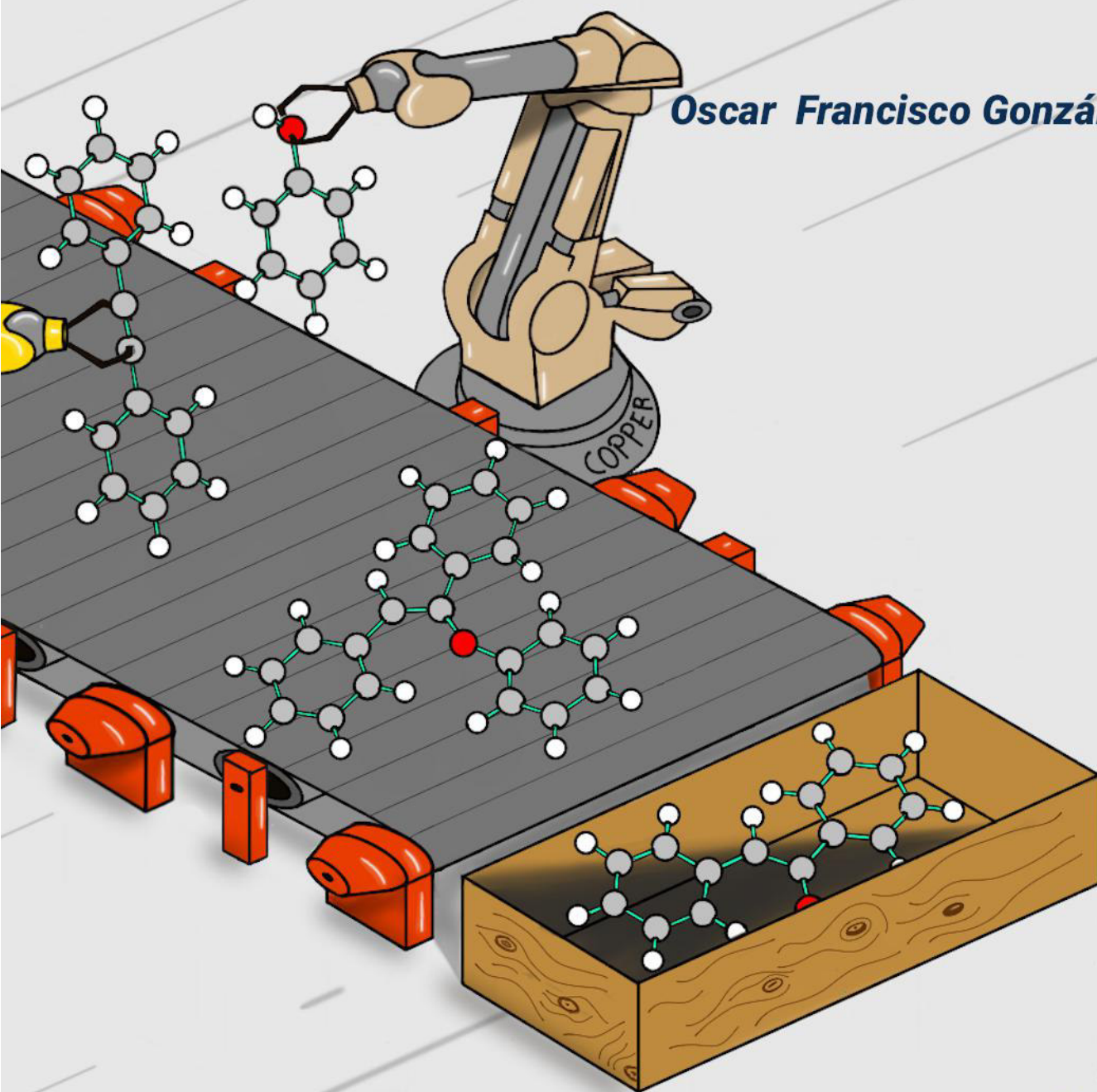


The Role of the Metal in the in the Dual-Metal Catalyzed Hydrophenoxylation of Alkynes

Oscar Francisco González Belman



Master Thesis

The Role of the Metal in the Dual-Metal
Catalyzed Hydrophenoxylation of Alkynes

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2018

Double degree program: Master in Chemical
Sciences/Master in Advanced Catalysis and Molecular
Modelling



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Dedicated to my girlfriend and family.

Acknowledgements

First of all, I want to give many thanks to my parents Ma. Guadalupe Belman Hernández, Martín González Juárez, and my brother Jesus Manuel González Belman for the unconditional support throughout my professional life. Another important person who had an important contribution to undertake this project is my girlfriend Andrea Palacios Rodríguez, I cannot thank her enough to be my cheerleader when I need it. Other appreciated members of my family to whom I want to give my sincere thanks are my aunts María Leobarda Belman Hernández, Martina Belman Hernández, and my cousin Samara Mendoza Belman.

I would like to express my deepest thanks to Dr. J. Oscar C. Jiménez Halla (University of Guanajuato) and Dr. Albert Poater (University of Girona), for support me throughout the development of this project. It was a great honor to work under their supervision.

I would also like to express my gratitude to Prof. Holger Braunschweig and his workgroup (University of Würzburg), for giving me the opportunity to broaden my knowledge in boron chemistry with our last collaboration works.

Many thanks for the scholarship to:



Finally, I would like to Thank institutions below for giving me the opportunity to belong to the double degree program: Master in Chemical Sciences and Master in Advanced Catalysis and Molecular Modelling.



List of Publications

The thesis is based in the following publications:

1. Casals-Cruañas, E., González-Belman, O. F., Besalú-Sala, P., Nelson, D. J., and Poater, A. "The preference for dual-gold(I) catalysis in the hydro(alkoxylation *vs.* phenoxylation) of alkynes". *Org. Biomol. Chem.* 15(2017), 6416–6425.
2. González-Belman, O. F., Jimenez-Halla, J. O. C., Nahra, F., Cazin, C., and Poater, A. "The role of the metal in the dual-metal catalysed hydrophenoxylation of diphenylacetylene". *Catal. Sci. Technol.* (2018) DOI: 10.1039/C8CY00510A

Other publications:

1. Hofmann, A., Lamprecht, A., González-Belman, O. F., Dewhurst, R. D., Jimenez-Halla, J. O. C., Kachel, S., and Braunschweig, H. "Dialumination of unsaturated species with a reactive bis(cyclopentadienyl) dialane". *Chem. Commun.* 54(2018), 1639–1642.
2. Winner, L., Hermann, A., Bélanger-Chabot, G., González-Belman, O. F., Jimenez-Halla, J. O. C., and Braunschweig, H. "Cleavage of BN Triple Bonds by Main Group Reagents". *Chem. Commun.* (2018) DOI: 10.1039/C8CC02317D
3. Böhnke, J., Brückner, T., Hermann, A., González-Belman, O. F., Arrowsmith, M., Halla-Jimenez, J. O. C., and Braunschweig, H. "Single and double activation of acetone by isolobal $B\equiv N$ and $B\equiv B$ triple bonds". *Chem. Sci.* 9(2018), 5354–5359.

Congresses where “The Role of the Metal in the Dual-Metal Catalyzed Hydrophenoxylation of Alkynes” was presented:

1. Poater, A., Casals, E., Besalú, P., Luque-Urrutia, J. A., and Belman, O. “Dual Metal Catalysts vs the Traditional Monometal catalysis” (invited talk); EMN Meeting on Catalysis, Dubrovnik (Croatia); May 3-7th, 2017.
2. González-Belman, O. F., Poater, A., and Jiménez-Halla, J. O. C. “The role of the metal in the dual-metal catalyzed hydrophenoxylation of diphenylacetylene” (poster); Mexican Meeting of Theoretical Physicochemistry, Puebla (Mexico); November 16-18th, 2017.
3. González-Belman, O. F., Jiménez-Halla, J. O. C., Nahra, F., Cazin, C. S. J., and Poater, A. “The role of the metal in the dual-metal catalyzed hydrophenoxylation of diphenylacetylene” (poster); Girona Seminar 2018: Predictive Catalysis, Transition-Metal Reactivity by Design, Girona (Spain), April 3-6th, 2018.
4. Besalú-Sala, P., Casals-Cruañas, È., González-Belman, O. F., Nelson, D. J., and Poater, A. “The preference for dual-gold(I) catalysis in the hydro(alkoxylation vs. phenoxylation) of alkynes” (poster); Girona Seminar 2018: Predictive Catalysis, Transition-Metal Reactivity by Design, Girona (Spain), April 3-6th, 2018.

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List of abbreviations

<i>Ac</i> : Acetyl	<i>PE</i> : Potential Energy
<i>BINAP</i> : 2,2'-bis(diphenylphosphino)-1,1'-binaphthyl	<i>PES</i> : Potential Energy Surface
<i>Bn</i> : Benzyl	<i>PSC</i> : Phosphinosilyl carbene
<i>Boc</i> : <i>tert</i> -Butyloxycarbonyl	<i>rds</i> : rate-determining step
<i>bpy</i> : Bipyridyl	<i>SIMes</i> : 1,3-dimesityl-4,5-dihydro-1 <i>H</i> -imidazol-3-ium-2-ide
<i>BSSE</i> : Basis Set Superposition Error	<i>STO</i> : Slater-Type Orbital
<i>CAAC</i> : Cyclic (Alkyl)(Amino)Carbenes	<i>THF</i> : Tetrahydrofuran
<i>CD</i> : Circular Dichroism	<i>TST</i> : Transition State Theory
<i>cod</i> : 1,5-cyclooctadiene	<i>XC</i> : Exchange-Correlation
<i>DFT</i> : Density Functional Theory	
<i>DMAP</i> : 4-Dimethylaminopyridine	
<i>dmpe</i> : 1,2-Bis(dimethylphosphino)ethane	
<i>ECP</i> : Effective Core Potential	
<i>EPR</i> : Electron Paramagnetic Resonance	
<i>GGA</i> : Generalized Gradient Approximation	
<i>GTO</i> : Gaussian-Type Orbital	
<i>HAR</i> : Hydroalkoxylation reaction	
<i>HEG</i> : Homogeneous Electron Gas	
<i>HF</i> : Hartree-Fock	
<i>HPR</i> : Hydrophenoxylation reaction	
<i>IMe</i> : 1,3-dimethyl-1,3-dihydro-2 λ^2 -imidazole	
<i>IMes</i> : 1,3-dimesityl-1 <i>H</i> -imidazol-3-ium-2-ide	
<i>iPr</i> : Isopropyl	
<i>IPr</i> : 1,3-bis(2,6-diisopropylphenyl)-1 <i>H</i> -imidazol-3-ium-2-ide	
<i>IPr*</i> : 1,3-bis(2,6-dibenzohydril-4-methylphenyl)-2,3-dihydro-1 <i>H</i> -imidazole	
<i>LA</i> : Lewis acid	
<i>LB</i> : Lewis base	
<i>LDA</i> : Local Density Approximation	
<i>LG</i> : Leaving group	
<i>MBO</i> : Mayer Bond Order	
<i>MCD</i> : Magnetic Circular Dichroism	
<i>MTBE</i> : Methyl <i>tert</i> -butyl ether	
<i>NBO</i> : Natural Bond Orbital	
<i>NHC</i> : <i>N</i> -heterocyclic carbene	
<i>NMR</i> : Nuclear Magnetic Resonance	

Abstract

Poly vinyl ethers are compounds with an immense value in coating industry due to their properties such as: high viscosity, soft adhesiveness, and solubility in water and organic solvents. However, the main challenge in this field is the synthesis of vinyl ether monomers that can be synthesized by several methodologies such as vinyl transfer, reduction of vinyl phosphate ether, isomerization, hydrogenation of acetylenic ethers, elimination, addition of alcohols to alkyne species, etc. The most successful strategy to access to vinyl ether derivatives is the addition of alcohols to alkynes catalyzed by transition-metals such as: molybdenum, tungsten, ruthenium, palladium, platinum, gold, silver, iridium and rhodium, where gold-*N*-heterocyclic carbene (Au-NHC) catalysts have shown the best results in vinyl ether synthesis. Recently, the hydrophenoxylation reaction (HPR) has been reported as a digold-assisted process where the species that determine the rate of the reaction are PhO-[Au(IPr)] and alkyne-[Au(IPr)]. In addition, Cazin and co-workers reported the improvement of the hydrophenoxylation reaction by using the Cu-NHC and Au-NHC catalyst.

The present thesis is a computational study via Density Functional Theory of the rate-determining step (rds) proposed by Poater *et al.* for the potential initial reagents (PhO-[M] and alkyne-[M] species) in the [Cu]/[Au] catalytic system, to obtain a more cost-effective method for the hydrophenoxylation reaction. Silver was also included in order to understand the effect of the metal center. Moreover, the steric sensitivity of the rds was investigated with less sterically demanding NHC ligands such as IMes, SIMes, and IMe. In the search of bringing down the rds energy barrier, we substituted NHCs by Cyclic (Alkyl)(Amino)Carbenes (CAAC) (Pyrrolidin-ylidenes L¹ and L²) and Phosphinosilyl carbene (PSC) ([bis(diisopropylamino)phosphanyl](trimethylsilyl)carbene) ligands for extending the hetero-dual-catalysed HPR. Additionally, we performed computational studies for the hetero-dual and heteroleptic IPr/(L²) system, taking into account that catalysts bearing those ligands generate good electrophiles and nucleophiles.

Our results indicate that the [Cu(IPr)]/[Au(IPr)] system is better than the [Au(IPr)]/[Au(IPr)] system, but the [Ag(IPr)]/[Au(IPr)] couple exhibits the lowest energy barrier for the rds. On the other hand, the study of the metal effect in the rds shows that, by exchanging IPr for CAAC ligand (which stands for L¹), the couples [Cu(L¹)]/[Au(L¹)] and [Ag(L¹)]/[Au(L¹)] are equally capable catalysts for decreasing the energy activation. Moreover, when we added the bulky CAAC ligand L² to observe the steric effect in the [Cu]/[Au] system, this was also sterically influenced as in the case of the catalysis involving NHC ligands. On the other hand, in the hetero-dual and heteroleptic study, it showed the [Au(IPr)(PhCCPh)]⁺/[Cu(L²)(OPh)] couple as the best one. In fact, those species displayed the lowest energy barriers for the rds regarding to all the studied species in this thesis. In the case of the PSC ligand, the pre-activated species [Cu(PSC)(OPh)]/[Au(PSC)(PhCCPh)]⁺ displayed a lower energy barrier than the species bearing the IPr ligand. Yet, all these results allowed us to broaden

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the heterometallic catalysis. In summary, the rds turned out to be quite sensitive to the sterical hindrance of carbene ligands.

Resumen

Los polímeros de éteres de vinilo son compuestos de gran valor en la industria del recubrimiento, debido a que presentan propiedades como: alta viscosidad, adhesividad suave, solubilidad en agua y solventes orgánicos. No obstante, el principal reto en esta área es la síntesis de los monómeros de éteres de vinilo, los cuales pueden ser sintetizados empleando metodologías tales como la transferencia del grupo vinilo, la reducción de éteres de vinil fosfato, la isomerización de éteres alílicos, la hidrogenación de éteres acetilénicos, la eliminación de grupos salientes, la adición de alcoholes a especies alquínicas, etc. La estrategia más exitosa a través de la cual es posible acceder a los derivados de vinilo es la adición de alcoholes a alquinos catalizada por metales de transición como: molibdeno, tungsteno, rutenio, paladio, platino, oro, plata, iridio y rodio, donde los catalizadores de oro-carbeno *N*-heterocíclico (Au-CNH) han mostrado los mejores resultados en la síntesis de vinil éteres. Recientemente, la reacción de hidrofenoilación (RHP) ha sido descrita como un proceso doblemente asistido por oro, donde las especies que determinan la velocidad de la reacción son PhO-[Au(IPr)] y alquino-[Au(IPr)]. Además, Cazin y colaboradores han reportado la mejora de la reacción de hidrofenoilación tras el empleo de catalizadores de Cu-CNH y Au-CNH.

Esta tesis es un estudio computacional vía Teoría de Funcionales de la Densidad de la etapa determinante de la reacción (edr) propuesta por *Poater et al.* para los potenciales reactivos de partida (especies PhO-[M] y alquino-[M]) en el sistema catalítico [Cu]/[Au], para obtener un método más económico para la reacción de hidrofenoilación. También se incluyó la plata para entender el efecto del centro metálico. Además, se estudió la sensibilidad estérica de la etapa determinante de la reacción empleando ligandos NHC menos voluminosos como el IMes y SIMes en lugar del IPr. En búsqueda de disminuir la barrera energética de la edr, sustituimos los ligandos CNHs por los Carbenos de (Alquil)(Amino) Cíclicos (CAAC) (Pirrolidin-ilidenos L^1 y L^2) y carbenos de fosfinosililo (CFS) ([bis(diisopropilamino)fosfanil](trimetilsilil)carbeno) con el objetivo de extender la RHP hetero-dual-catalizada. Además, realizamos los estudios computacionales para el sistema hetero-dual y heteroléptico IPr/ L^2 , tomando en cuenta que la catálisis que involucra estos ligandos produce buenos electrófilos y nucleófilos.

Nuestros resultados indican que el sistema [Cu(IPr)]/[Au(IPr)] es mejor que el sistema [Au(IPr)]/[Au(IPr)], pero la pareja [Ag(IPr)]/[Au(IPr)] nos dio la barrera de energía más baja para la etapa determinante de la reacción. Por otro lado, el estudio del efecto del metal en la edr muestra que, al intercambiar el ligando IPr por CAAC (señalado como L^1), las parejas [Cu(L^1)]/[Au(L^1)] y [Ag(L^1)]/[Au(L^1)] son catalizadores igualmente capaces de disminuir la energía de activación. Además, cuando se adicionó el ligando voluminoso CAAC L^2 para observar el efecto estérico en el sistema [Cu]/[Au], este también se vio estéricamente influenciado al igual que en la catálisis que involucra ligandos CNH. Por otro lado, en el estudio hetero-dual y heteroléptico, este mostró la pareja [Au(IPr)(PhCCPh)]⁺/[Cu(L^2)(OPh)] como la mejor. De hecho, estas especies mostraron la

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barrera de energía más baja para la etapa determinante de la reacción respecto a las especies estudiadas en esta tesis. En el caso del ligando CPS, las especies pre-activadas $[\text{Cu}(\text{CPS})(\text{OPh})]/[\text{Au}(\text{CPS})(\text{PhCCPh})]^+$ mostraron una barrera energética más baja que las especies que contienen el ligando IPr. Así, todos estos resultados nos permitieron ampliar la catálisis heterometálica. En resumen, la etapa determinante de la reacción resultó ser bastante sensible al impedimento estérico de los ligandos de carbeno.

Resum

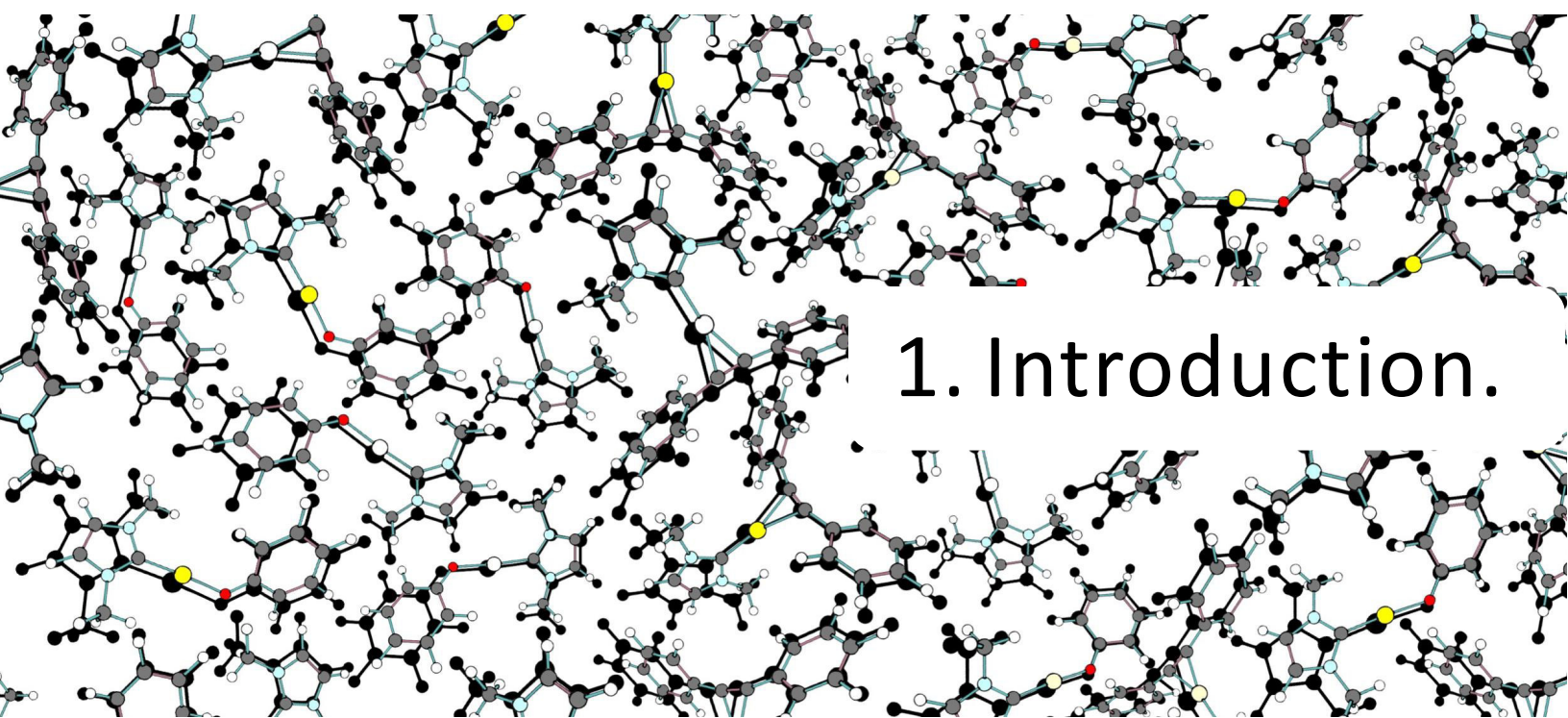
Els polímers de èters de vinil són compostos d'un gran valor a la indústria del recobriment, degut a que presenten propietats com: alta viscositat, adhesivitat suau, solubilitat en aigua i solvents orgànics. A més a més, el principal repte en aquesta àrea és la síntesi dels monòmers d'èters de vinil, els quals hi poden ser sintetitzats emprant metodologies com la transferència del grup vinil, la reducció d'èters de vinil fosfat, la isomerització d'èters al·lílics, la hidrogenació d'èters acetilènics, l'eliminació de grups sortints, l'adició d'alcohols a espècies alquíniques, etc. l'estratègia més reeixida a través de la qual és possible accedir als derivats de vinil és l'adició d'alcohols a alquins catalitzada per metalls de transició com: molibdè, tungstè, ruteni, pal·ladi, platí, or, argent, iridi i rodi, on els catalitzadors d'or-carbè *N*-heterocíclic (Au-CNH) han produït els millors resultats a la síntesi de vinil èters. Recentment, la reacció d'hidrofenoxilació ha estat descrita com un procés doblement assistit per or, on les espècies que determinen la velocitat de la reacció són PhO-[Au(IPr)] i alquí-[Au(IPr)]. A més, Cazin i col·laboradors van millorar la reacció d'hidrofenoxilació després de l'ús de catalitzadors de Cu-NHC i Au-NHC.

Aquesta tesi és un estudi computacional via Teoria de Funcionals de la Densitat de l'etapa determinant de la reacció (edr) proposada per *Poater et al.* Per als potencials (espècies PhO-[M] i alquí-[M]) en el sistema catalític [Cu]/[Au], per obtenir un mètode més econòmic per a la reacció d'hidrofenoxilació. També es va incloure provar l'argent per observar l'efecte del nucli metàl·lic. A més, es va analitzar la sensibilitat estèrica de l'etapa determinant de la reacció fent servir lligands NHC menys voluminosos com l'IMes i el SIMes en lloc de l'IPr. Tractant de disminuir la barrera energètica de l'edr, substituïm els lligands CNHs pels carbens d'(alquil)(amino) cíclics (CAAC) (Pirrolidin-ilidens L^1 i L^2) i carbè d'fosfinsilil (CPS) ([bis(diisopropilamino)fosfanil] (trimetilsilil)carbè) amb l'objectiu d'estendre la RHF hetero-dual-catalitzada. A més d'això, en varem realitzar els estudis computacionals pel sistema hetero-dual i heterolèptic IPr/(L^2), prenent en compte que la catàlisi que involucra aquests lligands produeix bons electròfils i nucleòfils.

Nostres resultats indiquen que el sistema [Cu(IPr)]/[Au(IPr)] és millor que el sistema [Au(IPr)]/[Au(IPr)], però la parella [Ag(IPr)]/[Au(IPr)] es va tornar la barrera d'energia més baixa per a l'etapa determinant de la reacció. Per altra banda, l'estudi de la influència del metall a l'edr mostra que, al intercanviar el lligand IPr per CAAC (designat com L^1), les parelles [Cu(L^1)]/[Au(L^1)] i [Ag(L^1)]/[Au(L^1)] són catalitzadors igualment capaços de disminuir l'energia d'activació. A més a més, quan es va addicionar el lligand voluminos CAAC L^2 per observar l'efecte estèric al sistema [Cu]/[Au], aquest també es va veure estèricament influenciat al igual que a la catàlisi que involucra lligands CNH. Per banda, al estudi hetero-dual i heterolèptic, aquest va mostrar a la parella [Au(IPr)(PhCCPh)]⁺/[Cu(L^2)(OPh)] com la millor. De fet, aquestes espècies van tenir la barrera d'energia més baixa per a l'etapa determinant de la reacció al respecte amb les espècies estudiades en aquesta tesi. Pel cas del lligand CPS, les espècies pre-activades

Abstract

[Cu(PSC)(OPh)]/[Au(PSC)(PhCCPh)]⁺ van presentar una barrera energètica més baixa que les espècies que contenen el lligand IPr. Així doncs, tots aquests resultats ens van permetre ampliar la catàlisi heterometàl·lica. En resum, l'etapa determinant de la reacció va resultar ser força sensible al impediment estèric dels lligands carbè.



1.1. Catalysis and petroleum industry.

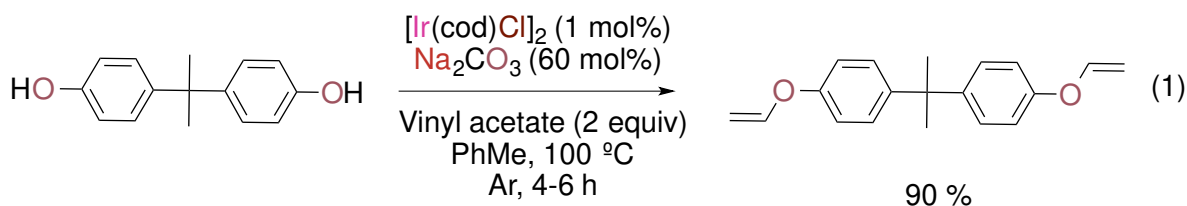
Along the time, alchemists and chemists have directed their efforts to control the chemical processes by using *species able to accelerate the rate of the reaction*. Since the 18th century, they have achieved significant advances in the catalysis field. Some contributions such as: sulphuric acid production, the conversion of starch to sugar purposed by Kirchoff, the first safety lamp for coal miners, and the catalyst definition by Berzelius marked the beginning of an era in this field.¹ At the beginning of the 19th century, Paul Sabatier reported the hydrogenation of unsaturated organic compounds catalysed by nickel.² Interestingly, this finding brought about the birth of the modern catalysis. At the same time, petroleum industry started to explode the catalysis goodness in processes such as catalytic cracking³ by the pioneer Eugene Houdry in 1922 and hydrocracking.⁴ The evolution of the petrochemical industry during the first half of the 19th century resulted into several advances in different industrial fields and the development of polymers area.

