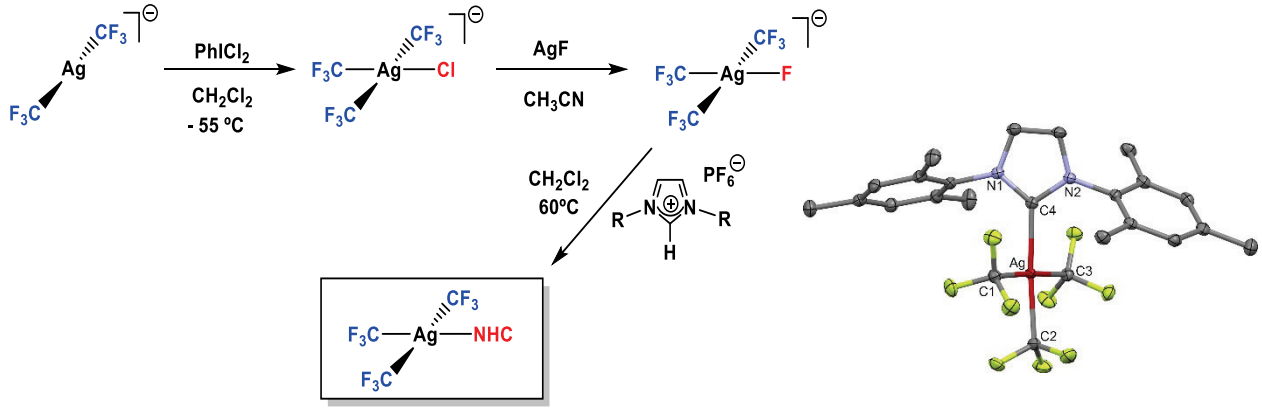

Figure 1. Ag^{III}-NHC synthetic path (left). Ag^{III}-NHC solid state structure (right).

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FP09

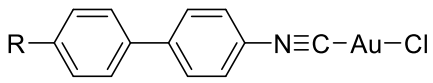
Liquid crystals based on gold(I) complexes with an uncommon molecular structure

Víctor Esteban, Manuel Bardají, Silverio Coco*

IU CINQUIMA / Departamento de Química Inorgánica, Facultad de Ciencias, Universidad de Valladolid, 47011-Valladolid, Spain
victor.esteban@uva.es

Classically, thermotropic liquid crystal synthesis has been based on the use of anisotropic structures composed of a centred rigid core and a number of flexible long alkyl chains at the periphery. However, among the large number of liquid crystals known, some exceptions to this model have been reported, in which mesomorphic compounds do not bear flexible long alkyl chains. In these cases the liquid crystal behavior is attributed, depending on the system, either by the presence of bulky or polarizable substituents [1,2,3]. However, there is still much to know about these unconventional liquid crystals.

In this communication we describe the unusual case of a series of gold(I) organometallic complexes with formula [AuCl($CNC_6H_4C_6H_4R$)] (R = OEt, OMe, Et, Me) (Fig. 1), which exhibit mesomorphism, despite not having long chains in contrast to classical examples. They have been structurally characterized by X-ray diffraction, and display a strongly luminescent behavior (in the solid state and in solution). The structural features, which determine the structure-properties relationships in these systems, will be discussed.



R = OEt, OMe, Et, Me

Figure 1.

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