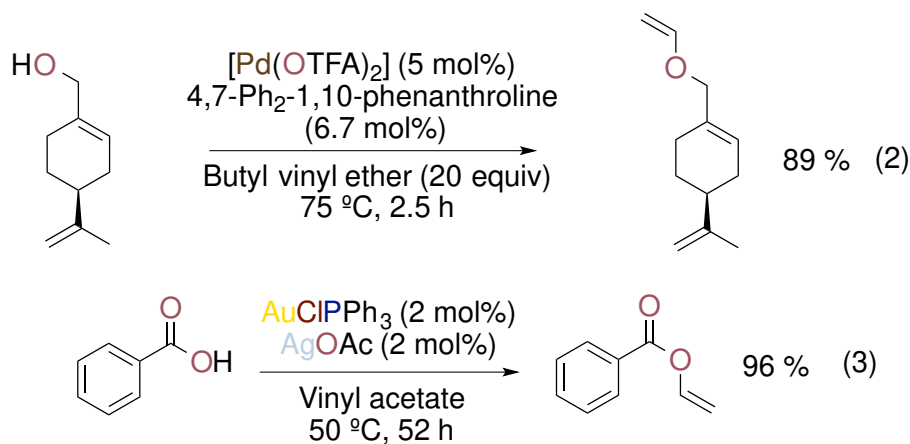
Businessmen started to explore this field, so the new business in chemical industry was born with the catalytic synthesis of building blocks of polymers such as acrylonitrile⁵ and vinyl chloride monomer.⁶ The exhaustive research in polymers area gave success to industries such as Du Pont, so since 20's, the company had positioned itself at the top in polymers marketplace with its polymeric films and synthetic fibres such as cellophane, rayon, nylon and polyester.⁷ Due to the properties such as high viscosity, soft adhesiveness, resistance to saponification, and solubility in water and organic solvents, the poly vinyl ethers have been the central focus in the polymers industry.⁸

1.2. Synthesis of vinyl ethers.

1.2.1. Vinyl transfer to alcohols.

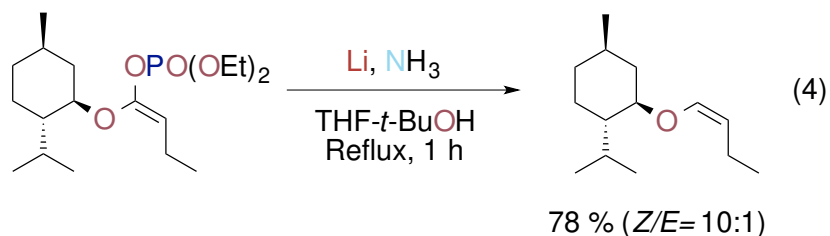
Chemists around the world have directed their efforts to improve the synthetic strategies to obtain vinyl ether monomers. Nevertheless, vinyl ethers can be synthesized through vinyl transesterification catalyzed by compounds such as $[\text{Ir}(\text{cod})\text{Cl}]_2$ (Eq. 1),⁹ $\text{Pd}(\text{OTFA})_2$ (Eq. 2),¹⁰ and AuClPPh_3 (Eq. 3),¹¹ where gold catalyst has shown the best effectivity for the vinylation of carboxylic acids.





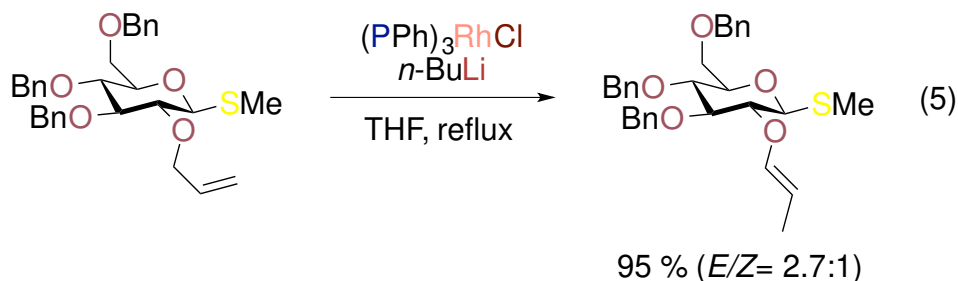
1.2.2. Reduction of vinyl phosphate ethers.

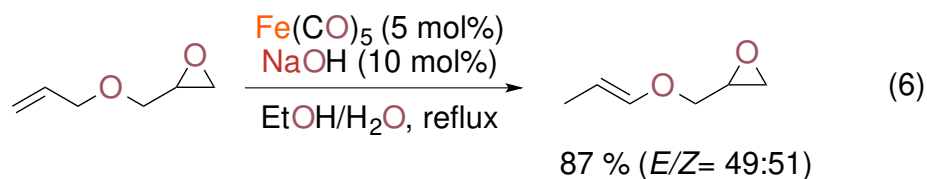
Other precursors of vinyl ethers are vinyl phosphate ethers. To obtain the desired vinyl compound, the phosphate group can be removed by using solutions of reductive metals. A clear example of the reductive cleavage of the C-P bond is Birch's methodology for the synthesis of chiral vinyl ethers (Eq. 4).¹²



1.2.3. Isomerization of allyl ethers to vinyl ethers.

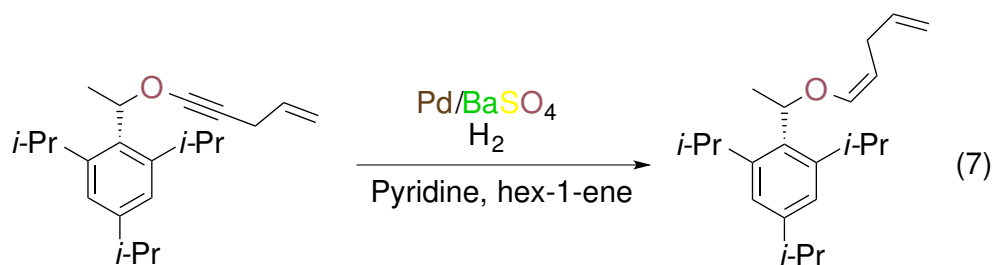
Allyl ethers tend to isomerize to vinyl ethers in the presence of a strong base such as potassium *tert*-butoxide.¹³ However, transition-metal species can also achieve the isomerization of allyl ether substrates. Catalysts such as $(\text{PPh})_3\text{RhCl}$ (Eq. 5)¹⁴ and $\text{Fe}(\text{CO})_5$ (Eq. 6)¹⁵ have shown good catalytic activity.





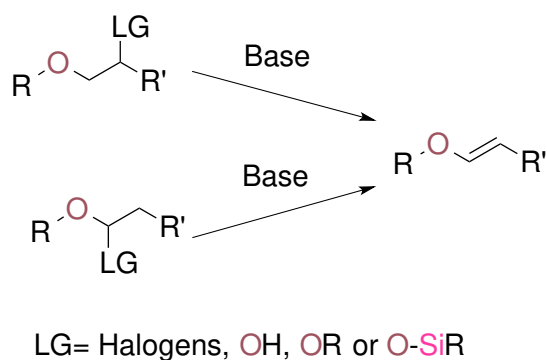
1.2.4. Hydrogenation of acetylenic ethers.

Hydrogen addition to π -bond in acetylenic ethers is another synthetic strategy to obtain vinyl ethers. Some transition metals such as palladium can achieve the hydrogenation of the unsaturated carbons (Eq. 7).¹⁶



1.2.5. Elimination.

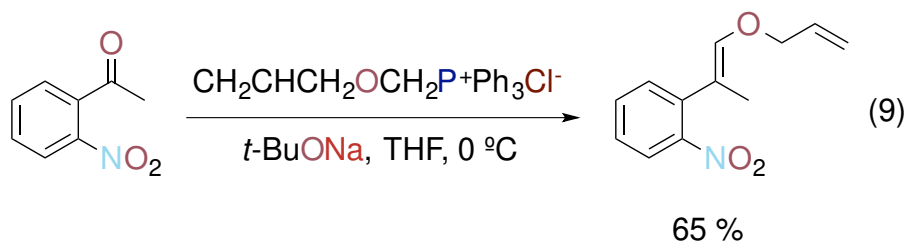
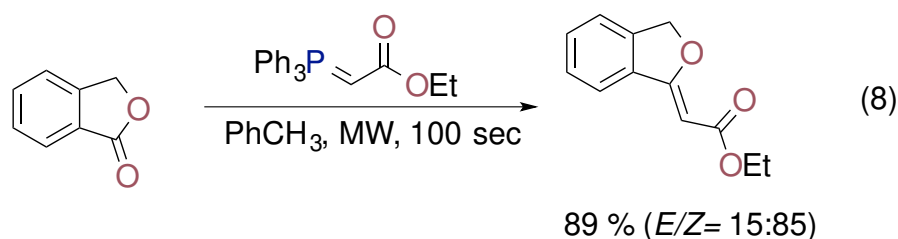
Ethers containing α or β leaving groups, such as halogens,¹⁷ hydroxyl,¹⁸ alkoxide¹⁹ and silyl oxide,²⁰ can carry out the elimination reaction in the presence of a strong base (see Scheme 1.2.1).



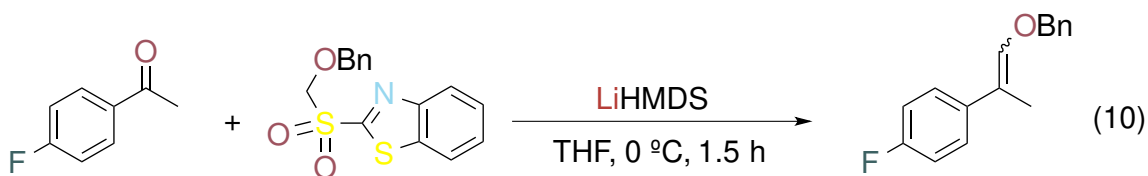
Scheme 1.2.1. Synthesis of vinyl ethers via elimination.

1.2.6. Olefination of carbonyl compounds.

Another way to access to vinyl ether is through carbonyl compounds. A carbon-oxygen double bond can be transformed into a carbon-carbon double bond by using the Wittig reaction or Julia olefination. However, carbonyl compounds such as lactones (Eq. 8)²¹ and ketones (Eq. 9)²² can be converted into vinyl ethers in the presence of phosphoranes.

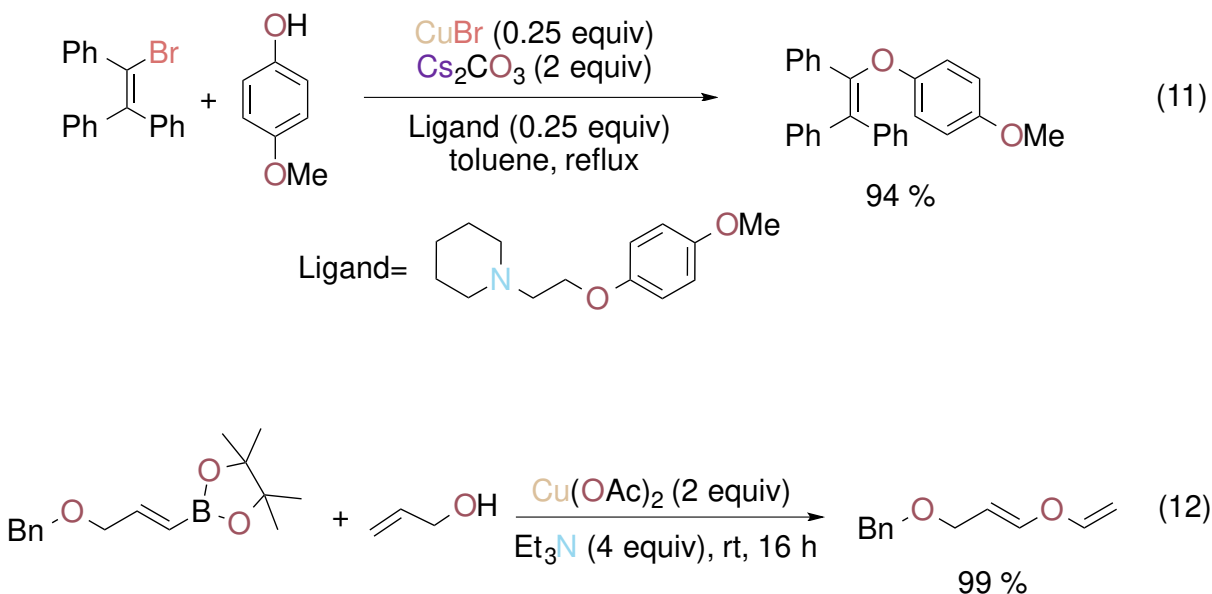


Julia olefination and its variants have become a versatile synthetic tool for the synthesis of vinyl ethers. On the other hand, Berthelette reported an efficient olefination process for aldehydes and ketones by using alkoxy sulfone anions (Eq. 10).²³



1.2.7. Addition of alcohols.

Synthesis of vinyl ethers can be achieved by a metal-mediated addition of alcohols to alkyne species. McDonald *et al.* reported the most successful, tungsten-assisted, cyclization of alkynols to obtain cyclic vinyl ethers.²⁴ Nevertheless, 1,3-dicarbonyl compounds tend to suffer keto-enol tautomerization, and enol species can be *O*-alkylated in acidic conditions to generate the desired vinyl ether product.²⁵ On the other hand, a metal-catalyzed carbon-oxygen coupling is another alternative way to synthesize alkoxyalkene species. The most remarkable results have been obtained with copper (I) (Eq. 11) and copper (II) catalysts (Eq. 12).^{26,27}



1.3. Stable carbenes and their applications.

Divalent and neutral carbon species have been pursued since 18th century due to its high reactivity. However, the research of carbenes began in 1945 with the unsuccessful Dumas' attempts to dehydrate methanol to generate free methylene and water.²⁸ One century later, in 1988, Bertrand accomplished the isolation of the first stable carbene²⁹ and, three years later, the first crystalline stable carbene was reported by Arduengo (see Figure 1.3.1).³⁰ A typical stable carbene contains at least one heteroatom covalently bonded to it that is capable of stabilizing by σ -donation to keep the neutral character.

Based on the stabilization provided by the substituents attached to the carbene, they can be classified as *push-push*, *push-pull*, and *pull-pull*. Groups bearing heteroatoms such as oxygen, nitrogen, or phosphorus are σ -donors that provide a strong electron density donation to the carbene. This behaviour is commonly named *push effect*, however, the opposite effect called *pull* is predominant and characteristic of π -acceptors groups such as SiR_3 , ^+PR , and halogenated carbons, among others.³¹

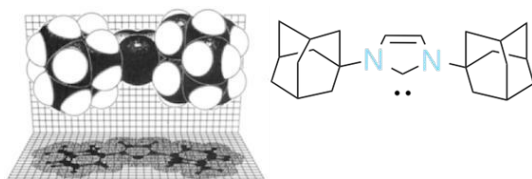


Figure 1.3.1. X-Ray structure of the crystalline stable carbene isolated by Arduengo.³⁰

1.3.1. *Push-push* carbene species.

Cyclic diaminocarbenes or *N*-heterocyclic carbenes (NHCs) are the classic *push-push* type-carbene species (see Figure 1.3.2).³² Among these, NHCs are the most studied stable carbenes due to their applications as ligands³³ and organocatalysts³⁴. Other carbenic species that belong to this category are acyclic diaminocarbenes (ADCs),³⁴ *N,N'*-diamidocarbenes (DAC),³⁵ monoaminoamidocarbenes (MAACs),³⁶ diphosphinocarbene (PPC),³⁸ aminophosphinocarbene (APC)³⁹, cyclopropenylidene (CP),³⁹ aminooxycarbene (AOC),⁴⁰ aminothiocarbene (ATC),⁴⁰ and alkylaminocarbenes (AACs).⁴¹

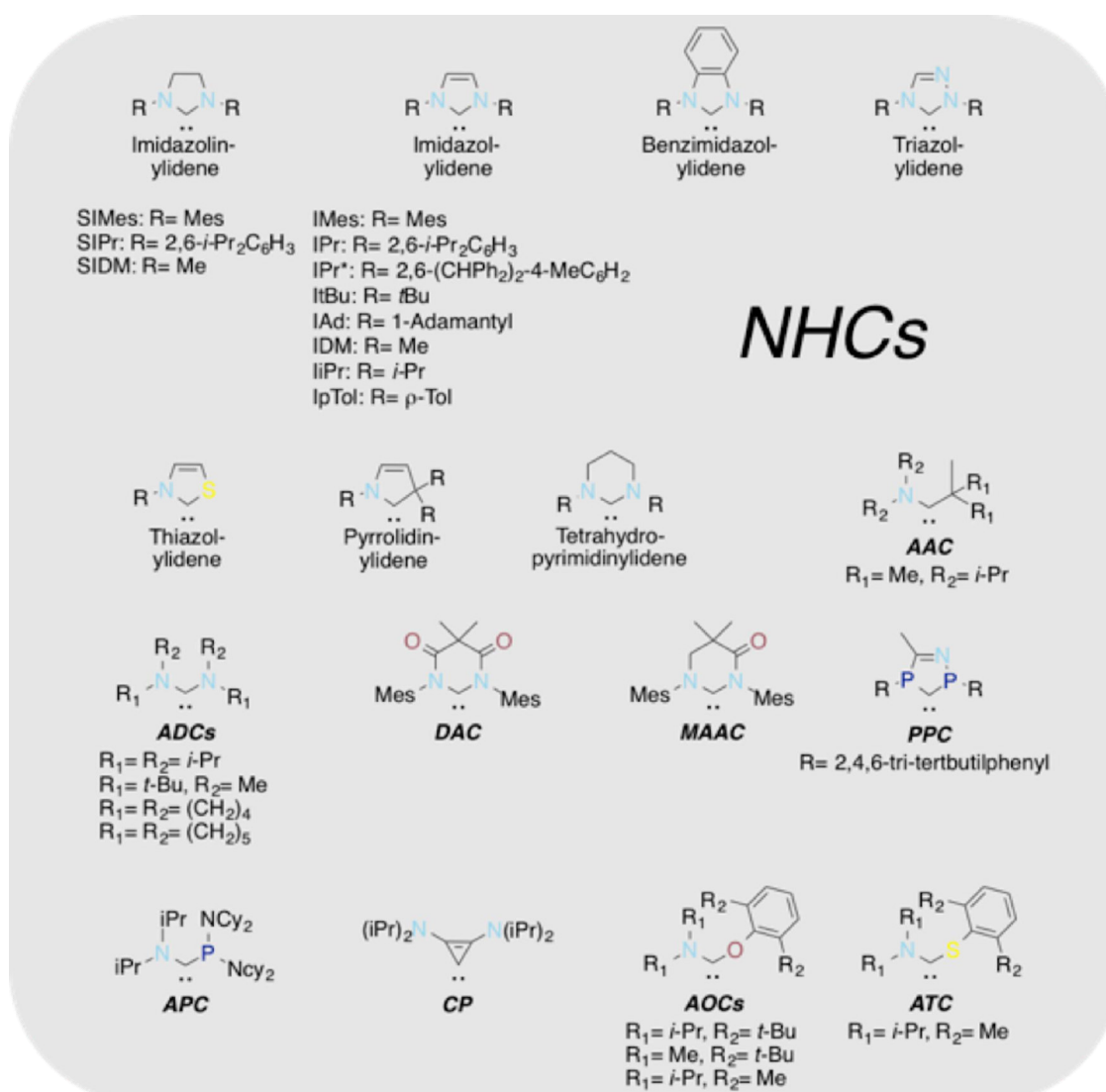


Figure 1.3.2. The most common *push-push* carbenes.

1.3.2. *Push-pull* carbene species.

On the other hand, species such as phosphinosilyl carbene (*PSC*),⁴² aminophosphonio- (*APC*⁺),⁴³ and phosphinophosphoniocarbenes (*PPC*⁺)⁴⁴ are considered as *push-pull* type. In these species, the carbene is stabilized by the σ -donation and π -accepting character of the substituents (see Figure 1.3.3).

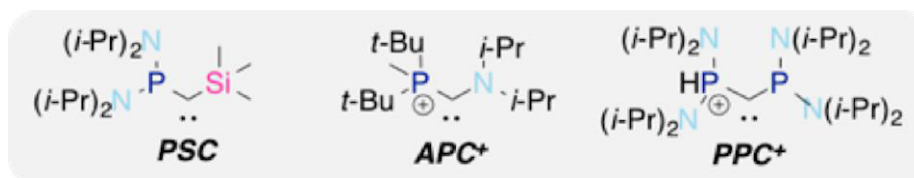


Figure 1.3.3. Synthesized *push-pull* species: phosphinosilyl carbene (*PSC*), aminophosphonio (*APC*⁺), and phosphinophosphoniocarbenes (*PPC*⁺).

1.3.3. *Pull-pull* carbene species.

The third stable carbene category is represented by borylmethyleneboranes (see Figure 1.3.4). Berndt and co-workers achieved the synthesis of boriranylideneboranes³¹ which are analogous to diborylcarbenes.

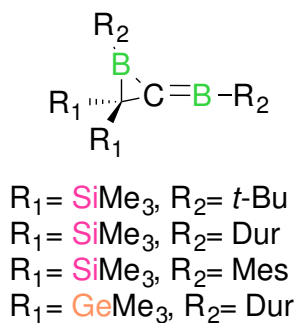


Figure 1.3.4. Synthesized boriranylideneboranes.

NHC-metal catalysts can assist transformations such as: hydrosilylation of ketones,⁴⁵ hydrogen transfer reduction of unsaturated bonds,^{46–48} cross-coupling,^{49–51} olefin metathesis,^{52,53} aryl amination of aryl halides, α -arylation of amides, ethylene/carbon monoxide copolymerization, olefin cyclopropanation, C-H bond activation, and arylation/alkenylation of aldehydes,⁵⁴ among others. On the other hand, CAAC type ligands have become the strongest rivals of NHCs due to their high versatility when are attached to transition metals. Also, some CAACs species display the lowest band-gap compared to *N*-heterocyclic carbenes which turn them out the best alternative to NHCs.

Therefore, CAAC-metal catalysts can assist a wide variety of processes such as, for instance, arylation and hydroamination reactions (see Figure 1.3.5).⁵⁵

Within the last years, stable carbenes have provided substantial improvements in different transformations; a clear example of them is the hydroalkoxylation process. The addition of alcohols to alkyne species has been totally benefited thanks to the use of gold catalysts bearing NHCs species. Gold-NHC catalysts combine the back-donation^{56,57} and the relativistic effects⁵⁷ to generate electrophilic π -complexes in the presence of alkynes. These studies will be discussed in the following subtopics.

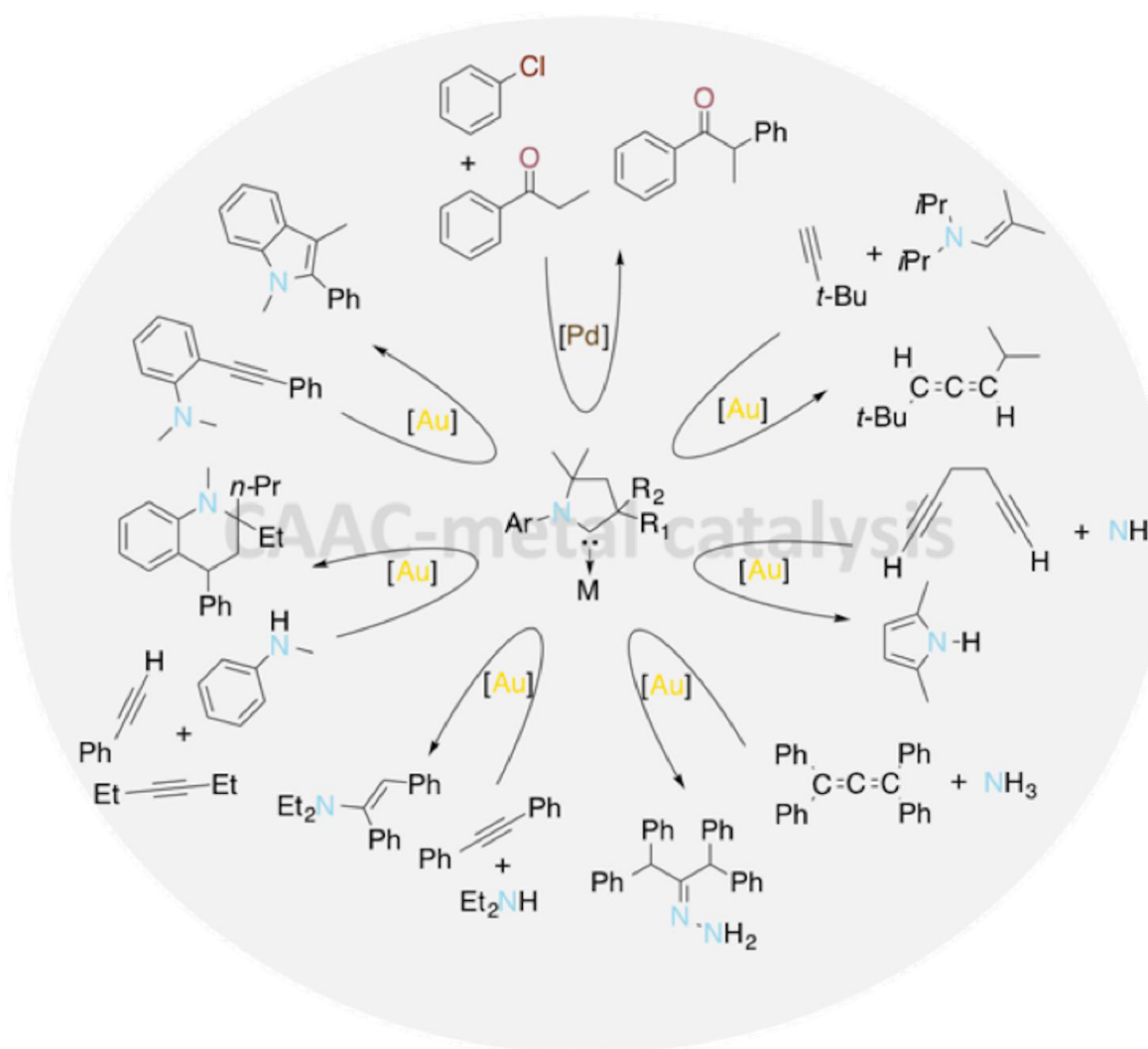
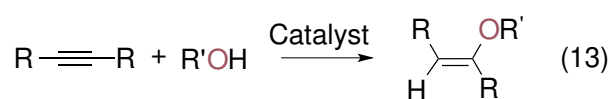


Figure 1.3.5. Transformations assisted by CAAC-metal catalysts.⁵⁵

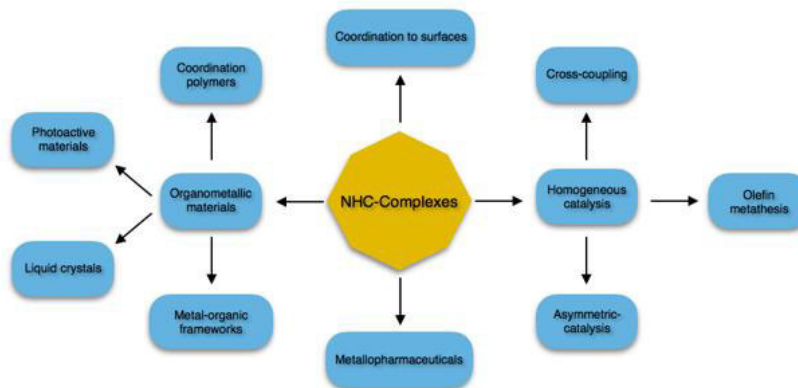
1.4. Hydroalkoxylation.

The hydroalkoxylation (Eq. 13) of alkynes is a synthetic tool by which vinyl ethers can be obtained. These vinyl compounds have significant importance into the chemical industry due to their applications as building blocks of polymers that are then used in the production of adhesives, paints, plasticizers, thickeners, and inks.⁸ Usually, this reaction needs to be catalyzed by using molybdenum⁵⁸, tungsten^{59,60}, ruthenium^{61,62}, and palladium^{63,64}. On the other hand, platinum^{65,66}, gold⁶⁷⁻⁶⁹, silver^{70,71}, iridium⁷²⁻⁷⁵, and rhodium-based⁷⁵ catalysts have been able to catalyze the alkoxylation reaction.



Nowadays, gold catalysts that bear *N*-heterocyclic carbene (NHC) ligands have been studied due to their high catalytic activity in the alkyne hydroalkoxylation field. Moreover, the well-studied Arduengo's carbene ligands have shown the ability to tune the electronic and steric properties that are attractive to the development of new NHC-transition-metal complexes with catalytic activity and even with pharmaceutical applications (see Scheme 1.4.1).^{76,77}

In the presence of alkyne compounds, gold catalysts containing NHC ligands can form π -complexes with electrophilic character to be able to carry out a nucleophilic attack by nucleophiles such as alcohols or amines to obtain vinyl ethers or amines, respectively.⁷⁸ Additionally, current reports have revealed that the steric demand from NHC-ligand and the solvent effect play a significant role in gold-mediated catalysis. For instance, Nolan *et al.* have reported the lower efficiency of large NHC-gold complexes in the intramolecular hydroalkoxylation of propargylic alcohol.⁷⁹



Scheme 1.4.1. Applications of NHC-Metal complexes.⁷⁷

Furthermore, these factors discussed above are not the only ones that can affect the catalysis. The counterion has been described as an important species in the catalysis. The best-known example of a counterion assistance was reported by Zuccaccia *et al.* (see Figure 1.4.1). In their extensive work, the counterion may help to achieve the nucleophilic attack due to their coordinating ability, basicity, and the morphology of the anion. Species with lower basicity, higher coordinating ability, and spherical form tend to decrease the catalytic activity. In summary, the most successful counterions that can achieve the nucleophile activation in an efficient way are: NTf_2^- , OTf^- , OTs^- , and OMs^- .⁸⁰

On the other hand, numerous research groups have focused their efforts in the intermolecular hydrophenoxylation of internal alkynes, since this transformation turns out to be entropically unfavorable. Efforts to improve its efficiency have provided major advances in the field. For instance, one of the most important reports was made by Kuram *et al.* They reported the hydrophenoxylation of symmetrical and unsymmetrical alkynes assisted by a gold catalyst in the presence of a mild or strong base (see Table 1.4.1).⁸²

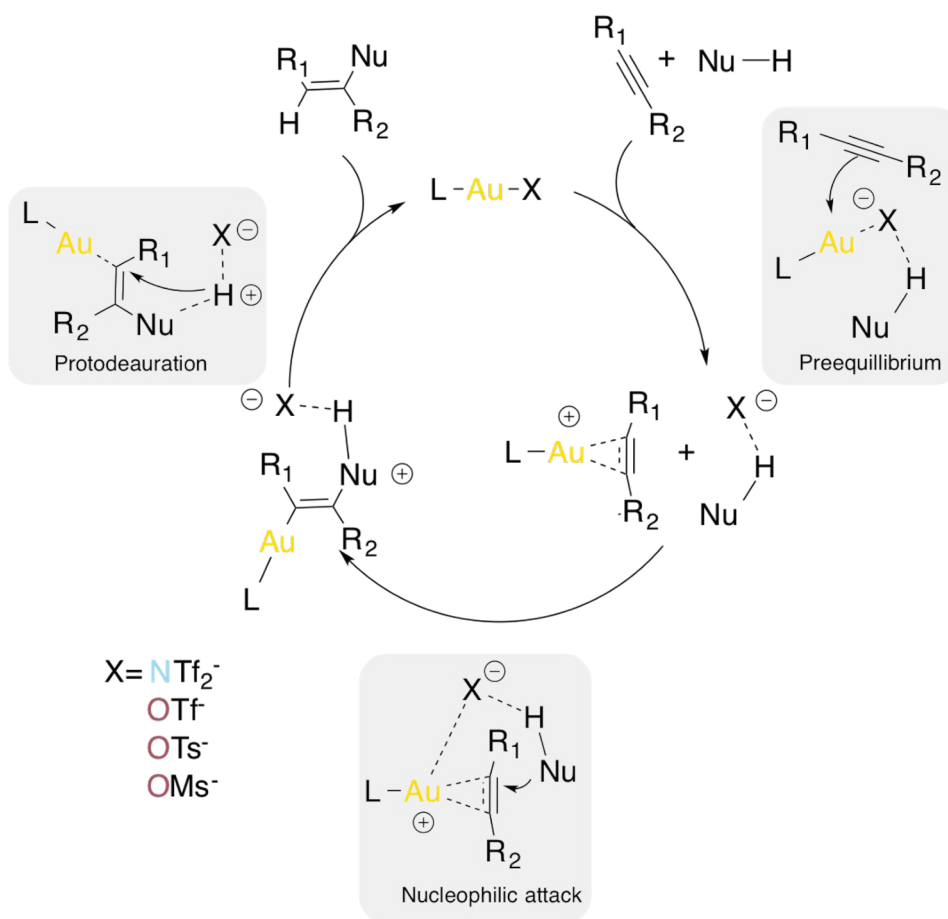
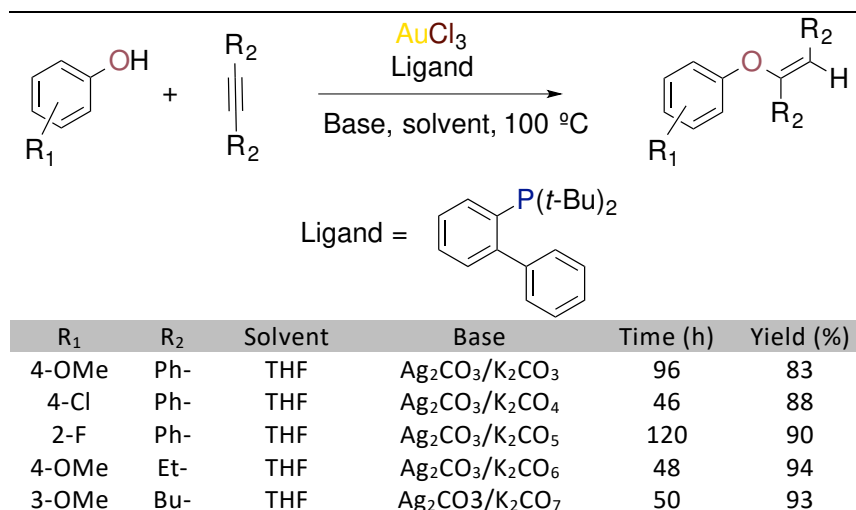


Figure 1.4.1. Proposed catalytic cycle for gold.⁸¹

Likewise, the use of gold catalysts containing sterically rich ligands has become a good methodology to achieve the addition of alcohols to unsaturated bonds. However, the steric hindrance of these ligands can affect the rate-determining step (rds).⁷⁹ While the rds increases by adding large ligands, the reaction rate is improved by the counter ion⁸¹ or the polar or protic species.⁸³ In 2010, Ujaque and co-workers reported the mechanism for addition of phenols to alkene compounds catalyzed by phosphine-gold catalysts. In their computational mechanistic studies, they proposed a process assisted by phenol and water.⁸³

Table 1.4.1. Hydrophenoxylation of symmetrical alkenes catalyzed by AuCl₃.



Mechanistically, they proposed the formation of the π -complex followed by the concerted addition and proton transfer from phenol to alkene moiety. Four possible cases were investigated for the rds (see Figure 1.4.3): 1) direct proton transfer, 2) proton transfer assisted by the counter ion, 3) proton transfer assisted by phenol and 4) proton transfer assisted by water. Thus, their results indicate that the pathway promoted by phenol and water proceeds through a concerted process. On the other hand, the direct and anion-assisted processes are unfeasible due to their higher energy barriers of 61.1 and 49.6 kcal/mol, respectively.⁸³

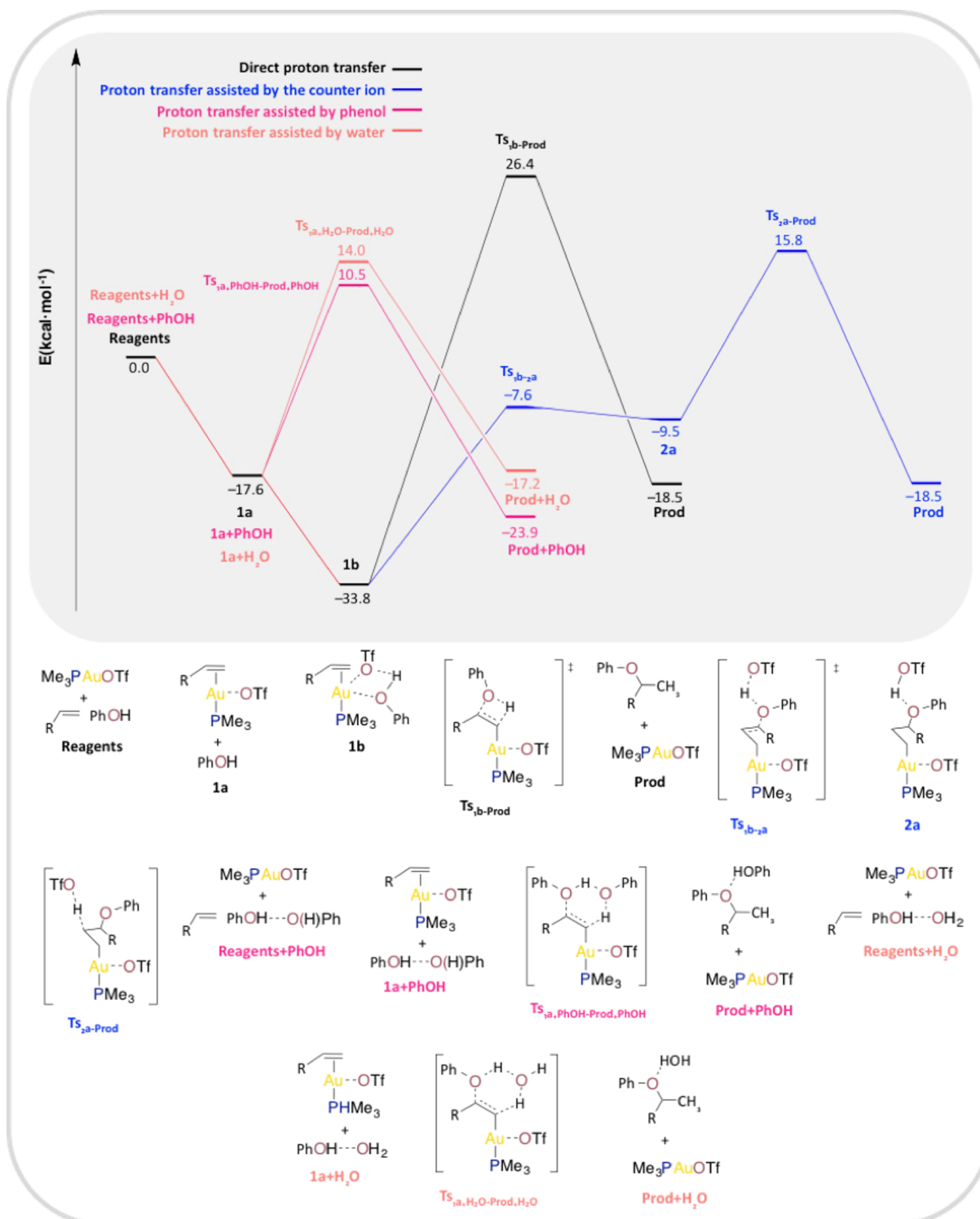
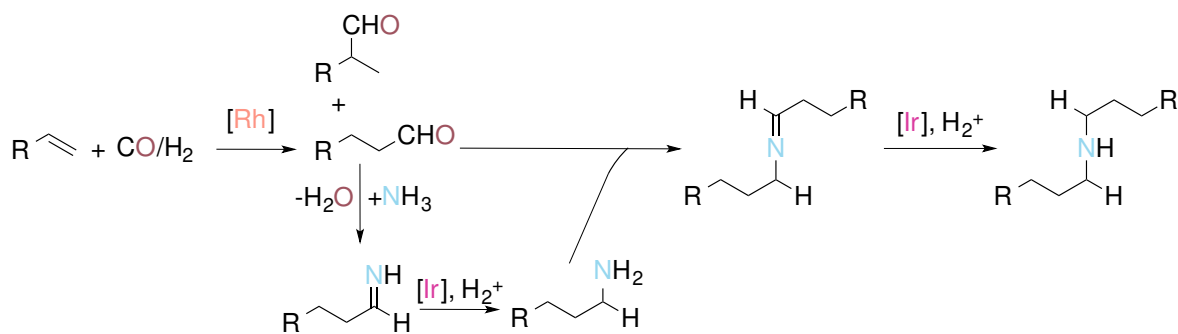


Figure 1.4.2. Possible pathways reported by Ujaque and co-workers for the addition of phenol to alkene species catalyzed by Me_3PAuOTf .⁸³

1.5. Dual catalysis: an efficient and versatile synthetic tool.

Dual catalysis has been expanding the catalysis field since the last century in processes such as hydroaminomethylation of olefins to obtain amines. This reaction was first performed for the synthesis of gas and ammonia in presence of [Rh/Ir] catalyst under formylation conditions in organic/aqueous phases (see Scheme 1.5.1). In addition, when exploring the solvent effect, Methyl tert-butyl ether (MTBE) was found as the best organic solvent to obtain selectively primary amines.⁸⁴ Another catalytic strategy that involves the synthesis of gas is the generation of green fuels such as methanol through the assistance of [Cu/ZnO] and 2-propanol under low temperature conditions.⁸⁵



Scheme 1.5.1. Generation of the primary and secondary amines in the hydroaminomethylation of olefins assisted by a dual rhodium-iridium catalytic system.⁸⁴

Another process influenced by the dual catalysis is the C-C cross-coupling. In 2010, Bera *et al.* published the Suzuki and Heck cross-coupling catalyzed by dipalladium(I) catalyst.⁸⁶ Two years later, Schönebeck and co-workers reported the catalytic activity of dipalladium(I) complexes bridged by halide ligands. In their report, the C-C cross-coupling catalyzed by palladium(I) dimer was described as a homo-dual assisted process.^{87,88} However, C-C cross-coupling can be achieved even by using hetero-dual-metal catalysis. A clear example of this is the cross-coupling assisted by [Pd(dmpe) or (PMe₃)₂] and vinyl-gold species (see Figure 1.5.1).⁸⁹

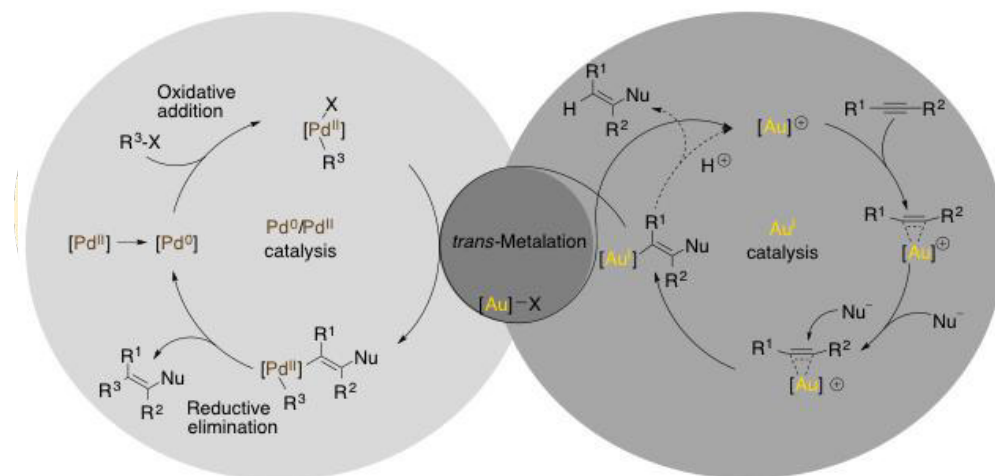


Figure 1.5.1. C-C cross-coupling assisted by palladium and gold catalyst.⁸⁹

In the area of polymers, dual-catalytic systems have provided interesting results. One of the published reports is on the ring-opening polymerization of ω -pentadecanone catalyzed by 4-Dimethylaminopyridine (*DMAP*) Brønsted base and magnesium halides (see Figure 1.5.2).⁹⁰ Another achievement in the field has been the polymerization of methacrylate catalyzed by the $[\text{Et}_3\text{SiH}]/[\text{Et}_3\text{Si(L)}]^+[\text{B}(\text{C}_6\text{F}_5)_4]^-$ couple, which was described as a good methodology to produce linear polymethacrilates.⁹¹

Some fields in chemistry have been impacted in a quite positive way by the dual-assisted process such as the asymmetric synthesis. In 2004, Jacobsen *et al.* achieved the addition of hydrogen cyanide to unsaturated imides assisted by aluminium and lanthanide chiral complexes. In this study, the enantioselectivity was improved by the lanthanide species.⁹² Three years later, the field of dual-assisted catalysis was broadened with the enantioselective alkylation of α -amino esters catalyzed by a chiral Brønsted acid and silver acetate.⁹³ More interesting works were added to this field, such as the enantioselective [2+2] photocycloaddition between two unsaturated ketones. The cycloaddition reaction was promoted with visible light in presence of a ruthenium catalyst and a chiral Lewis acid (see Figure 1.5.3).⁹⁴

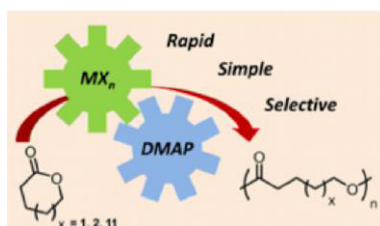


Figure 1.5.2. Ring-opening polymerization of lactones.⁹⁰

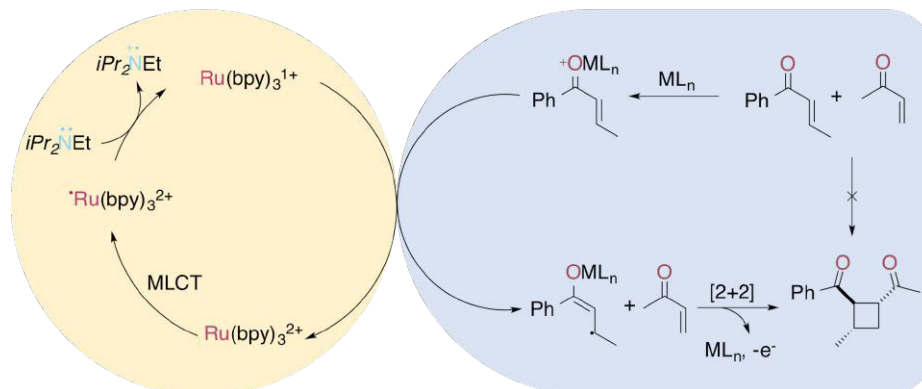


Figure 1.5.3. Enantioselective [2+2] cycloaddition.⁹⁴

Thereby, a Brønsted acid in conjunction with a Lewis acid can catalyze enantioselective reactions, but also a Lewis acid in combination with a Schiff base can carry out a large variety of homo-dual- and hetero-dual-assisted processes providing a wide range of asymmetric transformations. For instance, asymmetric reactions such as amination, Mannich, and aziridine opening were achieved by using bimetallic complexes bearing Schiff bases and obtaining products with a higher percentage of enantiomeric excess (see Figure 1.5.4).⁹⁵

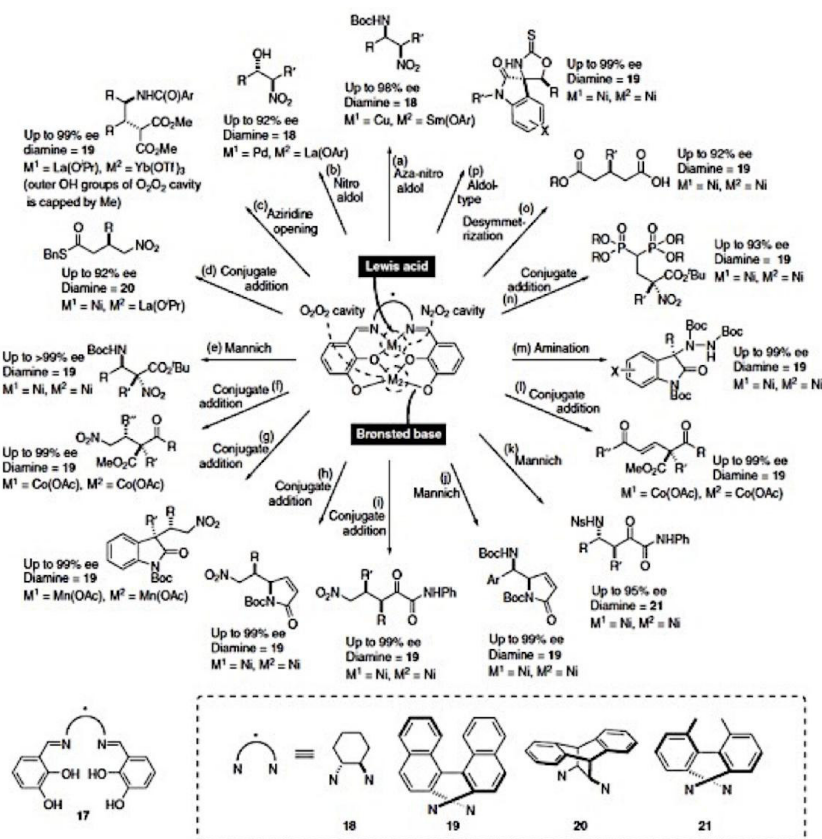


Figure 1.5.4. Asymmetric transformations catalyzed by a Lewis acid/Brønsted base pair.⁹⁵

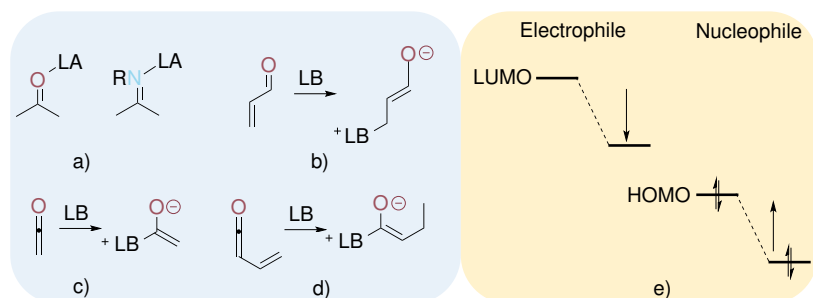


Figure 1.5.5. a) Activation of the electrophile by a Lewis acid; b-d) Activation of the nucleophile by a Lewis base, and e) Frontier orbitals of the activated nucleophile and electrophile.¹⁰²

Catalysis involving a Lewis acid and/or base is able to promote a widely variety of processes where these species interact and activate the substrate via electron donating or electron withdrawing processes (see Figure 1.5.5). Some of them are the enantioselective reduction of ketones catalyzed by borane/oxazaborolidines,⁹⁶ alkylation of aldehydes⁹⁷ and ketones⁹⁸ assisted by Zn-salen catalyst, enantioselective allylation of aldehydes directed silver-(*R*)-BINAP complex,⁹⁹ and even diastereoselective condensation reactions such as aldol¹⁰⁰ and Mannich.¹⁰¹

On the other hand, cooperative catalysis has also been applied to carry out processes such as the asymmetric hydrogenation of ketones, where the ligand and the metal assist the reaction synergistically. The most known catalysts reported are Ru-(phosphine)₂-amine¹⁰³ and Fe-amine(imine)diphosphine.^{104,105} This kind of catalysts are able to achieve the hydrogen transfer through a metal-nitrogen dual-assisted process (see Figure 1.5.6).

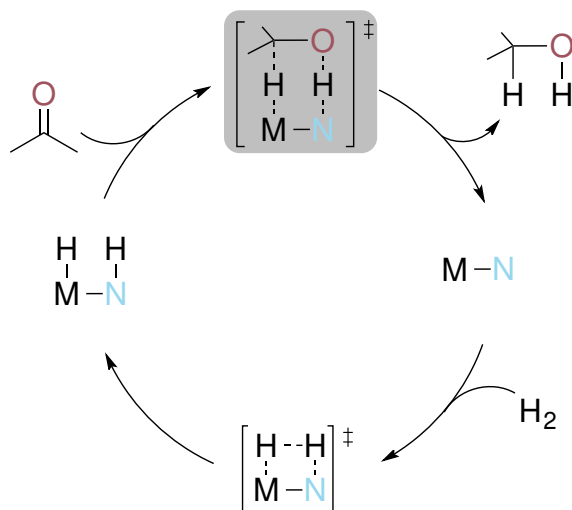
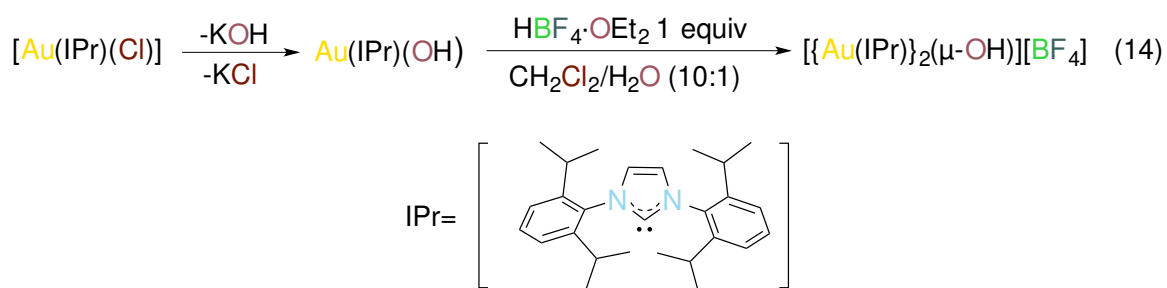


Figure 1.5.6. Metal-nitrogen activation in asymmetric hydrogenation of non-symmetric ketones.¹⁰⁵

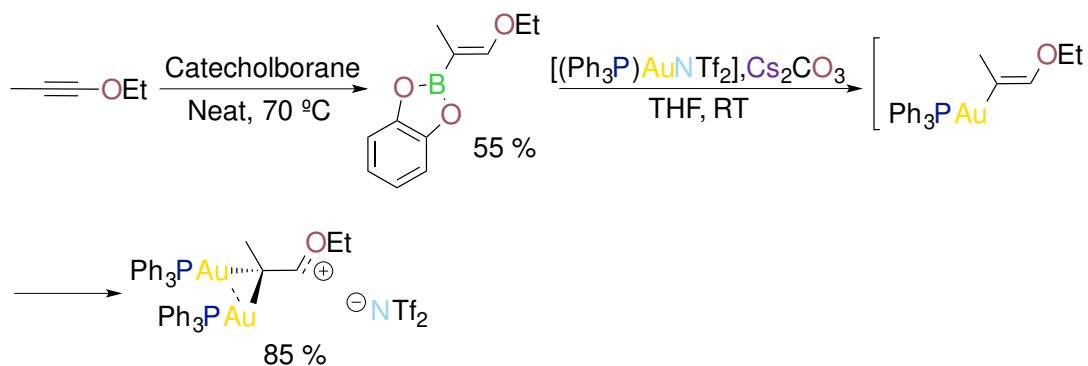
Moreover, dual-cooperative catalysis has been explored in the field of biomimetic chemistry. On this field, an enzyme in conjunction with a metal are capable to carry out a wide variety of synergistic processes such as regeneration of nicotinamide,¹⁰⁷ bio-transformations like enantioselective hydrolysis of esters,¹⁰⁸ acylations,¹⁰⁹ asymmetric polymerizations,¹¹⁰ epoxidations of fatty acids,¹¹¹ and conversions of *N*-acetyl amino acrylates to amino acids.¹¹²

1.6. Dual-assisted hydroalkoxylation process.

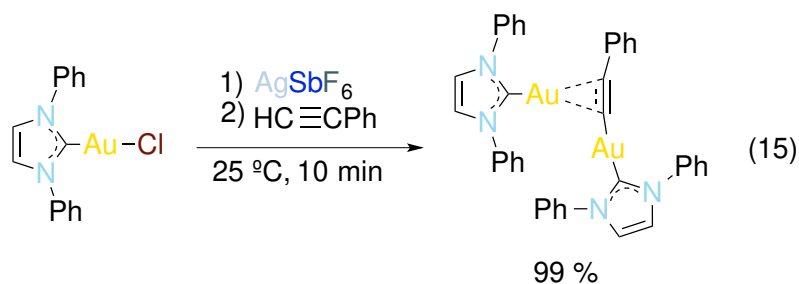
During the last years, dual or cooperative catalysis has been described as a powerful tool that improves selectivity and reactivity in organic reactions.¹¹³⁻¹¹⁵ In 2008, Toste *et al.* published the dual-gold-catalyzed cycloisomerization of 1,5-allenynes.¹¹⁶ In 2010, inspired by these results, Nolan and co-workers succeeded with the synthesis of *gem*-digold $[\{\text{Au}(\text{PPh}_3)\}_2(\mu\text{-OH})]^+[\text{BF}_4]^-$ complex that provided a new overview for gold catalysis (Eq. 14).¹¹⁷ In the same year, Fürstner and co-workers reported the synthesis of an air-stable *gem*-diaurated complex (Scheme 1.6.1).¹¹⁸



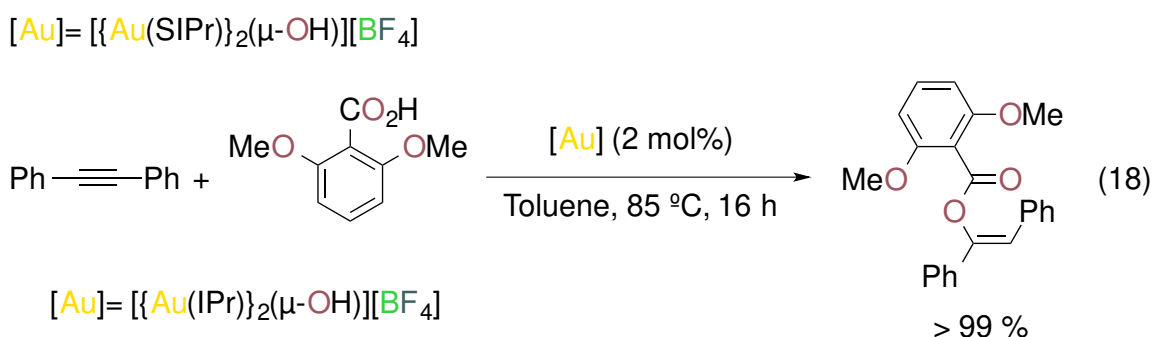
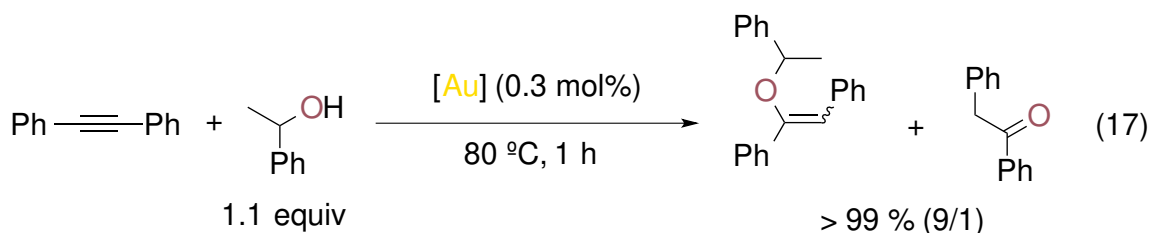
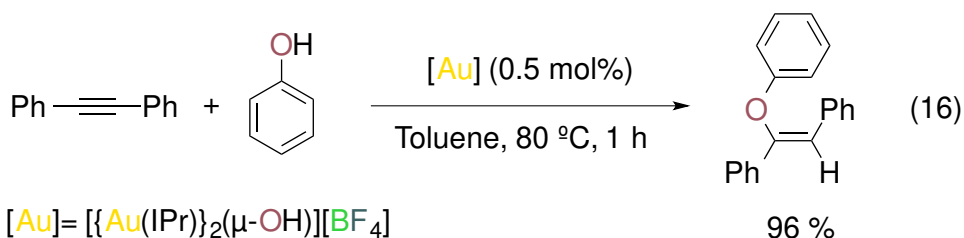
Later, Widenhöfer *et al.* achieved the σ,π -alkyne activation (Eq. 15).¹¹⁹ Di-gold σ,π -acetylide complexes in the absence of a base were synthesized. Due to their easy access and interesting properties, they are considered as intermediates in digold catalysis involving terminal alkynes.



Scheme 1.6.1. Synthetic pathway of the air-stable *gem*-diaurated complex.¹¹⁸



Later, in 2013, the synthesis of a *gem*-digold compound by Nolan *et al.* allowed the alkyne hydrophenoxylation (Eq. 16), catalyzed by this di-gold hydroxide species under relatively mild conditions.¹²⁰ The passion for vinyl ethers synthesis inspired Nolan's group to achieve the intermolecular hydroalkoxylation¹²¹ (Eq. 17) and hydrocarboxylation¹²² (Eq. 18) of internal alkynes.



Promising progress in dual-gold-assisted catalysis attracted the attention of Roithová and co-workers focussing their efforts in the exploration of the hydroalkoxylation mechanism by Electro Spray Ionization Mass Spectrometry (ESI-MS) and Density Functional Theory (DFT)

calculations. They observed a competitive mono- and di-gold mechanism for hydromethoxylation of 1-phenyl-propyne, due to the success of this methodology. In 2015, they reported a new computational-experimental strategy to analyze the intermediates in gold catalysis (see Figure 1.6.1).^{123,124}

In the same year, another interesting computational mechanistic study about dual-gold catalysis was published by Hashmi *et al.* They discussed the improvement of the rate-determining step via mono- or di-gold catalyst transfer from C-[M]₂ compounds to non-activated terminal alkyne species. Focusing on the proton transfer, they found a higher energy barrier for the single gold catalyst transfer pathway (46.9 kcal/mol), being more favored the dual-assisted process (29.5 kcal/mol) (see Figure 1.6.2).¹²⁵

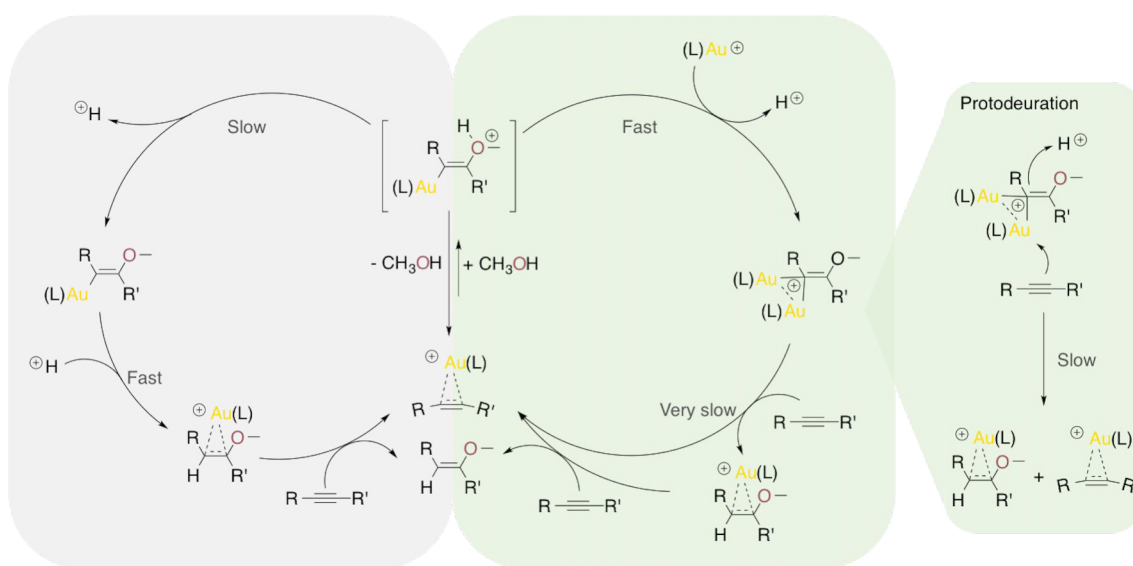


Figure 1.6.1. Reaction mechanism of alkyne hydromethoxylation assisted by mono- or di-aurated species containing hindered ligands.¹²⁴

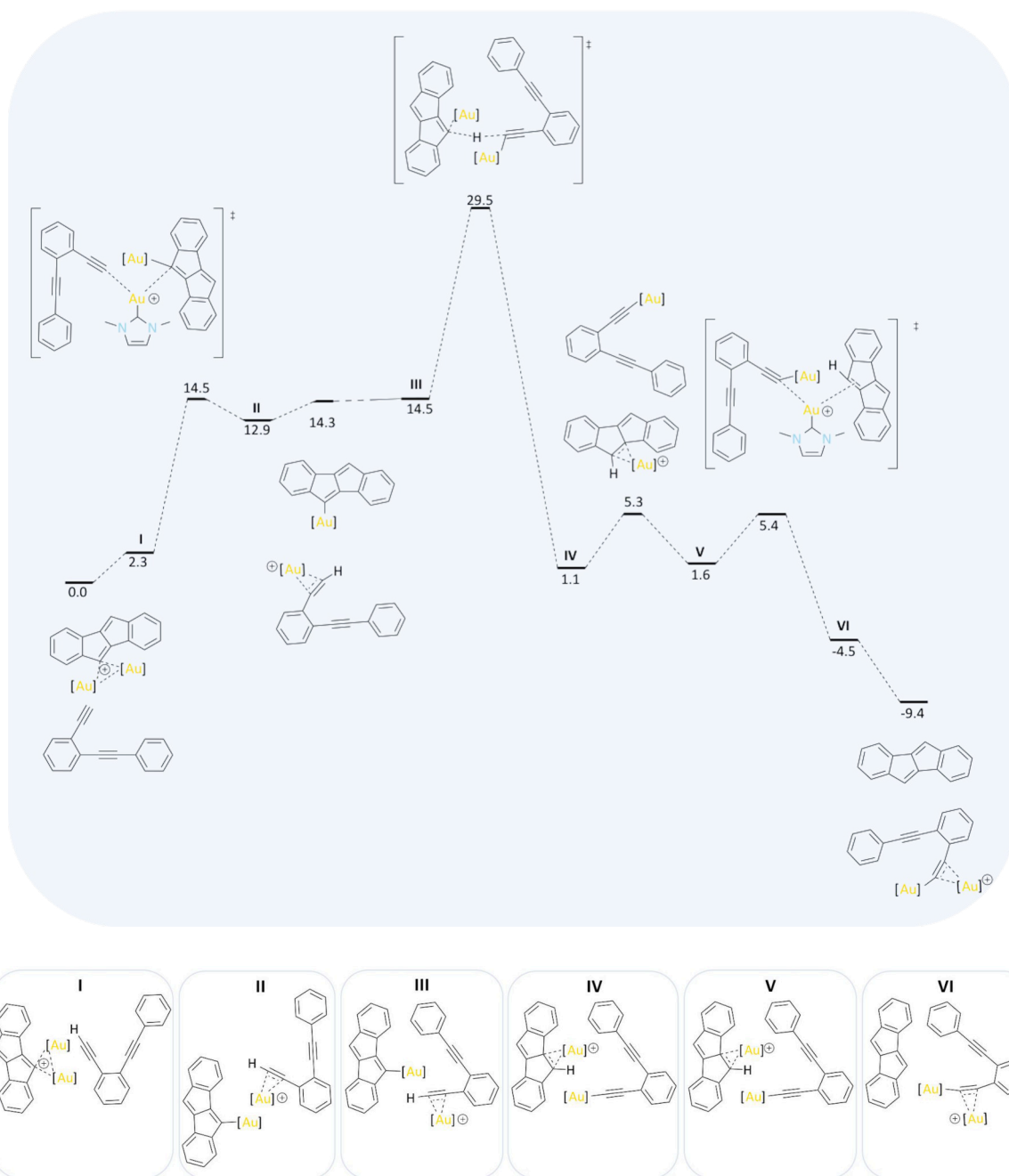


Figure 1.6.2. Energy profile of the dual-catalyzed transfer process (in kcal/mol).¹²⁵

Taking as starting point the equilibrium between the *gem*-digold compound and the alkyne-gold complex, Poater *et al.* proposed a mechanism that involves the active species included in Figure 1.6.3. On the reaction pathway, the reactive species alkyne-[Au] and PhO-[Au] are formed in the initiation part and regenerated during the catalytic cycle. Overall, the process is described as a nucleophilic attack followed by displacement and protonation reactions. Moreover, the nucleophilic attack that involves the C-O bond formation was found to be the rate-determining step.¹²⁶

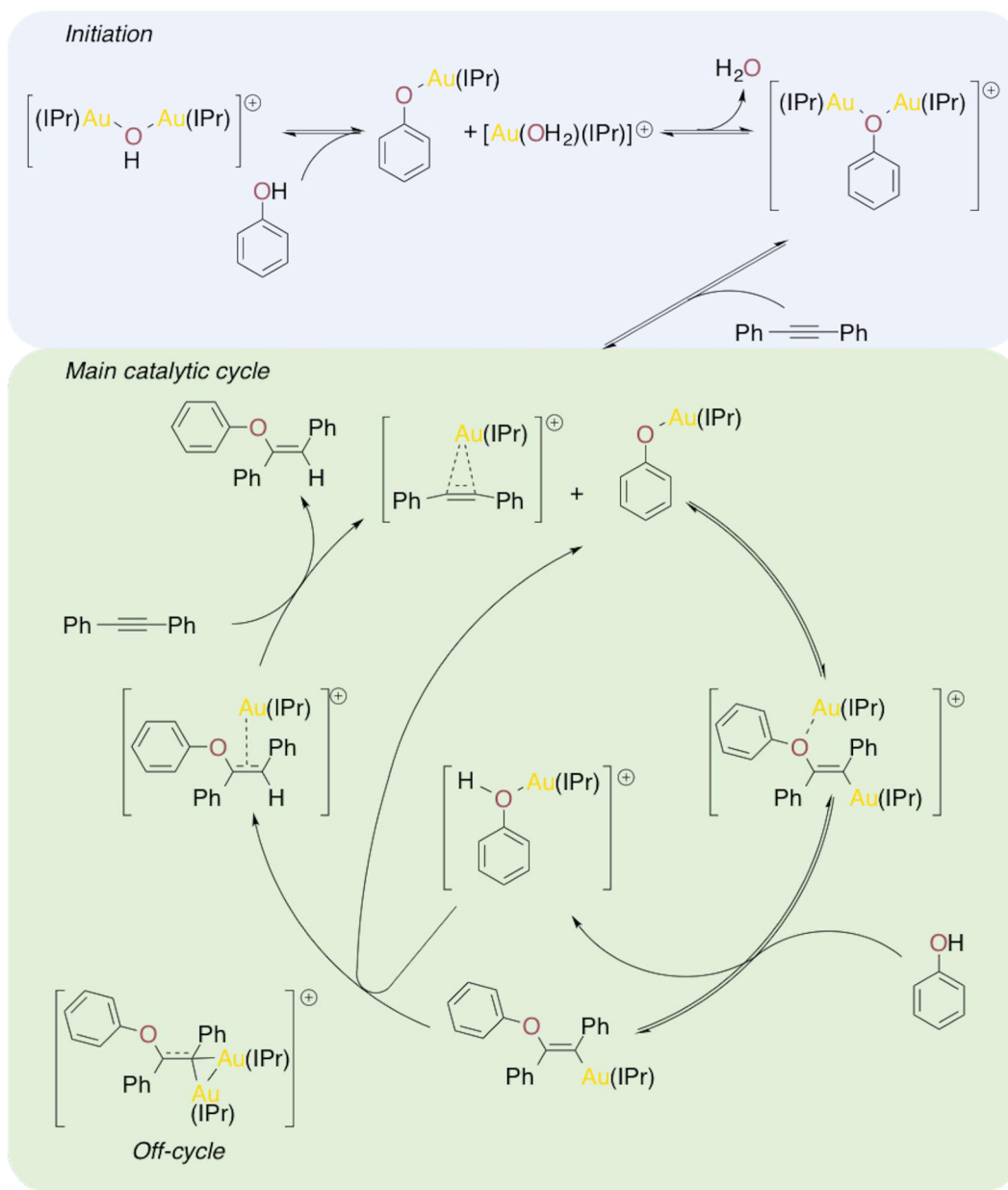
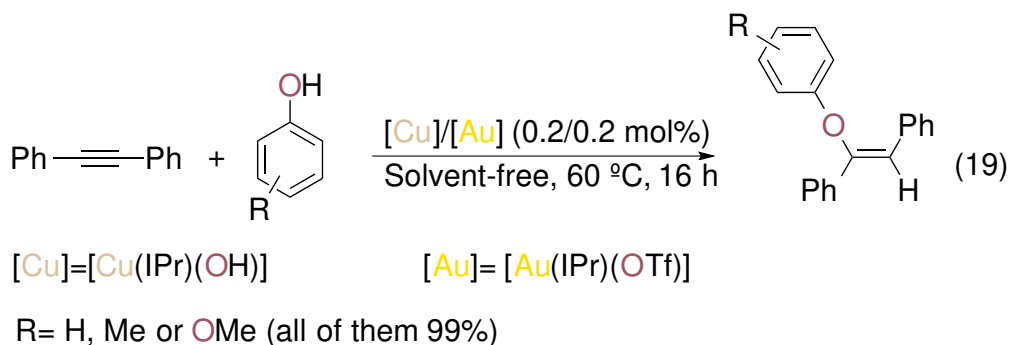


Figure 1.6.3. Reaction mechanism for di-gold-assisted hydrophenoxylation of diphenylacetylene.¹²⁶

Recently, Cazin *et al.* have reported the hydrophenoxylation of diphenylacetylene catalyzed by the Cu(NHC)/Au(NHC) dual system. They performed experimental studies to determine the solvent and temperature effects in the hydrophenoxylation reaction and found a higher conversion to the desired product under free solvent conditions. At the optimal conditions, they tested the addition of substituted phenols to diphenylacetylene observing conversions of up to 90% of the desired vinyl ether (Eq. 19).¹²⁷



Additionally, Cazin and co-workers performed some kinetic studies to elucidate the mechanism by which the reaction proceeds (see Figure 1.6.4). The stoichiometric reactions revealed the generation of the activated species ($[\text{Cu}(\text{IPr})(\text{OPh})]$ and $[\text{Au}(\text{IPr})(\text{PhCCPh})]$) and their importance in the catalytic process.¹²⁷

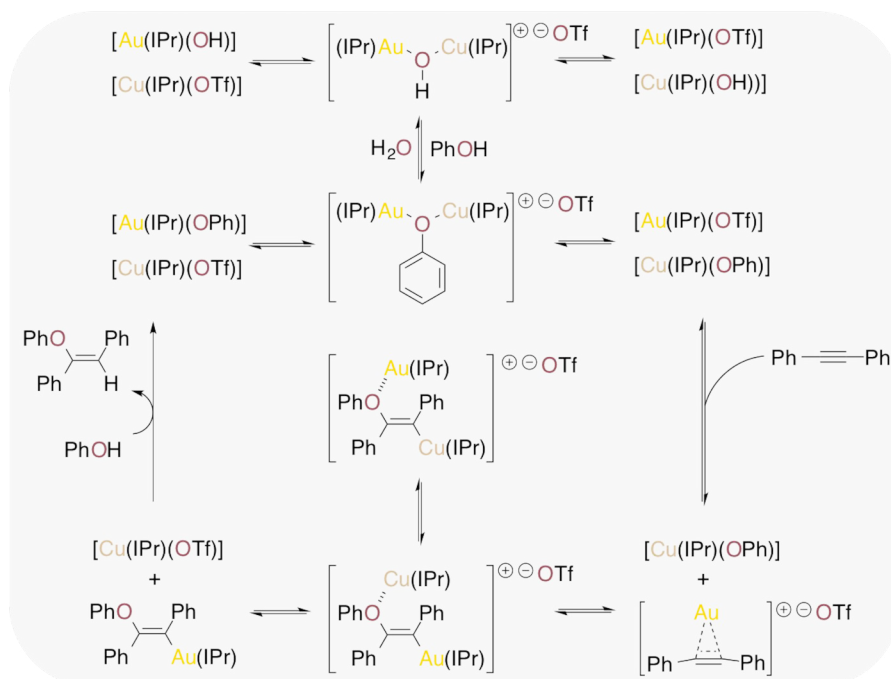
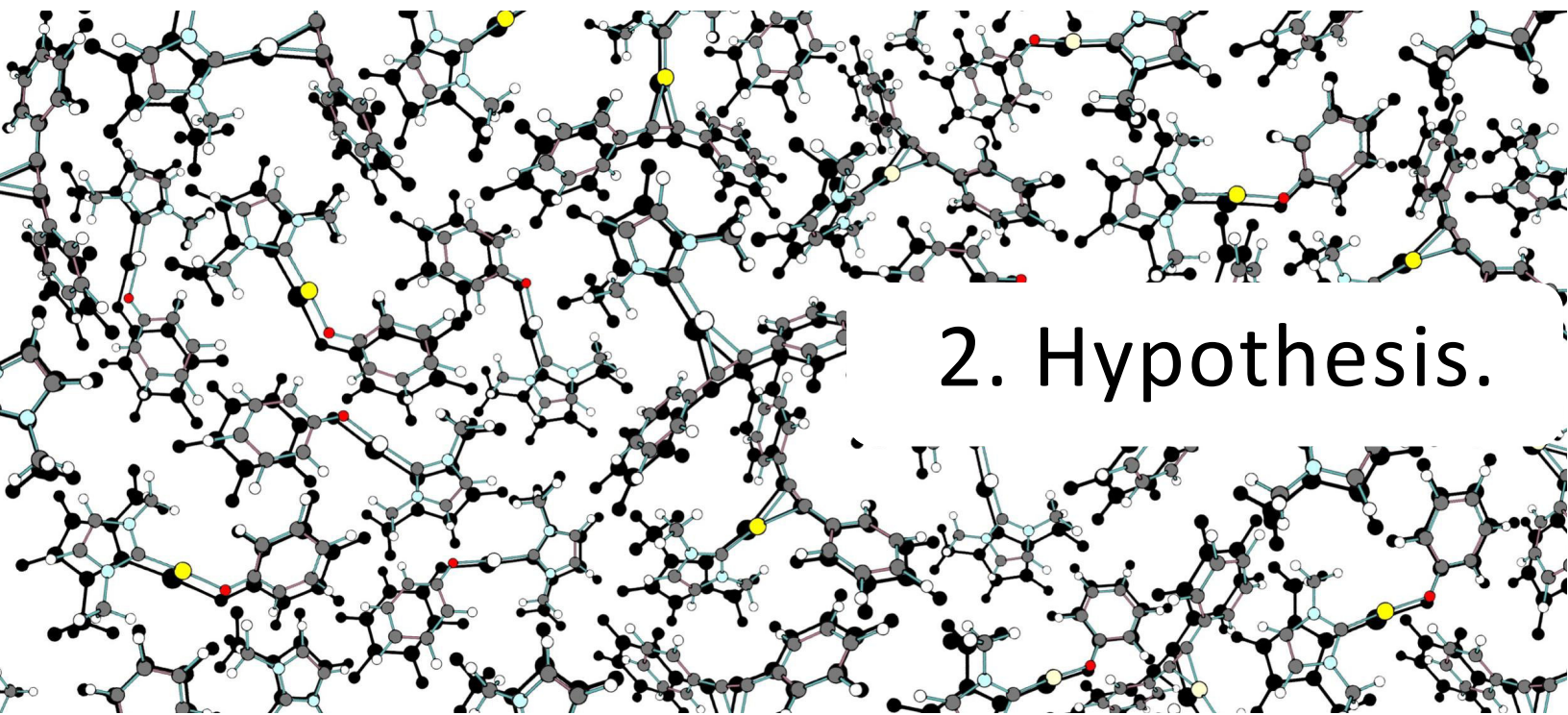
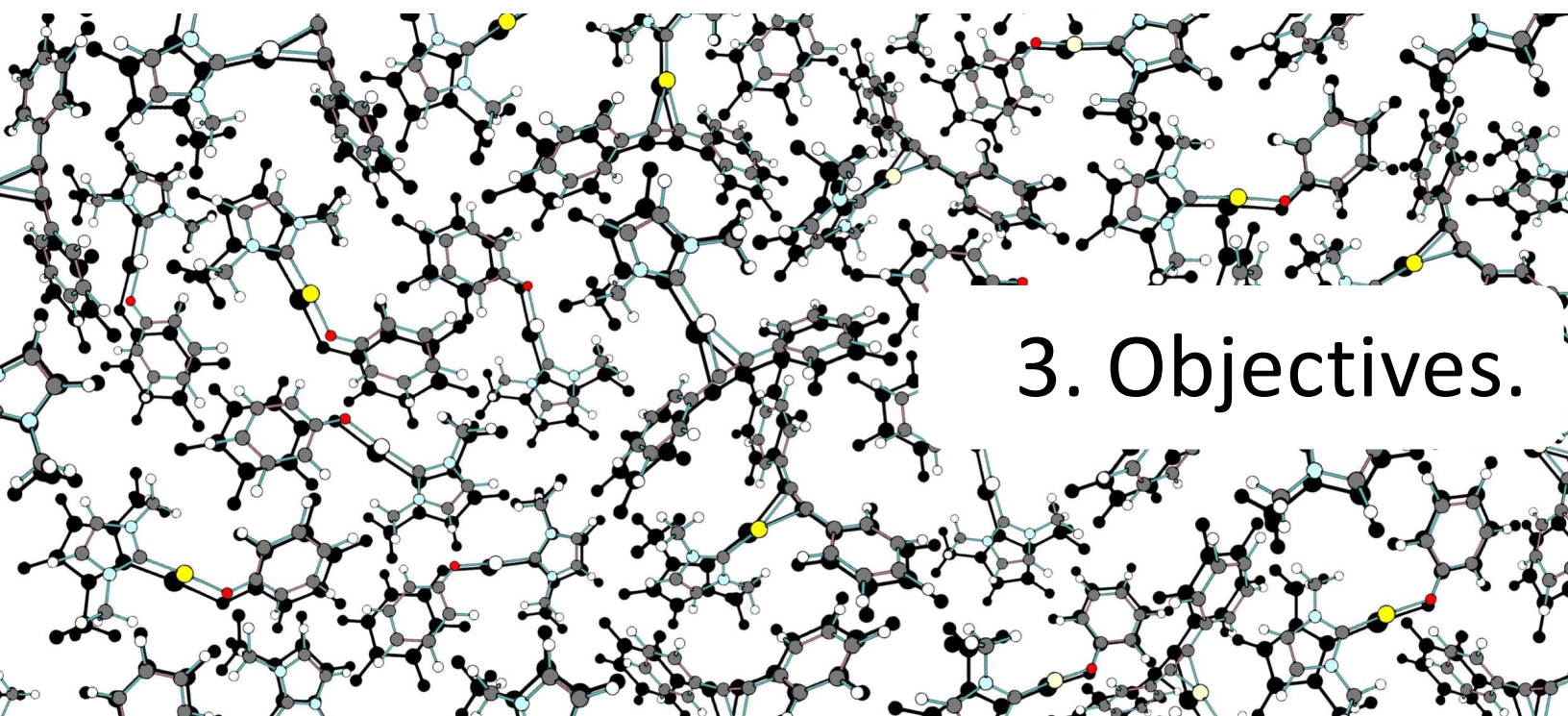


Figure 1.6.4. Mechanism for the hydrophenoxylation of internal alkynes assisted by gold/copper catalysts.¹²⁷



Hypothesis

The experimental results by Cazin and co-workers gave a clear hint that the dual-metal mechanism will be favored with respect to any monometallic one. However, the role of each metal here is unknown. Based on past experiments, it is thought that the copper moiety will bear the phenoxy group whereas the gold will bond to the triple C-C bond of the alkyne and computationally this might be due to the increased nucleophilicity of the phenoxide when not bonded to gold, but copper.



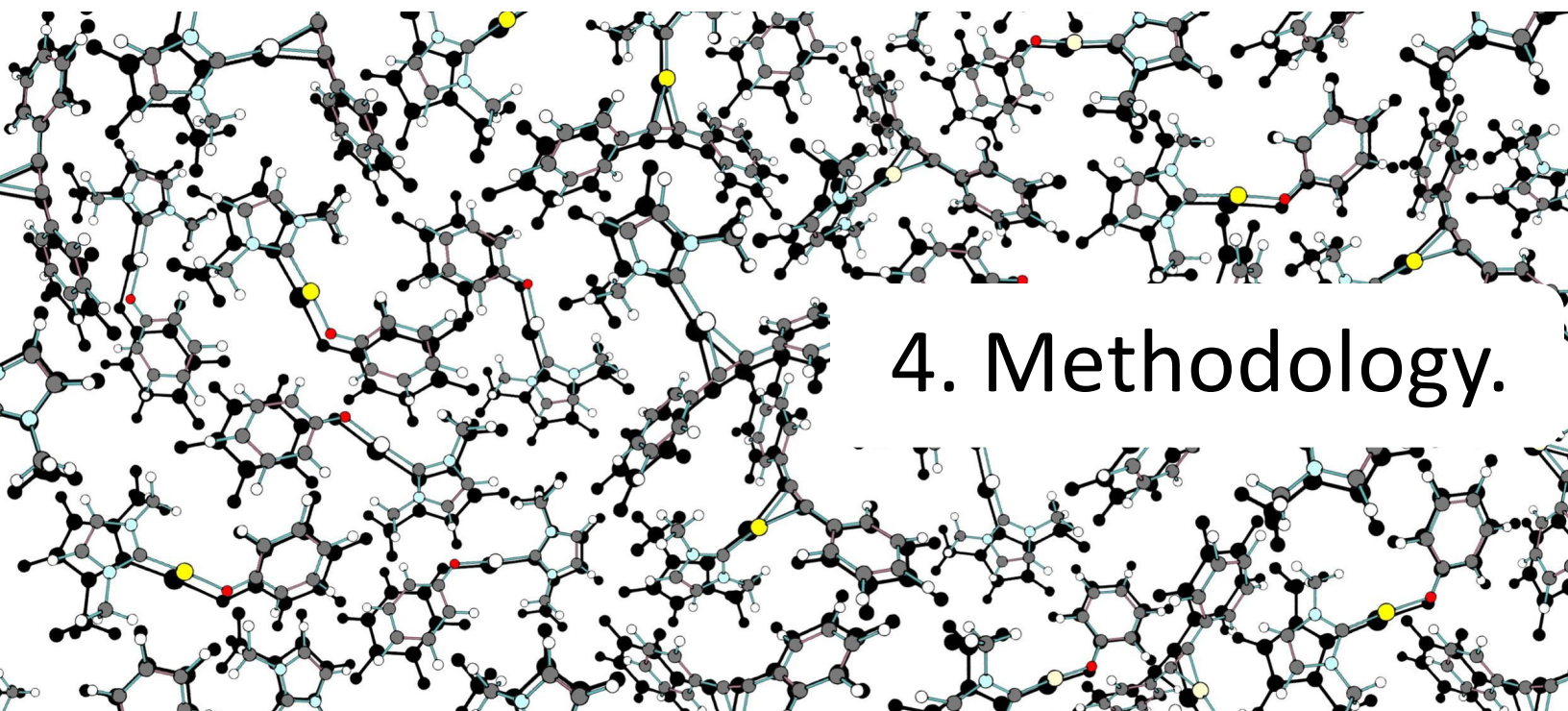
3. Objectives.

Objectives

The general aim of this thesis is to get a kinetically cheaper method for the hydrophenoxylation of alkynes using a novel bimetallic catalytic system, different than the existing ones, by means of exchange the metal (gold by copper) or the ligand bonded to the metal (NHC).

Particular Aims:

- To assess the effect of exchanging gold by copper in $[M(\text{IPr})(\text{OH})]$.
- To investigate the effect of exchanging gold by copper in $[M(\text{IPr})(\text{PhCCPh})]^+$.
- To report the hydrophenoxylation of alkynes via a dual activation process, using a heterobimetallic system consisting of Cu(I)- and Au(I)-NHC (NHC = N-heterocyclic carbene) complexes.
- To see the effect of exchanging the IMe, IMes, SIMes, and IPr* NHC ligands by the real IPr NHC ligand.



4. Methodology.

4.1. Density Functional Theory (DFT).

Nowadays, Density Functional Theory has become a powerful and versatile approach to explore chemical systems. This quantum mechanical method can predict molecular geometries, transition states, harmonic vibrational frequencies, Raman spectroscopy, optical spectroscopy (UV/Vis, CD, MCD), X-ray absorption spectroscopy, EPR and NMR spectroscopy, among others.¹²⁸ The most highlighted DFT industrial applications are the mechanistic study of the ammonia production using ruthenium nanoparticles and the impurity influence in physical properties of metals.¹²⁹

The DFT formalism started with the research of Thomas and Fermi in 1920s. They assumed an uniform distribution of electrons in a six-dimensional phase space, in which electrons can move on a rate of two for each h^3 by the help of an effective potential between the nucleus and electron distribution, so they proposed the energy expression for an atom in terms of electron density (Eq. 20). We must consider that the second term had to be properly modified for molecules.¹³⁰

$$E_{TF}[\rho(\mathbf{r})] = C_F \int \rho^{\frac{5}{3}}(\mathbf{r}) d\mathbf{r} - Z \int \frac{\rho(\mathbf{r})}{r} d\mathbf{r} + \frac{1}{2} \iint \frac{\rho(\mathbf{r}_1)\rho(\mathbf{r}_2)}{|\mathbf{r}_1 - \mathbf{r}_2|} d\mathbf{r}_1 d\mathbf{r}_2 \quad (20)$$

This is the energy functional of the Thomas-Fermi theory of atoms. We assume that in the ground state of an atom, the energy functional (Eq. 20) is minimized by the electron density. This is done through the incorporation of the constraint, given by Eq. (21) and using the method of Lagrange multipliers that leads to the Euler-Lagrange equation (see Eq. 22), where $\phi(\mathbf{r})$ is the electrostatic potential at point \mathbf{r} (Eq. 23).

$$N = N[\rho(\mathbf{r})] = \int \rho(\mathbf{r}) d\mathbf{r} \quad (21)$$

$$\mu_{TF} = \frac{\delta E_{TF}[\rho]}{\delta \rho(\mathbf{r})} = \frac{5}{3} C_F \rho^{\frac{2}{3}}(\mathbf{r}) - \phi(\mathbf{r}) \quad (22)$$

$$\phi(\mathbf{r}) = \frac{Z}{r} - \int \frac{\rho(\mathbf{r}_2)}{|\mathbf{r} - \mathbf{r}_2|} d\mathbf{r}_2 \quad (23)$$

Equations (22) and (23) can be solved together and the resulting electron density is then inserted into Equation (20) to get the total energy of the atom.

However, Thomas-Fermi theory was considered by Hohenberg and Kohn (HK) as an approximation to the Density Functional Theory. In 1964, they proposed the following two theorems:¹³¹

Theorem 1. *The ground state density $\rho(\mathbf{r})$ determines the external potential energy $v(\mathbf{r})$ with a difference as much as a trivial additive constant.*

Theorem 1 was proven by assuming that there were two external potentials v and v' differing by more than a constant, and each of them provides the same $\rho(\mathbf{r})$ for its ground state. Considering last suppositions, we would have the Hamiltonians H and H' , the same ground-state densities and two different normalized wavefunctions Ψ and Ψ' . Using Ψ' as the function for \hat{H} , we obtain Eq. 24 where E_0 and E'_0 are the ground-state energies for H and H' , respectively.

$$E_0 < \langle \Psi' | \hat{H} | \Psi' \rangle = \langle \Psi' | \hat{H}' | \Psi' \rangle + \langle \Psi' | \hat{H} - \hat{H}' | \Psi' \rangle = E'_0 + \int \rho(\mathbf{r}) [v(\mathbf{r}) - v'(\mathbf{r})] d(\mathbf{r}) \quad (24)$$

Now, we consider Ψ as the trial function for the H' case,

$$E'_0 < \langle \Psi | \hat{H}' | \Psi \rangle = \langle \Psi | \hat{H} | \Psi \rangle + \langle \Psi | \hat{H}' - \hat{H} | \Psi \rangle = E_0 + \int \rho(\mathbf{r}) [v'(\mathbf{r}) - v(\mathbf{r})] d(\mathbf{r}) \quad (25)$$

If we combine Eq. 24 and Eq. 25 we obtain that $E_0 + E'_0 < E'_0 + E_0$, which is an argument to absurdity. It has not sense because two different $v(\mathbf{r})$ cannot provide the same $\rho(\mathbf{r})$ for their ground states. In addition, N , $v(\mathbf{r})$ and all properties of the ground-state are determined by $\rho(\mathbf{r})$. Some examples are the kinetic energy, the potential energy and the total energy in Eq. 26, where $F_{HK} = T[\rho] + V_{ee}[\rho]$ and $V_{ee}[\rho] = J[\rho] + \text{nonclassical therm.}$

$$E_v[\rho] = T[\rho] + V_{ne}[\rho] + V_{ee}[\rho] = \int \rho(\mathbf{r}) v(\mathbf{r}) d\mathbf{r} + F_{HK} \quad (26)$$

$$E[\Psi] \geq E_0 \quad (27)$$

Theorem 2. *Energy Variational Principle (Eq. 27): The ground-state density $\rho(\mathbf{r})$ can be determined from the ground-state energy functional $E[\rho]$ by variation of the density.*

To prove Theorem 2, we take Eq. 26 and the trial wave function $\tilde{\Psi}$, hence we obtain Eq. 28.

$$\langle \tilde{\Psi} | \hat{H} | \tilde{\Psi} \rangle = \int \tilde{\rho}(\mathbf{r}) v(\mathbf{r}) d\mathbf{r} + F_{HK}[\tilde{\rho}] = E_v[\tilde{\rho}] \geq E[\rho] \quad (28)$$

When applying the variational principle, the ground state must satisfy the stationary principle (Eq. 29).

$$\delta\{E_v[\rho] - \mu[\int \rho(\mathbf{r}) d\mathbf{r} - N]\} = 0 \quad (29)$$

From Eq. 29, we obtain the Euler-Lagrange expression (Eq. 30),

$$\mu = \frac{\delta E_v[\rho]}{\delta \rho(\mathbf{r})} = v(\mathbf{r}) + \frac{\delta F_{HK}[\rho]}{\delta \rho(\mathbf{r})} \quad (30)$$

If we keep focusing on the chemical potential (Eq. 30), we can realize that $F_{HK}[\rho]$, the exact expression for the ground state, does not depend of $v(\mathbf{r})$; therefore, $F_{HK}[\rho]$ is called the exact and universal functional of $\rho(\mathbf{r})$. Equation 30 can be applied to a wide variety of systems. Under the HK approach, this equation is the main expression of the DFT formalism that helps to minimize the energy and obtain the ground-state density. Since $F_{HK}[\rho]$ is composed by the unknown terms $T[\rho]$ and $V_{ee}[\rho]$, many approximations have been applied (like that for the ideal electronic gas phase, which is the base for the Thomas-Fermi model) but none has been enough accurate yet. To solve the problem, in 1965 Kohn y Sham (KS) proposed an innovating procedure to calculate the energy from electron density¹³². In this methodology, they assumed a non-interacting system of N electrons that moves under an external potential $v_s(\mathbf{r})$ that gives a wave function ψ . Furthermore, this wave function holds the same density as the real system.

KS methodology seems to be quite similar to the Hartree-Fock (HF) method, since its Hamiltonian (Eq. 31) contains the mono-electronic terms and the exact wave function is the Slater determinant (Eq. 32). Moreover, molecular orbitals are obtained as solutions of HF equations (Eq. 32). Hence, the exact electron density and the kinetic energy are defined as $\rho(\vec{r}) = \sum_{i=1}^{N_{occ}} |\chi_i(\vec{r})|^2$ and $T_s[\rho] = \sum_{i=1}^{N_{occ}} \langle \chi_i | -\frac{1}{2} \nabla^2 | \chi_i \rangle$, respectively.

$$\hat{H}_s = \sum_{i=1}^N \hat{h}(i) = \sum_{i=1}^N \frac{1}{2} \nabla^2(i) + \sum_{i=1}^N \hat{v}_s(i) \quad (31)$$

$$\psi_s = \frac{1}{\sqrt{N!}} |\chi_1(1)\chi_2(2)\chi_3(3) \cdots \chi_N(N)| \quad (32)$$

$$\left[-\frac{1}{2} \nabla^2 + \hat{v}_s(\vec{r}) \right] \chi_i = \varepsilon_i \chi_i \quad ; \quad \langle \chi_i | \chi_j \rangle = \delta_{ij} \quad (33)$$

In fact, if Eq. 30 is solved along with Eq. 34, it must lead to the exact non-interacting electron density above mentioned. On the other hand, the $V_{ee}[\rho]$ term must be added in the energy expression (Eq. 34) for a real system where the N electrons are interacting. Moreover, $v_s(\vec{r})$ must be replaced by $v_n(\vec{r})$.

$$E_v[\rho] = \sum_{i=1}^{N_{occ}} \varepsilon_i = T_s[\rho] + \int \rho(\vec{r}) v_s(\vec{r}) d\vec{r} \quad (34)$$

By defining $T[\rho] - T_s[\rho] = T_C[\rho]$ and $V_{ee}[\rho] - J[\rho] = W_{XC}[\rho]$, we can obtain $E_{XC}[\rho] = T_C[\rho] + W_{XC}[\rho]$. This last expression is the total exchange-correlation energy.

$$E_v[\rho] = \sum_{i=1}^{N_{occ}} \varepsilon_i = T_s[\rho] + \int \rho(\vec{r}) v_s(\vec{r}) d\vec{r} + J[\rho] + (T[\rho] - T_s[\rho]) + (V_{ee}[\rho] - J[\rho]) \quad (35)$$

Considering the Eq. 35 for an interacting system, the coulombic repulsion $\frac{1}{2} \iint \frac{\rho(\vec{r}_1)\rho(\vec{r}_2)}{|\vec{r}_1 - \vec{r}_2|} d\vec{r}_1 d\vec{r}_2$, and the total exchange-correlation energy, we obtain Eq. 36.

$$E_v[\rho] = T_s[\rho] + \int \rho(\vec{r}) v_n(\vec{r}) d\vec{r} + \frac{1}{2} \iint \frac{\rho(\vec{r}_1)\rho(\vec{r}_2)}{|\vec{r}_1 - \vec{r}_2|} d\vec{r}_1 d\vec{r}_2 + E_{XC}[\rho] \quad (36)$$

Then, applying Eq. 30 to Eq. 36,

$$\mu = \frac{\delta E_v[\rho]}{\delta \rho(\vec{r})} = \frac{\delta T_s[\rho]}{\delta \rho(\vec{r})} + \left[v_n(\vec{r}) + \int \frac{\rho(\vec{r}_2)}{|\vec{r}_1 - \vec{r}_2|} d\vec{r}_2 \right] + \frac{\delta E_{XC}[\rho]}{\delta \rho(\vec{r})} \quad (37)$$

Coulomb potential $\phi(\vec{r})$

X-C potential $v_{XC}(\vec{r})$

And so,

$$\mu = \frac{\delta T_s[\rho]}{\delta \rho(\vec{r})} + v_{eff}(\vec{r}) \quad (38)$$

As we can realize, Eq. 38 is similar to the non-interacting system expression $\mu = \frac{\delta T_s[\rho]}{\delta \rho(\vec{r})} + v_s(\vec{r})$. This means that the solution of Eq. 38 will be the same than that of the non-interacting case. To obtain the solution of the interacting system, analogous HF equations must be solved (Eqs. 39, 40). Kohn-Sham orbitals (χ_i) in eq. 39 allow to obtain the electronic density $\rho(\vec{r}) = \sum_{i=1}^{N_{occ}} |\chi_i(\vec{r})|^2$, the $v_{eff}(\vec{r})$, and finally solve $\hat{h}_{KS}\chi_i = \varepsilon_i\chi_i$. Thus, Kohn-Sham process is carried out in an iterative manner until satisfying the convergence criteria.

$$v_{eff}(\vec{r}) = v_n(\vec{r}) + \int \frac{\rho(\vec{r}_2)}{|\vec{r}_1 - \vec{r}_2|} d\vec{r}_2 + v_{XC}(\vec{r}) \quad (39)$$

$$\hat{h}_{KS}\chi_i = \varepsilon_i\chi_i: \quad \hat{h}_{KS} = -\frac{1}{2}\nabla^2 + v_{eff}(\vec{r}) ; \quad \langle \chi_i | \chi_j \rangle = \delta_{ij} \quad (40)$$

To obtain the exact ground-state energy, the exchange-correlation functional $E_{XC}[\rho]$ must be well-defined. Unfortunately, XC-functional is unknown, but there is a first approximation named *Local Density Approximation (LDA)* which gives a starting point for the electronic structure by assuming a homogeneous electron gas (HEG) (Eq. 41).¹³³ However, under the LDA approach, electrons are moving on a homogeneous and positive background charge density that neutralizes the electron gas charge.

$$E_{XC}^{LDA}[\rho] = \int \rho(\vec{r}) \varepsilon_{XC}(\rho(\vec{r})) d\vec{r}; \quad \varepsilon_{XC}(\rho(\vec{r})) = \varepsilon_X(\rho(\vec{r})) + \varepsilon_C(\rho(\vec{r})), \quad \varepsilon_X = -\frac{3}{4} \sqrt{\frac{3\rho(\vec{r})}{\pi}} \quad (41)$$

Also, the correlation term ε_C has not a well-defined expression. Therefore, theoreticians had proposed several formulations to describe the correlation contribution. Among them, the most employed expression of ε_C was developed by Vosko, Wilk, and Nusair in 1980. Later in 1992, Perdew and Wang developed a most accurate formulation. Unfortunately, LDA overestimate atomization energies of molecules and solids.

However, this problem is solved by the method named “*Generalized Gradient Approximation (GGA)*” (Eq. 42), where the E_X^{GGA} term is described as $E_X^{LDA} + \sum_{\sigma} \int F(s_{\sigma}) \rho_{\sigma}^{4/3}(\vec{r}) d\vec{r}$, and $s_{\sigma}(\vec{r}) = \frac{|\nabla \rho_{\sigma}(\vec{r})|}{\rho_{\sigma}^{4/3}(\vec{r})}$ that is the local inhomogeneity. Thus, GGA approach is the most popular level of theory in computational chemistry. Because of its better accuracy than LDA, the gradient generalized treating can provide satisfactory results for covalent, ionic, metallic, and hydrogen bonds. Unfortunately, GGA and LDA approaches fail describing Van der Waals interactions.

$$E_{XC}^{GGA}[\rho_{\alpha}, \rho_{\beta}] = \int f(\rho_{\alpha}, \rho_{\beta}, \nabla \rho_{\alpha}, \nabla \rho_{\beta}) d\vec{r} = E_X^{GGA} + E_C^{GGA} \quad (42)$$

Continuous improvement of density functionals goes ever on, so, efforts by chemists and physics to provide more accurate formulations paid off by introducing a degree of freedom provided by the Kohn-Sham Kinetic Energy density $t_s(\vec{r}) = \frac{\hbar^2}{2m} \sum_i |\nabla \phi_i(\vec{r})|^2$, and so, the Meta-GGA level emerged (Eq. 43). This new degree of freedom can satisfy constraints such as a self-corrected correlation functional and a finite exchange potential at the nucleus. Unfortunately, MGGA-functionals cannot be performed for d -states in transition-metal oxides due to self-interaction errors.¹³⁴

$$E_{XC}^{MGGA}[\rho] = \int \rho(\vec{r}) \varepsilon_{XC}(\rho(\vec{r}), \nabla \rho(\vec{r}), t_s(\vec{r})) d\vec{r} \quad (43)$$

The exhaustive search for the holy grail in DFT led to increasingly better functionals such as the hybrid functionals (or hyper-GGA level). Moreover, the guess that in the lower limit of the coupling integration, the constant ($\lambda=0$) of $\bar{n}_{XC}(\mathbf{r}, \mathbf{r}') = \int_0^1 d\lambda n_{XC}^{\lambda}(\mathbf{r}, \mathbf{r}')$ is the exact exchange hole, allowed Becke to propose the combination of the exact exchange with the density functional exchange-correlation to solve this problem. The simplest E_{XC}^{hyb} is represented by (Eq. 44), where $a = 1/4$ provides good approaches for molecules. On the other hand, the a constant cannot be equal or close to 1 because of the incompatibility with GGA exchange.^{133,135} LDA, GGA, meta-GGA, hyper-GGA and DHDF are part of the famous “Jacob’s ladder” shown in Figure 4.1.1.

$$E_{XC}^{hyb} = E_X^{exact} + (1 - a)(E_X^{GGA} - E_X^{exact}) - E_C^{GGA} \quad (44)$$

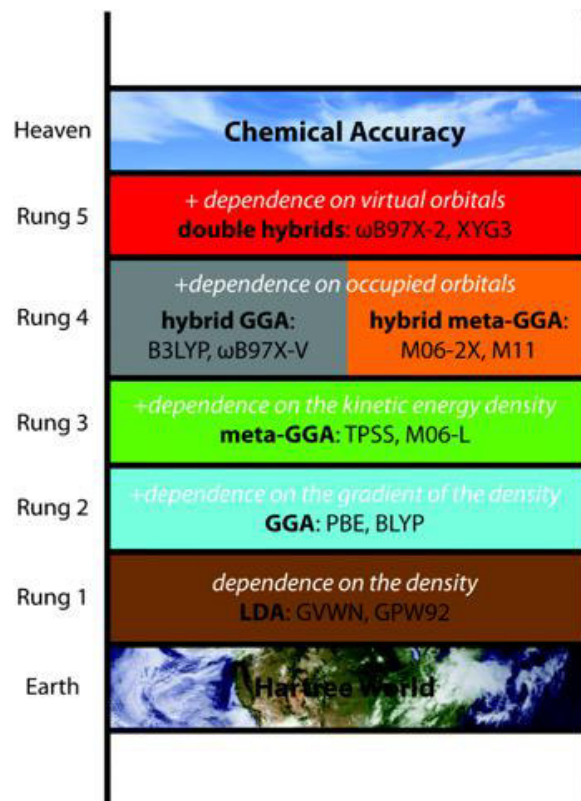


Figure 4.1.1. Jacob's ladder of density functionals.¹³⁶

4.1.1. Basis sets.

Another important concept in quantum mechanics is the basis set because this set of functions represents the atomic orbitals. Apart of planar waves and others not used in this thesis, there are two main types of basis sets, the Slater-type Orbitals (STOs)¹³⁷ (Eq. 45) and the Gaussian-type orbitals (GTOs)¹³⁸ (Eq. 46), where the specified functions Y_{lm} are the spherical harmonics which provide symmetry to the atomic orbitals (s, p, d, etc). The term $\exp(-r^2)$ is commonly known as the Gaussian primitive function. The contraction coefficients C_{ij} and the exponents ζ_{ij} are defined from a data base and do not change during the calculation. In fact, these coefficients and exponents are the so-called basis set. How does it work? By using these, the molecular orbital coefficients C_i are optimized during the self-consistent field (scf) procedure when solving the iterative KS equations.¹³⁹

$$\varphi_{STO} = NY_{lm} \sum_i C_i \sum_j C_{ij} r^{n-1} e^{-\zeta_{ij}} \quad (45)$$

$$\varphi_{GTO} = NY_{lm} \sum_i C_i \sum_j C_{ij} e^{-\zeta_{ij} r^2} \quad (46)$$

Nevertheless, Gaussian-type functions are preferred because of their low computational cost and efficiency. Unfortunately, the Gaussian-like shape of these functions is not close to the true behavior of atomic wave functions (cusp behavior) as compared to the Slater-type functions. Because of this, standard GTOs do not describe properly orbitals close to the nuclei unless a lineal combination of GTOs is used for a better description of the electron density around the nuclei.¹³⁹

Despite of that, GTOs and STOs can be classified as minimal basis sets, Pople's split-valence basis sets, correlation consistence basis sets, and other sub-types. Split valence basis sets are classified according to the number and type of basis sets that describe the atomic orbitals.¹⁴⁰

4.1.2. Minimal basis sets.

In this first category, we have one basis function for describing each atomic orbital. These basis sets are commonly called as single-zeta (single z, SZ). There are several minimal basis sets,¹⁴⁰ but the most common are the STO-*n*G developed by John Pople and co-workers.¹⁴¹ Each STO is composed by a linear combination of "*n*" GTOs or primitive orbitals. When the basis sets contain more than one GTO are considered as "contracted". The most known minimal basis set is the STO-3G, but there are some others as the STO-2G, the STO-4G, the STO-5G and the STO-6G.¹⁴⁰

4.1.3. Pople's basis sets.

This group includes the 3-21G¹⁴² (DZ), 6-21G¹⁴³ (DZ), 4-31G^{144,145} (DZ), 6-31G^{144,145} (DZ), and 6-311G¹⁴⁶ (TZ). This nomenclature describes a contraction scheme. The first number indicates the number of primitives used in the contracted core functions. The next numbers stand for the number of primitives used in the valence function. Moreover, polarization functions (*d*- or *p*-) are added while writing one or two asterisks, in parenthesis, after G letter. These ones provide more flexibility for the basis set in the valence region of the molecule to give a better description of the bonds. On the other hand, by adding diffuse functions to the basis set, it gets more flexible in regions far away from the nuclei, recovering extended electron density as for the case of anionic molecules (these are set up by writing one or two "+" signs before G letter).¹⁴⁰

4.1.4. Correlation consistent basis sets.

These ones are required in post HF methodologies. They add shells of polarization functions (*d, f, g, etc.*) to the valence region. Examples of these are cc-pVTZ (correlation-consistent valence triple-zeta), cc-pV5Z (correlation-consistent valence quintuple-zeta), and aug-cc-pVDZ (augmented correlation-consistent valence double-zeta), etc.¹⁴⁷⁻¹⁴⁹

Other split valence basis set are the ones developed by Ahlrichs and co-workers. Examples of these ones are SV(P) (SD), SVP (SZ), DZV (DZ), TZV (TZ), TZVPP (TZ plus two polarization functions), QZVP (QZ plus one polarization function) and their newer Def2 series (Def2-SV, Def2-SVP, etc.).¹⁵⁰⁻¹⁵³ These latter ones use a single function for orbitals which are not in the valence shell and two, three or four for the valence orbitals. In fact, these are the ones that we used to perform our computational studies, especially SVP and TZVP basis sets.

4.1.5. Basis set errors.

The basis set truncation errors are related to the difference between the real solution of the electronic Schrödinger equation and the experimental value corrected by non-bond orbital effects, and even relativistic corrections. On the other hand, the basis set superposition error is usually observed when two interacting atoms or molecules approach each other, and their basis sets overlap. The interaction energy for two atoms or molecules A and B is calculated by Eq. 47, where r_c indicates the distance between A and B in the adduct and r_e the size the separate reactants. However, this calculation gives large interaction energies that lead to complications for systems bound through dispersion interactions or hydrogen bonds.¹⁴⁰

$$E_{int} = E(AB, r_c) - E(A, r_e) - E(B, r_e) \quad (47)$$

Fortunately, the basis-set superposition error (BSSE) can be minimized by replacing the conventional Hamiltonian by one that may prevent the overlapping basis set by elimination of all the projector-containing terms that allow the basis set extension. On the other hand, the counterpoise method estimates the size of the BSSE by treating the separate monomers with a basis set of identical size. The counterpoise-corrected interaction energy is computed using Eq. 48, where the superscripts AB indicate that all the species are calculated with the same absolute basis.¹⁴⁰

$$E_{int}(CP) = E(AB, r_c)^{AB} - E(A, r_e)^{AB} - E(B, r_e)^{AB} \quad (48)$$

4.1.6. Effective core potentials.

Along the periodic table we can find heavy elements that are a real challenge for the molecular orbital theory, because the requirement of a big amount of functions for describing MOs. In 1935, Hellmann proposed the solution to this problem. He suggested the replacing of electrons and their basis functions in the wave function by analytical functions that represent accurately and efficiently the nuclear-electronic core and the valence electrons. Those functions are the effective core potentials (ECPs). Apart of reducing the computational cost, ECPs include the relativistic mass effect

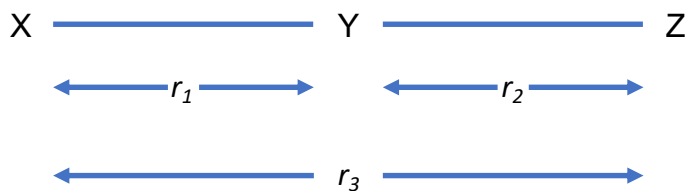
and the spin coupling terms that are quite important in the description of the environment near to the heavy nuclei.^{139,154,155}

Several ECP families are available for heavy atoms in the periodic table. Some of those families are Los Alamos National Laboratory (LANL) ECPs of Hay and Wadt,^{156–158} the consistent effective potential (CEP) by Stevens and co-workers,¹⁵⁹ the Ermeler-Christensen family,¹⁶⁰ and the Stuttgart-Dresden-Bonn (SDB) family^{161,162}. In this thesis, we used the Stuttgart-Dresden effective core potentials (SDD) to treat metal atoms (Cu, Ag and Au).

4.2. Transition State Theory.

Transition State Theory (TST), introduced by Eyring¹⁶³ and by Evans and Polanyi¹⁶⁴ in 1935, has been one of the most important contributions in chemistry. TST is a powerful tool that helps to describe the configurational and potential energy surface (PES) changes which occur when activated molecules react. The PES is divided in two regions: 1) reactants and products regions and 2) trajectories by which the reaction proceeds, through a transition state, once the reactants acquire enough energy. Moreover, once the system crosses the energy wall, it will turn back in a long time, in the order of k^{-1} , and this event does not affect the forward rate constant. The parameter that do not participate in the equilibrium is the concentration.^{165–167}

Considering a general reaction, *e.g.* $A + B \rightarrow C + D$, where reactants and products are polyatomic molecules, the potential energy surface for that system will be n -dimensional. However, an n -dimensional surface can be simplified into a three-dimensional $X + YZ \rightarrow XY + Z$, where X, Y and Z represent atoms. As shown in Scheme 4.2.1, there is an assumption of a linear approaching of X to XY and the recession of Z, where r_1 , r_2 and r_3 represent distances.¹⁶⁶



Scheme 4.2.1. Linear configurations for the three-dimensional surface.

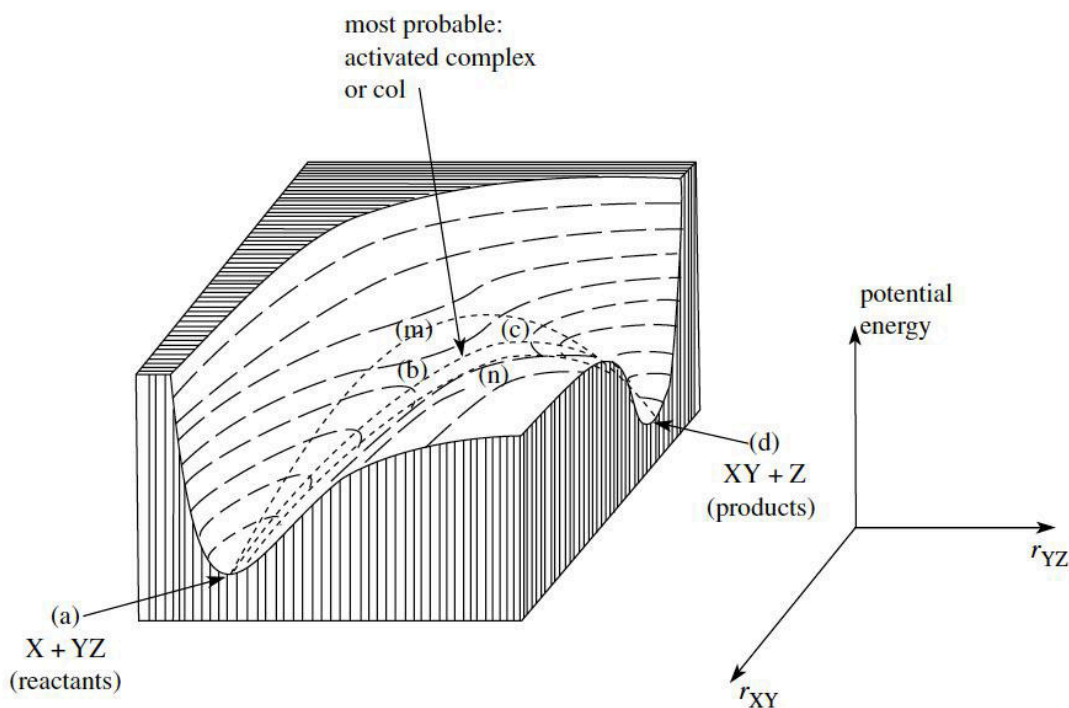


Figure 4.2.1. Three-dimension potential energy surface for $A + B \rightarrow C + D$.¹⁶⁶

As shown last page, when r_1 decreases, interactions between X and Y (YZ) becomes stronger than Y (XY) and Z. Therefore, these interactions are quite different along r_1 and can be plotted as the potential energy surface shown in Figure 4.2.1.

The sketched three-dimensional PES in Figure 4.2.1 has some properties that are important for TST; some of them are:¹⁶⁶

- A given reaction will have a unique PES, where the units (X---Y---Z) with the same configuration have the same potential energy (PE).
- For a diatomic molecule that vibrates as a harmonic oscillator, the PE is proportional to the square of the displacement from the equilibrium internuclear distance.
- At point (a), X is far away from YZ. This means that there is not interaction between X and XY. On the other hand, at point (d), Z has not interaction with XY. However, the most probable pathway that connects (a) with (d), is that one that has substantial number units (X---Y---Z).
- When we move away from points (a) or (b) in all directions, it gives an increment of the PE, giving the geometrical possible routes that connect each other through a maximum PE.

- The probability of a reaction path to be feasible decreases when PE increases.
- The maximum PE is called *the activated complex, the transition state* or *the critical configuration*.
- The vertical distance between (a) and *the activated complex* is the energy necessary for the reaction to proceed; likewise, the distance between (b) and *the activated complex* is the required energy to turn back the direction of the reaction.
- Changes in the dimensions of the activated complex along the reaction increase the PE.
- The reaction path on the PES gives a PE profile that shows the configurational changes along the reaction coordinate.
- Along the reaction pathway, a high energy intermediate can be formed in any step, but not as higher as *the transition state*.
- Molecules that have equal or larger energy than the transition state may be described as activated complexes.
- The rate of the reaction is determined by the total units/volume which pass through the transition state per unit time from reactants to products.

On the other hand, the rate at which the reaction passes through the critical configuration can be calculated from kinetic theory. The concentration of activated complexes can be calculated by using *partition functions* (translational, rotational, vibrational and electronic contributions) of *equilibrium statistical mechanics*, since $E_0 > kT$. The statistical form of the rate constant expression and the equilibrium constant for the formation of the activated complex are shown in Eq. 49 and Eq. 50, respectively.¹⁶⁶

$$k = \kappa \frac{kT}{h} \frac{Q^{**}}{Q_X Q_{YZ}} e^{\frac{-E_0}{RT}} \quad (49)$$

$$K^{**} = \frac{Q^{**}}{Q_X Q_{YZ}} e^{\frac{-E_0}{RT}} \quad (50)$$

Thus, κ is the transmission coefficient that defines the reactivity of each activated complex, k , h and E_0 are the Boltzmann constant, the Plank constant and the critical energy, respectively. On the other hand, Q^{**} , Q_X and Q_{YZ} are the partition function per volume unit for the activated complex and the reactants, respectively. It is worth to emphasize that K^{**} and Q^{**} quantities are not complete, these ones are missing the awkward terms: length along the reaction (δ) and the reduced mass (μ^\ddagger), nevertheless, these terms are factorized out to make it easy.¹⁶⁶

Sometimes, the partition function scheme is not useful as for reactions in solution, where the thermodynamic treatment works better. In this case, the thermodynamic quantities such as activation free energy (ΔG^\ddagger), activation enthalpy (ΔH^\ddagger), and activation entropy (ΔS^\ddagger) (Eq. 51–55), must be introduced.¹⁶⁶

$$\Delta G^\ddagger = -RT \log_e K, \quad K = \text{quotient of concentrations at equilibrium} \quad (51)$$

$$K = e^{\left(\frac{-\Delta G^\ddagger}{RT}\right)} = e^{\left(\frac{-\Delta H^\ddagger}{RT}\right)} e^{\left(\frac{+\Delta S^\ddagger}{R}\right)} \quad (52)$$

And so,

$$\Delta G^\ddagger = \Delta H^\ddagger + T\Delta S^\ddagger \quad (53)$$

$$d\Delta G^\ddagger = \Delta V^\ddagger dp - \Delta S^\ddagger dT \quad (54)$$

$$-\Delta S^\ddagger = \left(\frac{\partial \Delta G^\ddagger}{\partial T}\right)_p, \quad \Delta V^\ddagger = \left(\frac{\partial \Delta G^\ddagger}{\partial p}\right)_T, \quad +\frac{\Delta H^\ddagger}{RT^2} = \left(\frac{\partial \log_e K}{\partial T}\right)_p, \quad -\frac{\Delta V^\ddagger}{RT} = \left(\frac{\partial \log_e K}{\partial p}\right)_T \quad (55)$$

Eq, 54 shows a clear influence of pressure and temperature in the ΔG^\ddagger . On the other hand, the substitution of the equilibrium constant for the formation of the activated complex from reactants:

$$K^\ddagger = \frac{Q^\ddagger}{Q_X Q_{YZ}} e^{\frac{-\Delta U_0}{RT}} \text{ into } k = \kappa \frac{kT}{h} \frac{Q^\ddagger}{Q_X Q_{YZ}} e^{\frac{-E_0}{RT}} \text{ gives,}$$

$$k = \frac{\kappa kT}{h} K^{\ddagger*} \quad (56)$$

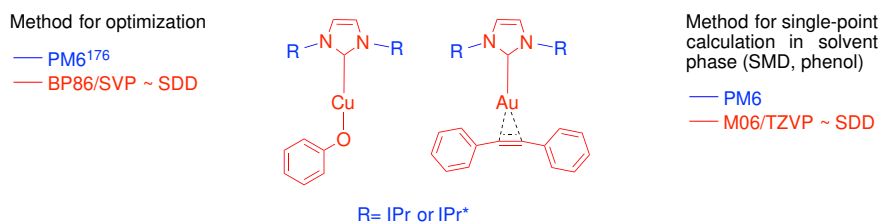
Then, applying $\Delta G^{\ddagger*}$, $\Delta H^{\ddagger*}$ and $\Delta S^{\ddagger*}$,

$$k = \frac{\kappa kT}{h} e^{\frac{-\Delta G^{\ddagger*}}{RT}} = \frac{\kappa kT}{h} e^{\left(\frac{-\Delta H^{\ddagger*}}{RT}\right)} e^{\left(\frac{+\Delta S^{\ddagger*}}{R}\right)} \quad (57)$$

Eq. 57 is the thermodynamic form of the equilibrium constant for the activated complex from reactants, where ΔG^{**} , ΔH^{**} and ΔS^{**} are the Gibbs free energy of activation, the enthalpy of activation, and the entropy of activation, respectively.

4.3. Computational details.

In this Master thesis, Density Functional Theory (DFT) has been applied to obtain relative energies, structural information, and properties such as the nucleophilic and electrophilic character of the generated species in alkyne hydrophenoxylation assisted by copper or silver-gold catalysts. The approaches to IMe, IMes, SIMes, IPr, CAAC (Pyrrolidin-ylidenes L^1 and L^2), and PSC ([bis(diisopropylamino)phosphanyl](trimethylsilyl)carbene) systems were performed at the GGA level by using the Becke-Perdew functional (BP86).¹⁶⁸ Carbon, hydrogen, nitrogen, and oxygen atoms were treated with the SVP basis set of Ahlrichs and co-workers,¹⁵⁰ and the quasi-relativistic Stuttgart/Dresden with their associated valence basis set (SDD keyword in G09) was employed for all metals.^{169–171} From the optimized geometries at the BP86/SVP~SDD level, single-point calculations were performed using the M06 functional¹⁷² in conjunction with the triple-zeta basis set of Weigend and Ahlrichs for main-group atoms (TZVP keyword in Gaussian),¹⁵² whereas for metal atoms the SDD basis set was still set up. Moreover, in these single-point calculations, the solvent effect was also added implicitly using the Truhlar and co-workers' SMD solvation model¹⁷³ with phenol as the solvent of the reaction. In the case of the system bearing the IPr* (and IPr ligand for the sake of comparison), the double-layer ONIOM model^{174,175} was used in order to compare the sterical hindrance effect. The methodology for these studies is shown in Scheme 4.3.1.



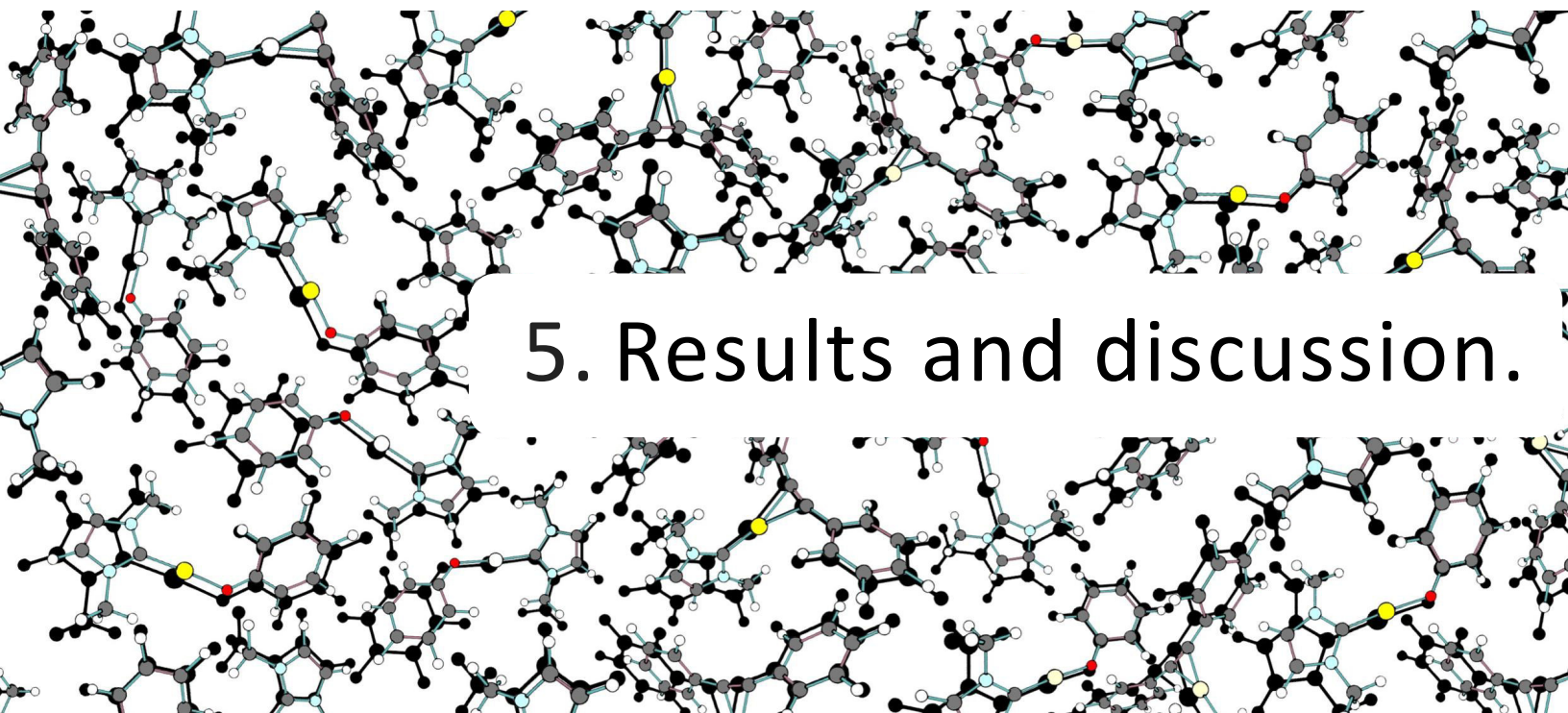
Scheme 4.3.1. Double-layer ONIOM model for the hetero-dual catalysis bearing the IPr* and IPr ligands.

The free energies reported in this work include energies obtained at the M06/TZVP and ONIOM (M06/TZVP:PM6) level of theory corrected with zero-point energies, thermal corrections, and entropy effects evaluated at 298 K and 1 atm.

To determine the steric hindrance around the metal, topographical steric maps of NHC, CAAC, and PSC ligands were obtained by the SambVca 2.0 tool, developed by Cavallo *et al.*¹⁷⁷ The radius of

Methodology

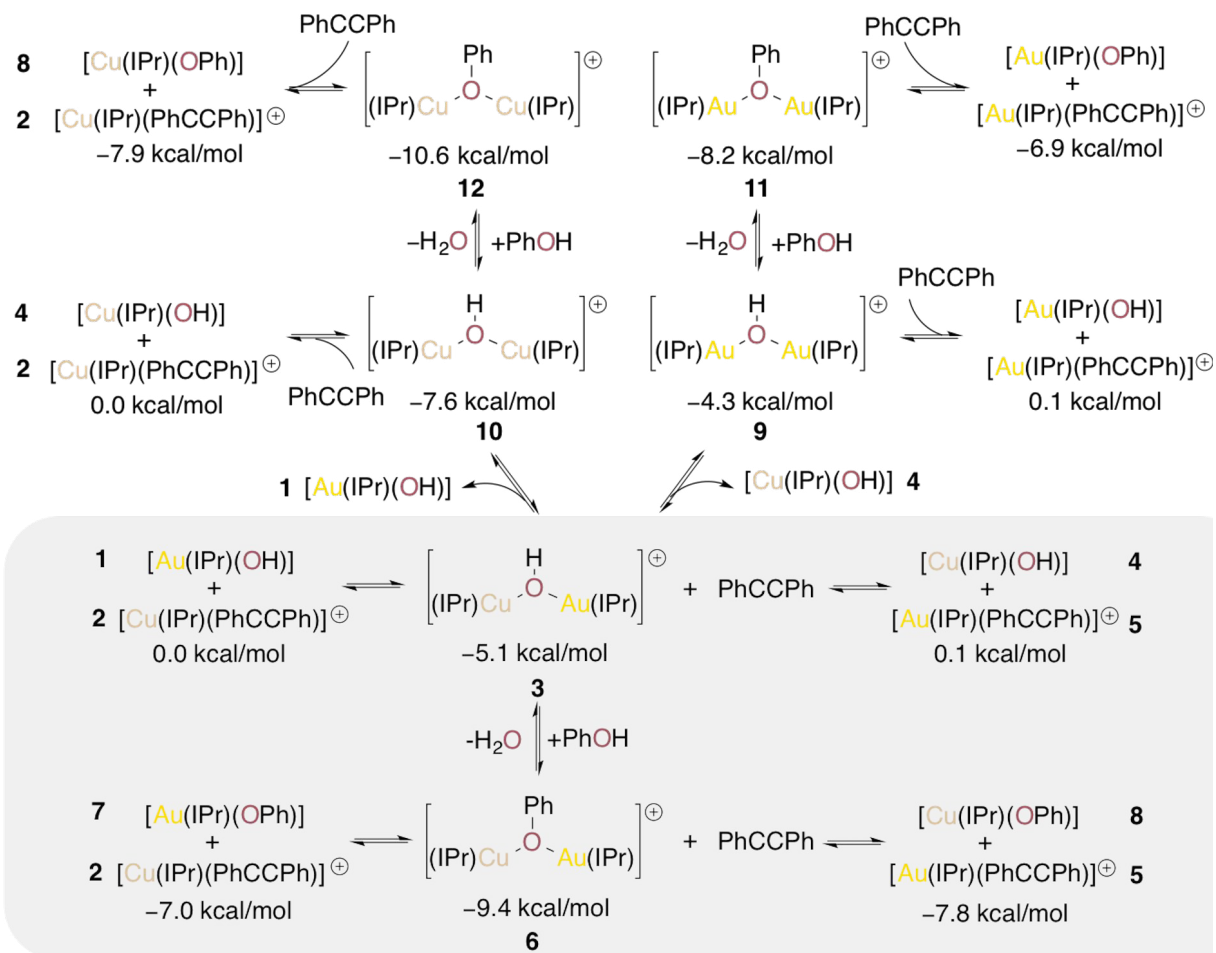
the sphere around the metal center was set to 3.5 Å, whereas for the other atoms we adopted the Bondi radii scaled by 1.17. Moreover, a mesh of 0.1 Å was used to scan the sphere for buried voxels.^{177–180}



5.1. Generation of σ - and π -activated species.

Hydroalkoxylation reaction is an important synthetic strategy that allows us to access to vinyl ethers that have a wide range of industrial applications. Thus, several scientists around the world have done their best to optimize the addition of alcohols to alkyne derivatives. Recently, mechanistic studies have described one where the σ - and π -activated compounds are generated in the initiation step.¹²⁶ These compounds carry out the catalytic cycle as follows: 1) nucleophilic attack by σ -species to the alkynic complex (rds); 2) *O*-deuration promoted by an external molecule of phenol; 3) α -protonation; and 4) a second deuration assisted by a molecule of the alkyne.

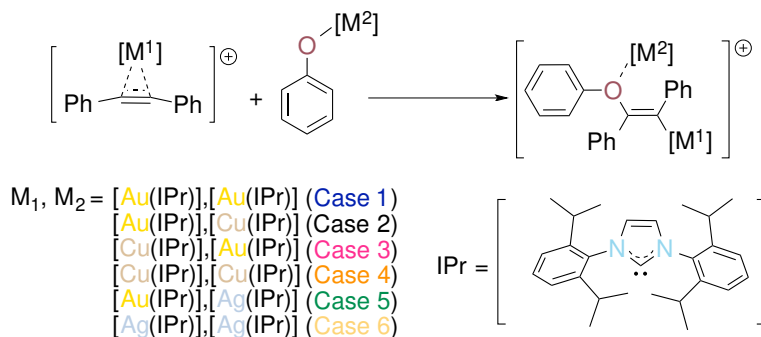
Herein, we discuss the full computational mechanistic study about the hydrophenoxylation of diphenylacetylene via a hetero-dual-assisted process. As we have mentioned above, the reactive σ - and π -species are generated during the initiation step. However, to explore the mechanistic pathway, we set ourselves the task of exploring this part of the reaction through the study of all the possible species that could be involved in the pre-activation step (see Scheme 5.1.1). Our results indicate that the stability of the *gem*-bimetal species increases as follows: **9** \ll **3** \ll **10**. Furthermore, when **10** reacts with a molecule of phenol, the most stable dimer **12** is generated; otherwise, the same reaction with the compound **3** produces dimer **6** that is lower in energy than dimer **11**. On the other hand, the analysis of $[M(\text{IPr})(\text{OPh})]/[M(\text{IPr})(\text{PhCCPh})]^+$ species shows that the $[\text{Cu}(\text{IPr})(\text{OPh})]/[\text{Cu}(\text{IPr})(\text{PhCCPh})]^+$ (-7.9 kcal/mol) and $[\text{Cu}(\text{IPr})(\text{OPh})]/[\text{Au}(\text{IPr})(\text{PhCCPh})]^+$ (-7.8 kcal/mol) are nearly isoenergetic and lower in energy than $[\text{Au}(\text{IPr})(\text{OPh})]/[\text{Au}(\text{IPr})(\text{PhCCPh})]^+$ (-6.9 kcal/mol). Thus, due to the stability of **6** and $[\text{Cu}(\text{IPr})(\text{OPh})]/[\text{Au}(\text{IPr})(\text{PhCCPh})]^+$ species, the hetero-dual system will be favoured, as proposed in the experimental report.



Scheme 5.1.1. Possible species involved in the initiation step.

5.2. Metal effect in the rate-determining step.

Inspired by the recent experimental studies of digold catalysis and heterometallic dual catalysis,¹²⁷ we proposed three possible pairs of nucleophile-electrophile species (see Scheme 5.2.1, Cases 2, 3, and 4) to describe the improvement of the hydroalkoxylation process by using dual-heterometallic catalysis. The digold specie (case 1) was considered as the reference case. Moreover, we expect that the Case 3 display the lowest energy barrier for the nucleophilic attack, as proposed experimentally in the literature. Accordingly, we found interesting computational results that help us to understand and support the proposal in the experimental report.



Scheme 5.2.1. Possible starting species in hydrophenoxylation assisted by gold-, copper- and silver-IPr catalysts.

The set of energy profiles in Figure 5.2.1 shows the results of the different possible cases for the starting species in the catalytic system and their corresponding energy barriers for the C-O bond formation step. We observed that the Cases 3 and 4 exhibit energy barriers of 20.7 and 19.4 kcal/mol, respectively. However, these latter barriers are larger than for Case 1, that has an energy barrier of 17.8 kcal/mol. In addition, the provided information allowed us to discard the cases σ -gold/ π -copper and σ -copper/ π -copper, leading us to the Cazin's proposal.

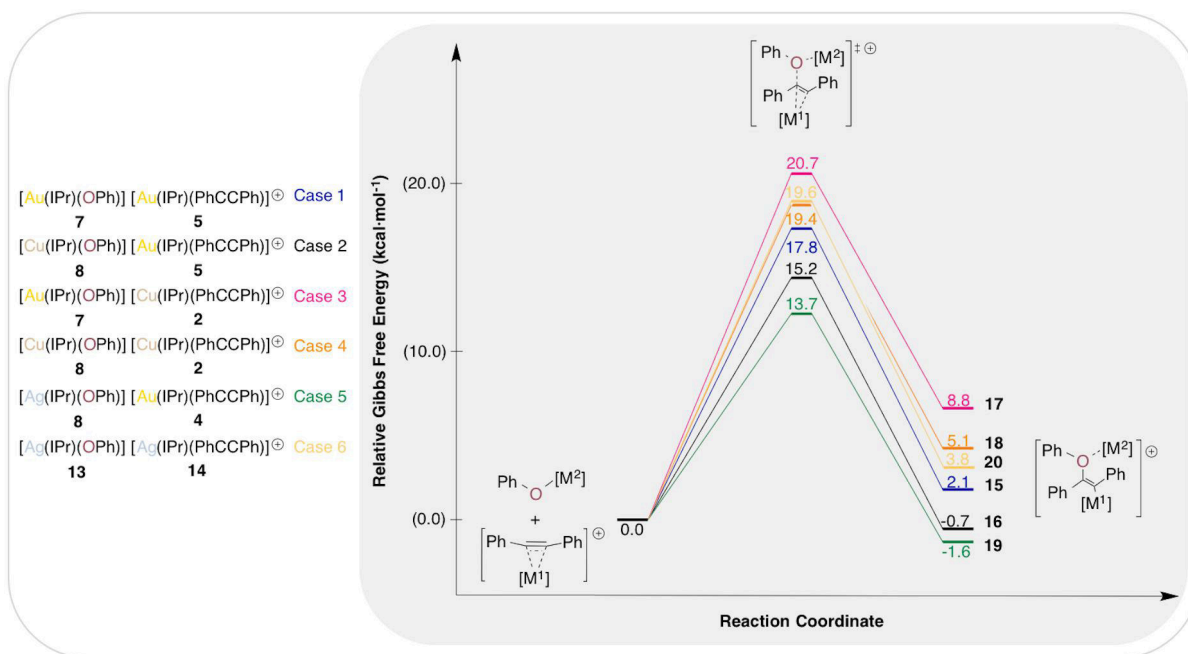


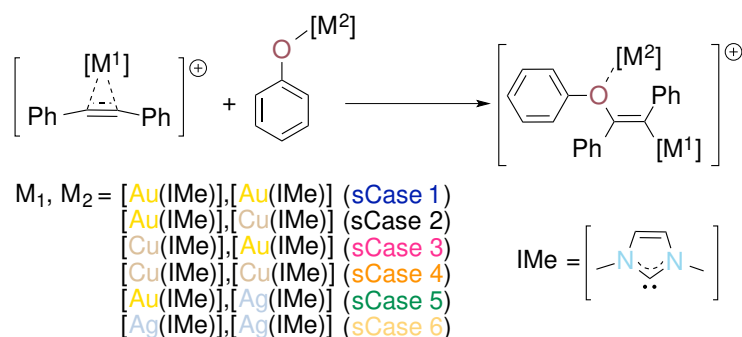
Figure 5.2.1. Influence of the metal-NHC catalyst in the rds (Gibbs free energies in solvent are given in kcal/mol).

On the other hand, we found the lowest energy activation (15.2 kcal/mol) for the Case 2 that includes **8** and **5** as starting species. This means that the hetero-metal-dual catalysis proposed by Cazin and co-workers will be favored.¹²⁷ Moreover, after the analysis of the intermediates generated in each case, we found that the intermediate **16** (produced in the Case 2) is the one with lowest energy, thus, it is also thermodynamically favored.

Once that we found the σ/π couple that improves the hetero-dual process, we decided to explore the influence of the metallic atom. Thus, we performed the calculations for the rds with silver instead copper (see Scheme 5.2.1, Case 5) and the σ -Ag/ π -Ag system (see Scheme 5.2.1, Case 6). Nonetheless, the silver/silver case showed an energy barrier of 19.6 kcal/mol that turns out to be higher than for the Cases 1, 2 and 5. Moreover, focused on the ΔG_{TS} for homo-dual cases, we observed an interesting trend along the group 11 as follows: **13/14** > **8/2** > **7/5**. Further, from a thermodynamic point of view, the intermediate generated in each case follows the next behavior: **8** > **20** > **16**. Regarding the Case 5, this has the lowest energy activation and thus this electrophile-nucleophile couple could carry out the hydrophenoxylation reaction in a more efficient way than the Case 2. Additionally, the intermediate **19** generated in the latter case is the most stable with -1.6 kcal/mol in comparison with the intermediate associated to **8/5** system which exhibits an energy stabilization of -0.7 kcal/mol.

5.3. Metal effect in the rate-determining step using IMe instead of IPr ligand.

To determine the main reason of why the species **13** reacts with compound **5** in a more efficient way than species **8**, we performed the calculations for σ -M/ π -M systems involving the IMe ligand instead of IPr, which is one of the most hindered NHC-ligands in this computational work. The cases for the simplified σ - and π -species are shown in Scheme 5.3.1.



Scheme 5.3.1. Possible starting species in the hydrophenoxylation assisted by gold-, copper- and silver-IMe catalysts.

Figure 5.3.1 shows the set of energy profiles for all the possible combinations of the π -[M(IMe)]/ σ -[M(IMe)] couples. Interestingly, the **29/22** couple displays the lowest energy barrier for the C-O bond formation. Moreover, the intermediate **30** generated in this case is the lowest in energy such as **19** in the metal-IPr system. In general, the metal-IMe energy profiles manifest similar tendencies to the metal-IPr profiles (see Figure 5.2.1), except for the **24/22** couple which exhibits a higher energy barrier (13.6 kcal/mol) than the homo-dual sCase 1 (12.3 kcal/mol).

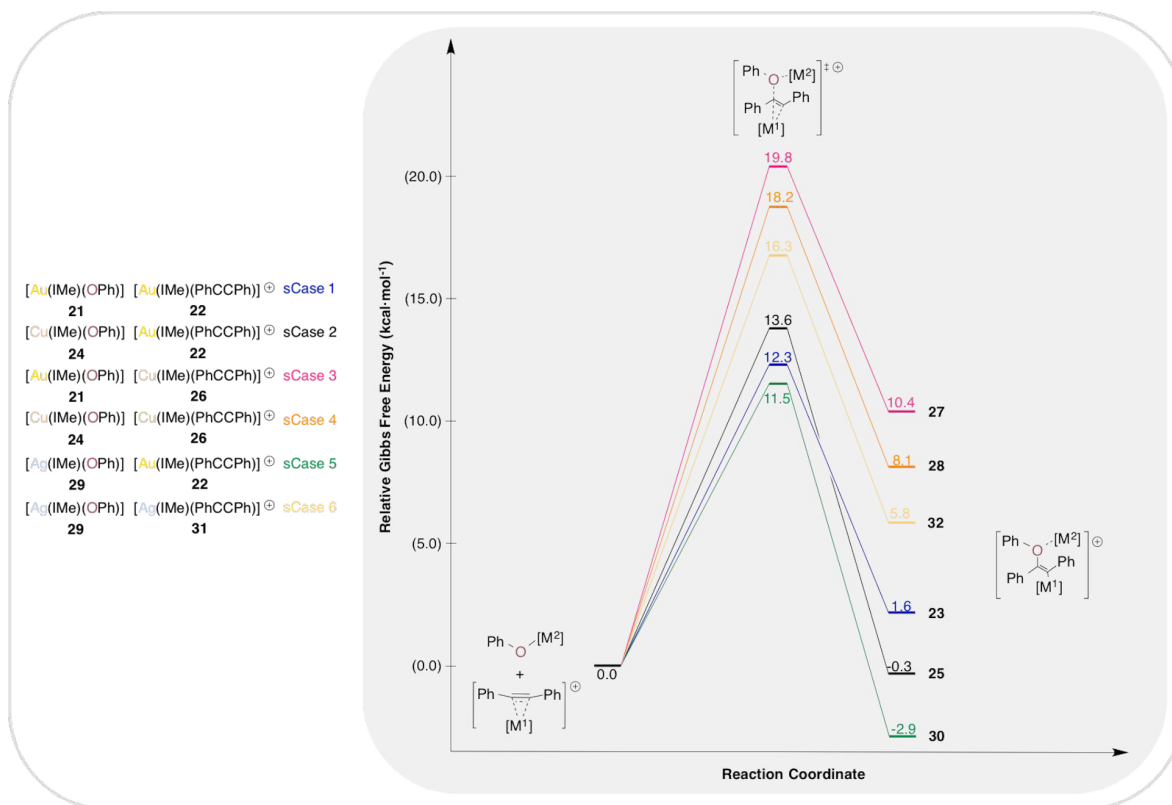


Figure 5.3.1. Influence of the metal center in the rds for the simplified cases in Scheme 5.3.1 (Gibbs free energies in solvent are given in kcal/mol).

5.4. Structural and electronic data analysis of σ - and π -activated species in hetero-metal-assisted catalysis involving IMe and IPr ligands.

To find out the effect of the metal core, we analyzed the structural data for the π -metal species involving the IPr and IMe ligands. The results showed that the C-C bond length of the alkynic fragment increases in the species π -species as follows: π -Ag < π -Cu < π -Au. This means that the alkyne compound is more activated by gold catalyst than copper and silver catalysts. Likewise,

Mayer Bond Orders (MBO) confirm that the gold achieves a better activation of the alkyne compound in comparison with silver or copper. By contrast, the gold-carbon bonds exhibit the highest MBO values in IMe and IPr (0.572 and 0.651, respectively). Moreover, the MBO values follow the same tendency as the C-C bond length (see Table 5.4.1), *i. e.* the larger the MBOs, the longer the C-C bond.

Table 5.4.1. Structural data for π -species, C-C bond lengths (in Å), and MBO index for metal-carbon (M-C) bonds.

Species	MBO (C-M)	d (C-C) (Å)
[Au(IPr)(PhCCPh)] ⁺	0.651	1.267
[Cu(IPr)(PhCCPh)] ⁺	0.498	1.260
[Ag(IPr)(PhCCPh)] ⁺	0.473	1.255
[Au(IMe)(PhCCPh)] ⁺	0.572	1.268
[Cu(IMe)(PhCCPh)] ⁺	0.527	1.259
[Ag(IMe)(PhCCPh)] ⁺	0.394	1.254

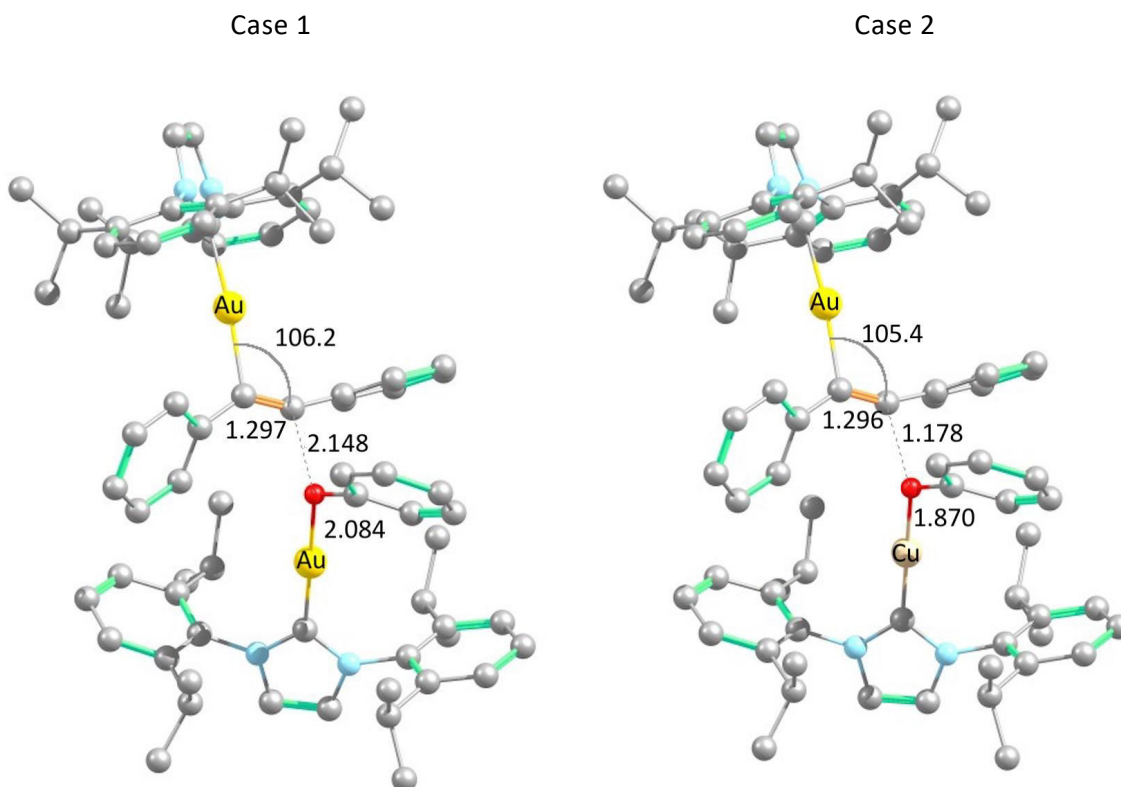
Additional information that contribute to the description of the improvement of the hydroalkoxylation process is the C-O bond strength in the intermediates generated in IPr and IMes systems (see Schemes 5.2.1 and 5.3.1). Focusing on the IPr cases, Mayer atomic bond orders (MBO) indicated that the intermediate in Case 5 has the strongest C-O bond with a value of 0.826 (see Table 5.4.2). Moreover, when we substituted IPr by IMe, we observed the highest MBO for the C-O bond in the sCase 5.

Table 5.4.2. Mayer bond orders and C-O bond lengths for the intermediates generated in the cases shown in Figures 5.2.1 and 5.3.1.

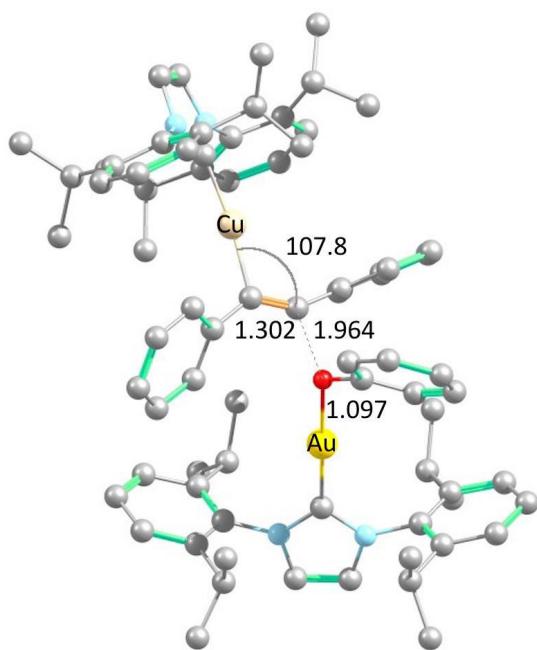
Species	MBO (C-O)	d (C-O) (Å)
[Au(IPr)(OPh)(PhCCPh)(IPr)Cu] ⁺	0.763	1.484
[Cu(IPr)(OPh)(PhCCPh)(IPr)Cu] ⁺	0.758	1.481
[Au(IPr)(OPh)(PhCCPh)(IPr)Au] ⁺	0.791	1.476
[Cu(IPr)(OPh)(PhCCPh)(IPr)Au] ⁺	0.821	1.474
[Ag(IPr)(OPh)(PhCCPh)(IPr)Au] ⁺	0.826	1.466
[Ag(IPr)(OPh)(PhCCPh)(IPr)Ag] ⁺	0.806	1.476
[Au(IMe)(OPh)(PhCCPh)(IMe)Cu] ⁺	0.766	1.483
[Cu(IMe)(OPh)(PhCCPh)(IMe)Cu] ⁺	0.760	1.479
[Au(IMe)(OPh)(PhCCPh)(IMe)Au] ⁺	0.795	1.474
[Cu(IMe)(OPh)(PhCCPh)(IMe)Au] ⁺	0.787	1.471
[Ag(IMe)(OPh)(PhCCPh)(IMe)Au] ⁺	0.832	1.462
[Ag(IMe)(OPh)(PhCCPh)(IMe)Ag] ⁺	0.809	1.472

In addition to the MBO analysis of the new C-O bond formed, we analyzed the C-O distance of the intermediates, as shown in Table 5.4.2. Thereby, we observed that the intermediates for Case 5 and sCase 5 display C-O distance values of 1.466 Å and 1.462 Å, respectively, which are the shortest and the ones that are closer to the C-O length in the product (1.389 Å). Moreover, in the IPr and IMe systems, the intermediates of homo-dual cases showed a decrease in the length distance as follows: Cu/Cu > Ag/Ag, Au/Au. On the other hand, when gold was substituted by copper or silver in the σ -species, we observed a reduction in the C-O bond length in the intermediates as follows: σ -gold/ π -gold > σ -copper/ π -gold > σ -silver/ π -gold.

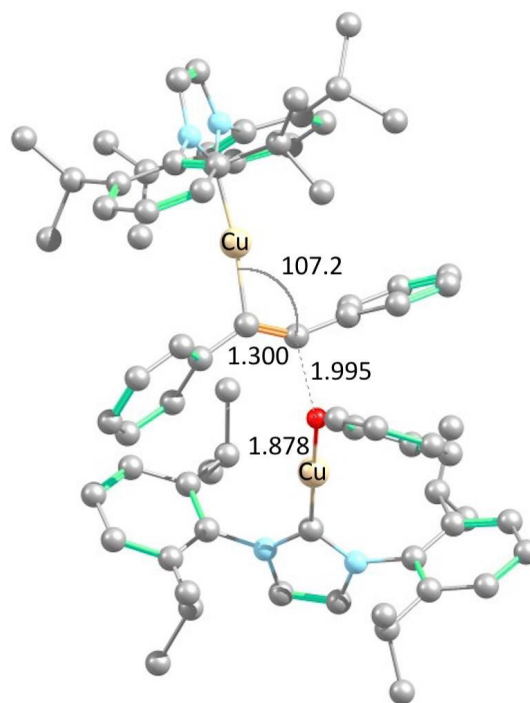
Other structural information that helped us to understand the influence of the metallic center was the C-O bond distance of the transition state. Figure 5.4.1 shows the structural information about the transition states involving different couples of σ -/ π -metal species containing IPr and IMe ligands, that appear to be geometrically similar. On the other hand, focusing on the C-O distance of each TS, we observe that these distances exhibit the following pattern for the IPr system: σ -gold/ π -copper < σ -copper/ π -copper < σ -gold/ π -gold < σ -copper/ π -gold < σ -silver/ π -silver < σ -silver/ π -gold. In the IMe systems, the C-O distance increases as follow: σ -gold/ π -copper < σ -copper/ π -copper < σ -silver/ π -silver < σ -gold/ π -gold < σ -copper/ π -gold < σ -silver/ π -gold.



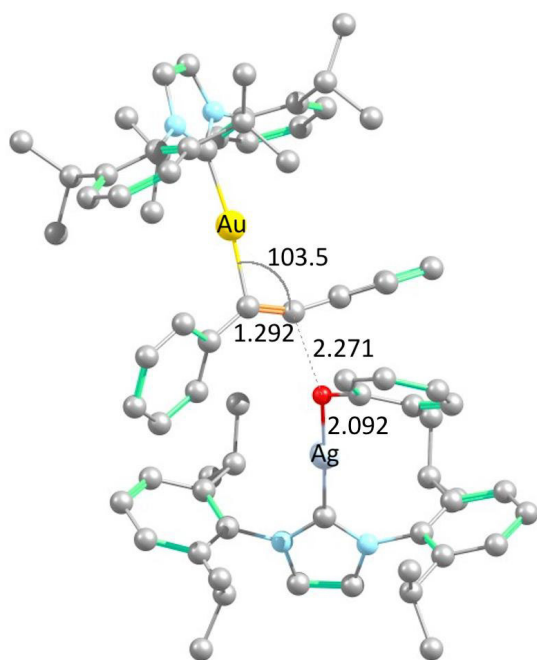
Case 3



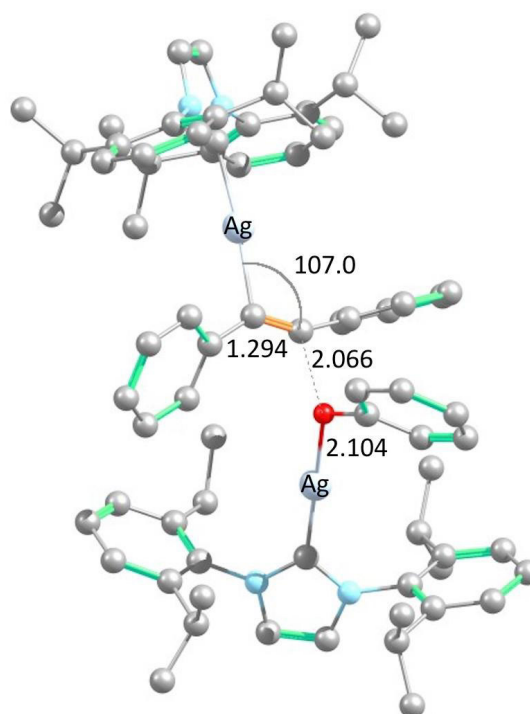
Case 4



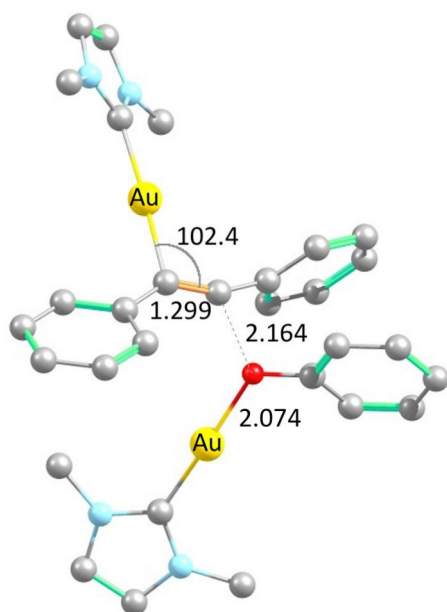
Case 5



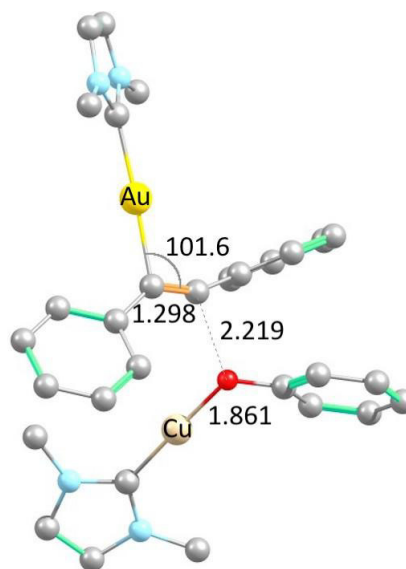
Case 6



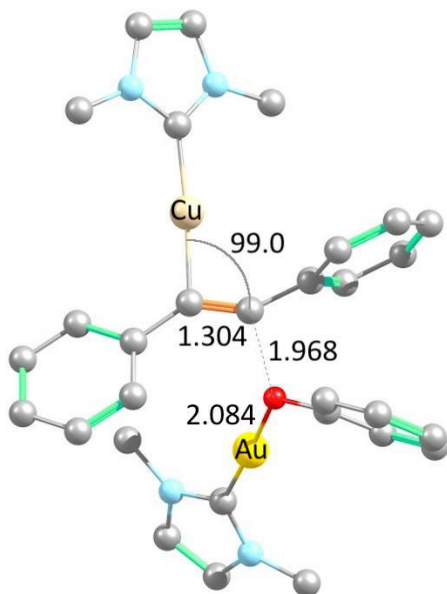
sCase 1



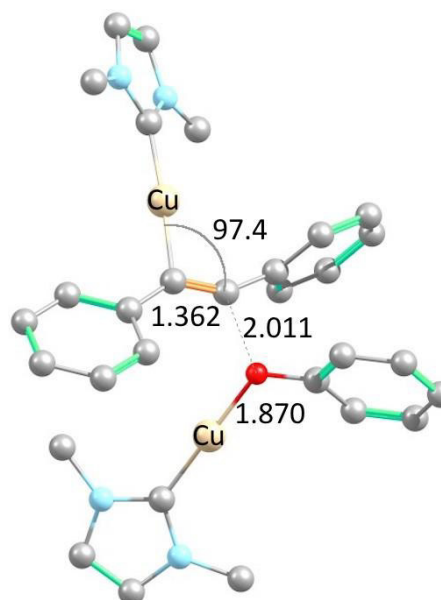
sCase 2



sCase 3



sCase 4



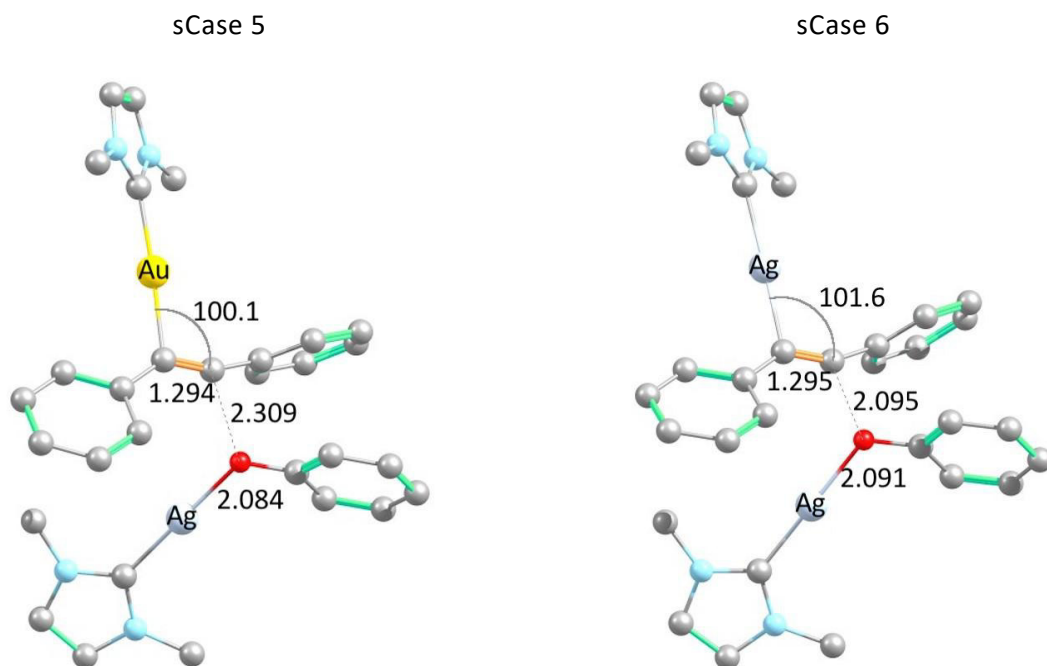


Figure 5.4.1. Molecular structures of the transition states shown in Figures 5.2.1 and 5.3.1 (Hydrogen atoms were omitted for a better view, selected distances are in Å and angles in degrees).

Beyond structural data, electronic information such as Natural Bond Orbital (NBO) charges and chemical hardness can provide the needed information to further support the improvement of the hydroalkoxylation reaction by using Ag-O and Cu-O species. In Table 5.4.3, we have thus the results of NBO charges and chemical hardness for the couples of σ - and π -species proposed in Figures 5.2.1 and 5.3.1.

Table 5.4.3. NBO charges and chemical hardness for the electrophile-nucleophile couples and intermediates shown in Figures 5.2.1 and 5.3.1.

Species	NBO (C)	NBO (O)	Chemical hardness (η) in eV
[Cu(IPr)(OPh)] ⁺	---	-0.801	2.07
[Ag(IPr)(OPh)] ⁺	---	-0.778	1.85
[Au(IPr)(OPh)]	---	-0.748	2.15
[Cu(IMe)(OPh)]	---	-0.757	2.26
[Ag(IMe)(OPh)]	---	-0.745	2.04
[Au(IMe)(OPh)]	---	-0.716	2.29
[Cu(IMe)(PhCCPh)] ⁺	-0.067	---	2.88
[Ag(IMe)(PhCCPh)] ⁺	-0.046	---	3.02
[Au(IMe)(PhCCPh)] ⁺	-0.041	---	3.02
[Cu(IPr)(PhCCPh)] ⁺	-0.079	---	3.05
[Ag(IPr)(PhCCPh)] ⁺	-0.054	---	3.07
[Au(IPr)(PhCCPh)] ⁺	-0.043	---	3.21

First, the NBO charges analysis gave us a couple of pieces of our puzzle, especially the nucleophilic and electrophilic character of the starting species. It was found that carbons in the former alkyne in $[\text{Au}(\text{IPr})(\text{PhCCPh})]^+$ species are more electrophilic than the homologous carbons in $[\text{Cu}(\text{IPr})(\text{PhCCPh})]^+$. On the other hand, the nucleophilic character of oxygen in $[\text{M}(\text{IPr})(\text{OPh})]$ was higher in the copper catalyst. Additionally, in order to support our findings for copper and gold, and then to establish a systematic trend, the NBO charges were recalculated replacing those metals with silver. The results obtained for the silver system revealed a linear trend along the group XI. Thus, the nucleophilicity of the phenoxyated species decreases going from copper to gold as a metal center, whereas the carbon atoms of the cationic $[\text{M}(\text{IPr})(\text{PhCCPh})]^+$ moiety increase their electrophilic character. This let us to explain why the Case 2 displays a lower energy barrier for the C-O bond formation than the Case 1.

Next, if we focus in the chemical hardness study, the results indicate that silver-phenoxide has the lowest chemical hardness in all cases. Thus, this one is more reactive than σ -copper and σ -gold species, whereby the silver and gold catalysts improve the energy barrier for the nucleophilic attack.

5.5. Full energy profile of the hetero-dual-metal-assisted catalysis using copper and gold catalysts bearing IPr ligand.

With the help of the results described in Sections 5.2 and 5.4 and the mechanistic studies of diaurated catalytic system reported by Poater *et al.*,¹²⁶ we computed the reaction mechanism shown in Figure 5.5.1. First, the mechanism shows the attack of oxygen for the C-O bond formation (**5+8-16**) as the rate determining step. Then, due to the oxophilia of copper, this is coordinated by a phenol molecule (**16-33+34**) to form the intermediate **33** and the species **34**. Next, the latter species will carry out the protonation reaction (**33+34-35**) to form the intermediate **35**. The experimental mechanistic studies reported by Cazin *et al.* allowed us to propose an alkyne coordination as the final step (**35-36**). Moreover, to support the profile of the reaction, we condensed in Figure 5.5.2 the geometries of the **16-33+34**, **33+34-35** and **35-36** transition states. As it can be seen, Cu-O distance (2.110 Å) in **16-33+34** is just 0.172 Å larger than the Cu-O bond length (1.938 Å) in $[\text{Cu}(\text{IPr})(\text{OHPh})]^+$, whereas C-H distance (1.420 Å) in **33+34-35** is 0.316 Å longer than C-H bond length in the intermediate **35** (1.104 Å) and the transition state for the deauration **35-36** step displays Au-C distances of 0.642 and 0.723 Å larger than the ones in compound **8** (2.234 Å).

Results and discussion

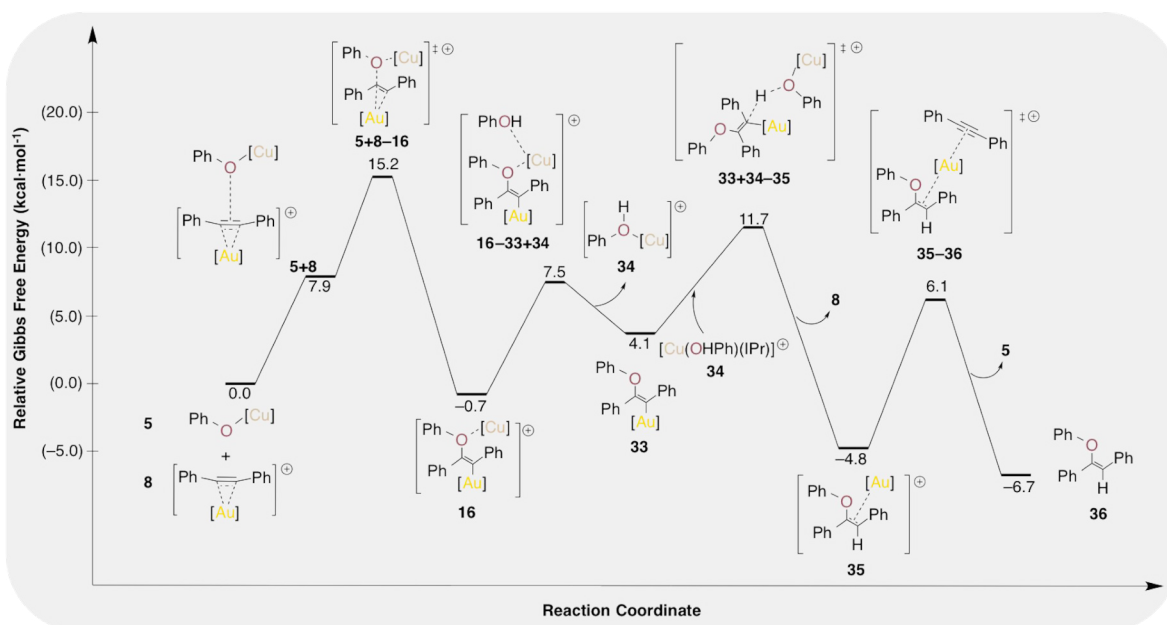
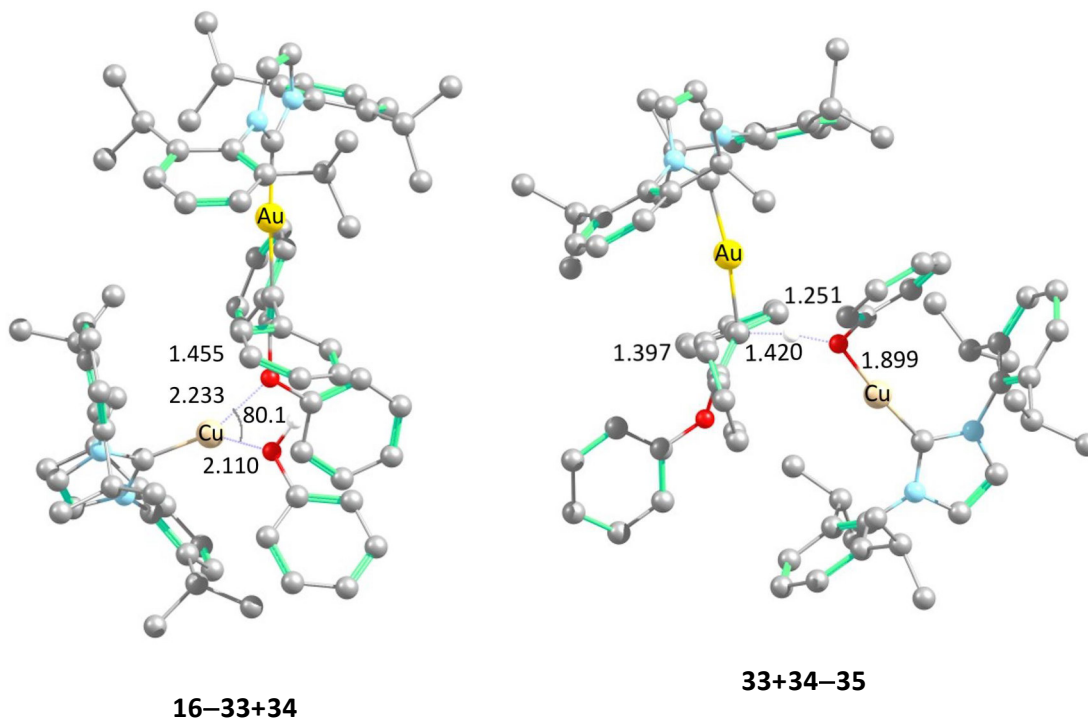
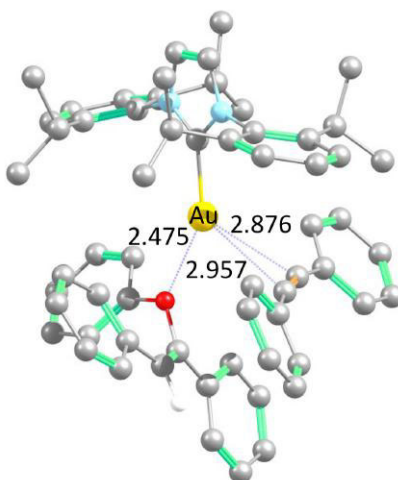


Figure 5.5.1. Reaction mechanism for the hydrophenoxylation of diphenylacetylene assisted by [Cu(IPr)(OPh)] and [Au(IPr)(PhCChPh)]⁺ catalytic moieties (Gibbs free energies in solvent are given in kcal/mol).





35–36

Figure 5.5.2. Molecular structures of the transition states: copper removal by a molecule of phenol (**16–33+34**), protonation by $[\text{Cu}(\text{IPr})(\text{OHPH})]^+$ species (**33+34–35**) and *O*-deauration assisted by an external alkyne species (**35–36**) (Hydrogen atoms were omitted for clarity, selected distances are in Å and angles in degrees).

Finally, the later mechanistic information about the hetero-dual-assisted hydrophenoxylation process allowed us to suggest the catalytic pathway for this process (see Figure 5.5.3). Thus, the full catalytic process schematized the initiation step, where pre-activated species $[\text{Cu}(\text{IPr})(\text{OPh})]$ and $[\text{Au}(\text{IPr})(\text{PhCCPh})]^+$ are produced. These species react as a nucleophile-electrophile reaction. It is worth emphasize that the *O*-attack to the π -species determines the rate of the reaction. Once the phenoxyated species is formed, $[\text{Cu}(\text{IPr})]$ moiety is removed by a phenol molecule to generate the gold-vinyl ether derivative and the $[\text{Cu}(\text{IPr})(\text{OHPH})]^+$ compound that behaves as the proton source. Later, the second species protonates the carbon attached to the $[\text{Au}(\text{IPr})]$ moiety in the gold-vinyl compound, and so, the $[\text{Au}]$ -vinyl coordination compound is formed. After that, a molecule of diphenylacetylene coordinates and removes the gold moiety from the $[\text{Au}]$ -vinyl derivative. In this step, the phenoxyated compound is released from the catalytic cycle, and the pre-activated species are regenerated on it. As it can be noticed, the catalytic pathway for the hetero-dual-assisted hydrophenoxylation reaction is quite similar to the mechanism for the homo-dual-assisted process reported by Poater *et al.*¹²⁶

On the other hand, we found that hetero-dual catalysis displayed a better performance than the homo-dual one. For that reason, we dare to say that this study has provided us with a new catalytic tool by which the addition of phenols and alcohols to unsaturated bonds is successfully achieved. Thus, the awesome success of the hetero-dual-assisted reaction is due to the fact that copper-phenoxide is better nucleophile than gold-phenoxide. Besides the nucleophilic character

from copper species, this one lowers the catalyst costs becoming the HP reaction a more profitable, attractive process to the coating industry.

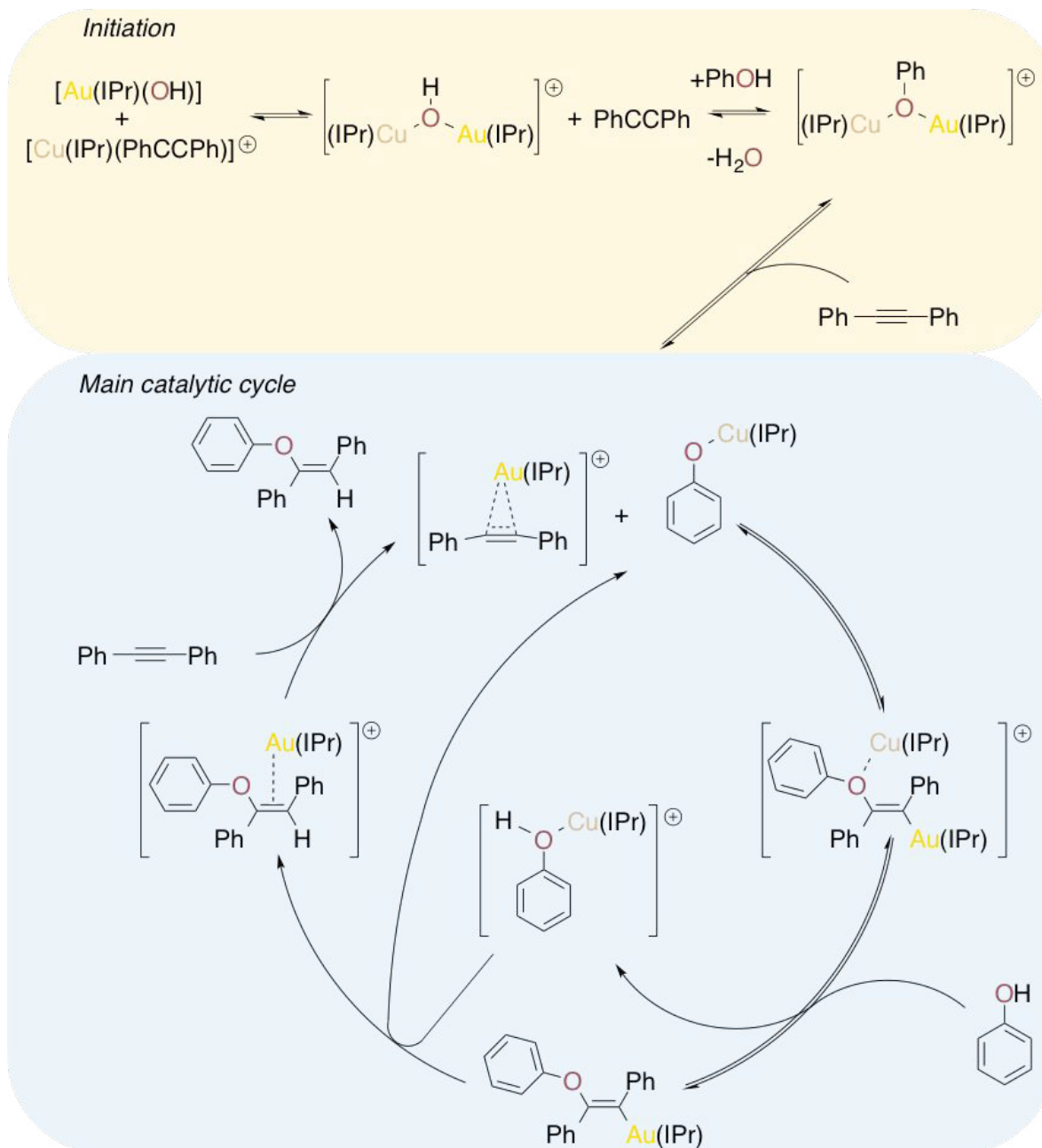
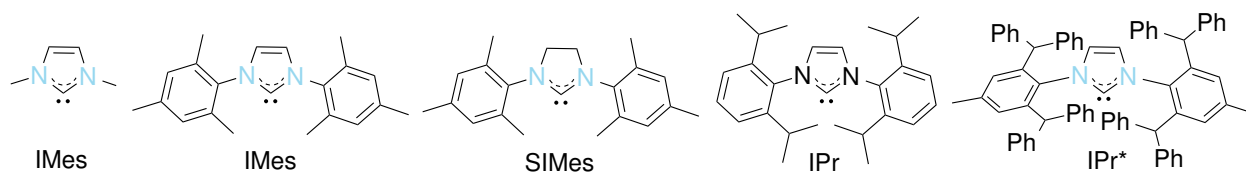


Figure 5.5.3. Catalytic pathway for the hetero-dual-assisted hydrophenoxylation of diphenylacetylene.

5.6. Sterical hindrance effect in the rate-determining step.

At this point, we determined the mechanism for gold and copper catalysts that bear an *N*-heterocyclic carbene like IPr which is relatively highly sterically demanding. To find out how the steric effect of the NHC ligand affects the rate-determining step, we performed the calculations for the rds employing NHCs such as IMes and SIMes, which are less sterically demanding than the IPr ligand. The larger IPr* ligand which is significantly bulkier than IPr (see Scheme 5.6.1) was also included. We found the lowest energy barrier for IMes system which is just 12.5 kcal/mol (see Figure 5.6.1). However, to support the study of the steric effect in rds, we measured the steric hindrance by using the buried volume maps.



Scheme 5.6.1. NHC ligands involved in the steric studies of the rds.

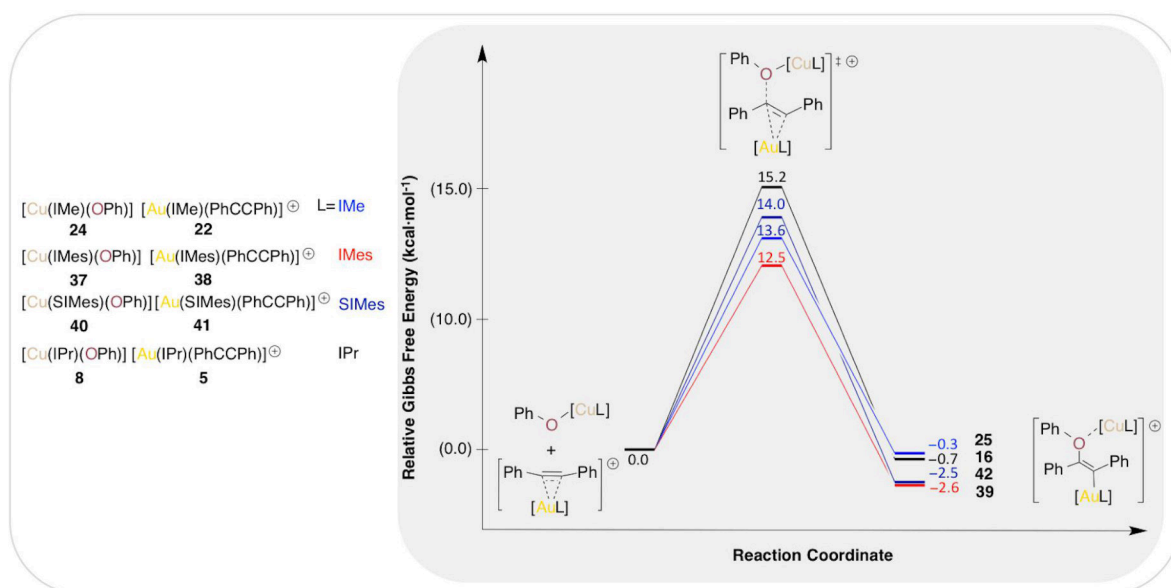


Figure 5.6.1. Rate-determining step for the dual systems: [Cu(IMe)(OPh)]/[Au(IMe)(PhCCh)]⁺ (in medium blue), [Cu(IMes)(OPh)]/[Au(IMes)(PhCCh)]⁺ (in red) and [Cu(SIMes)(OPh)]/[Au(SIMes)(PhCCPh)]⁺ (in midnight blue), to be compared with the corresponding [Cu(IPr)(OPh)]/[Au(IPr)(PhCCPh)]⁺ systems (in black) (Gibbs free energies in solvent are given in kcal/mol).

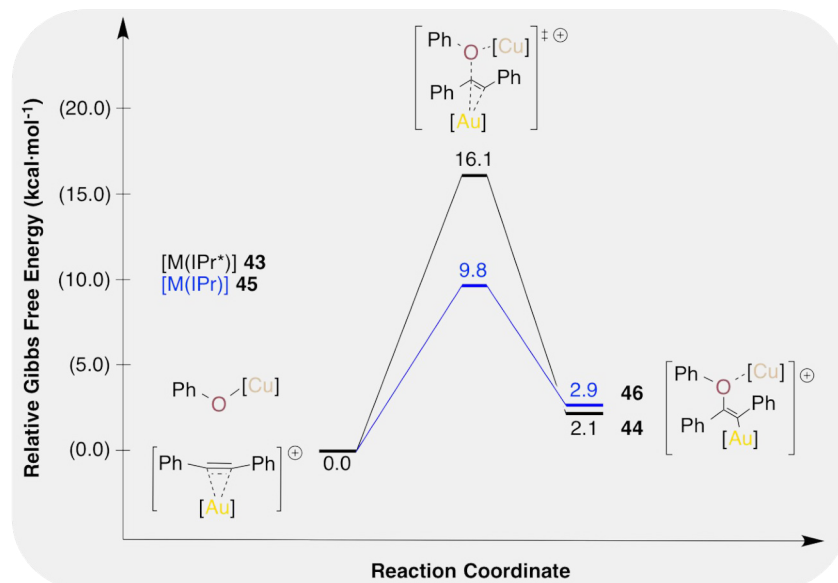


Figure 5.6.2. Rate-determining step for [Cu(IPr*)(OPh)]/[Au(IPr*)(PhCCPh)]⁺ couple (Gibbs free energies in toluene as solvent are given in kcal/mol).

On the other hand, the results obtained for IPr* via ONIOM scheme displayed a higher energy barrier than the IPr system (see Figure 5.6.2). Moreover, due to the obvious larger steric character of IPr* ligand, the intermediate next to the C-O bond formation turned out to be higher in energy as well as the TS. Last results confirm a clear hindrance effect in the rate-determining step, but also the little $\Delta\Delta G^\ddagger$ between each other leads to the guess that electronic characteristics of the catalyst can take part in the reactivity of each moiety.

Additionally, to support the influence of the steric effect in the rate-determining step, we performed the topographic steric maps. To further unravel how the sterical hindrance is important for the C-O bond formation, the simple IMe and the largest IPr* NHC ligands were also studied. As we can see in Figure 30, the steric character and the activation energy in the rds increase as follows: IMes \ll IMe < SIMes \ll IPr < IPr*. This means that the steric character by the catalyst is not the only factor that affects the C-O bond formation. Catalysts bearing highly hindered NHC-ligands can increase or decrease the energy barrier, according to the nucleophilic or electrophilic character of σ - and π -species, respectively.

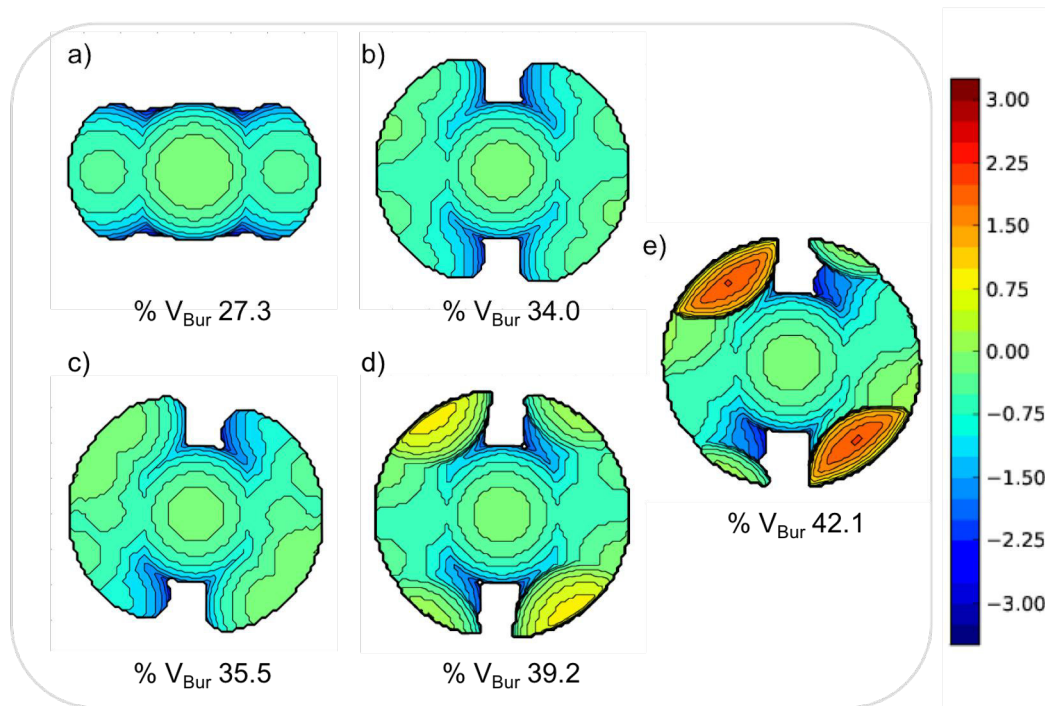


Figure 5.6.3. Topographic steric maps for the NHC ligands included in the gold, copper and silver catalysts: a) IMe; b) IMes; c) SIMes; d) IPr; and e) IPr*. The Au atom is at the origin and the Au-CNHC bond is aligned with the z-axis. The iso-contour curves of the steric maps are given in Å.

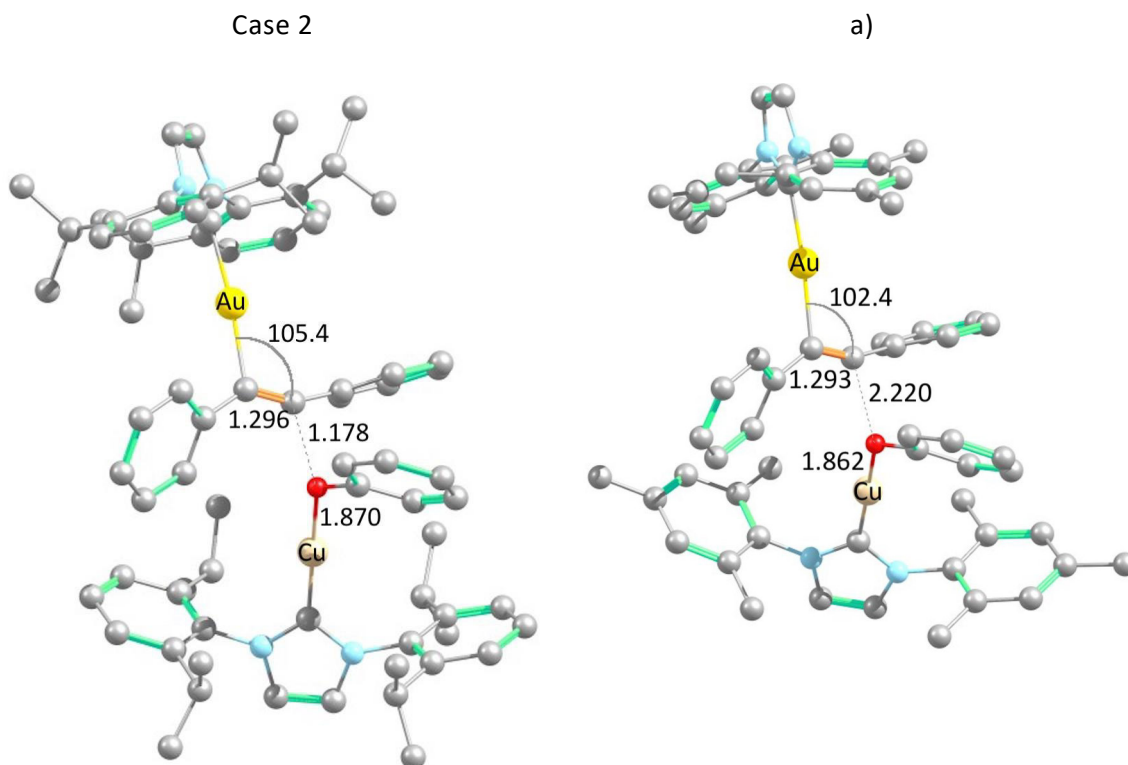
5.7. Comparative structural and electronic data analysis of σ - and π -activated species bearing IMe, IMes, SIMes, IPr and IPr* ligands.

To support the electronic effect by hindered NHC ligands in σ - and π -activated species, we carried out structural and electronic analysis such as: the length of the new formed C-O bond, NBO, MBO, and chemical hardness (η) of each activated moiety. First, in Table 5.7.1 we grouped the MBO data and C-O bond lengths for the intermediates mentioned in Figure 5.7.1. After the analysis of this structural information, we found that the bond strength increases as follows: IMes < IMe < SIMes < IPr. On the other hand, the bond length follows the next pattern: IMe < SIMes < IMes < IPr. As we can see in our results, the steric hindrance on the imidazole ring of the NHC ligand does not have an important impact on the new bond formed.

Table 5.7.1. MBO indexes and C-O bond lengths in the IMes, SIMes, and IMe intermediates (in Å).

Species	MBO (C-O)	d (C-O) (Å)
[Cu(IMes)(OPh)(PhCCPh)(IMes)Au] ⁺	0.785	1.473
[Cu(SIMes)(OPh)(PhCCPh)(SIMes)Au] ⁺	0.789	1.472
[Cu(IMe)(OPh)(PhCCPh)(IMe)Au] ⁺	0.787	1.470

Analyzing the geometries of the transition states shown in Figure 5.7.1, we found that even if the ligands are structurally different, their special arrangement seems to be similar to each other. Alternatively, focusing on the C-O length in the TSs, we found that the most hindered IPr system shows a value of 2.178 Å which is the shortest one regard to the less sterically demanding IMe system which exhibits a C-O distance of 2.219 Å.



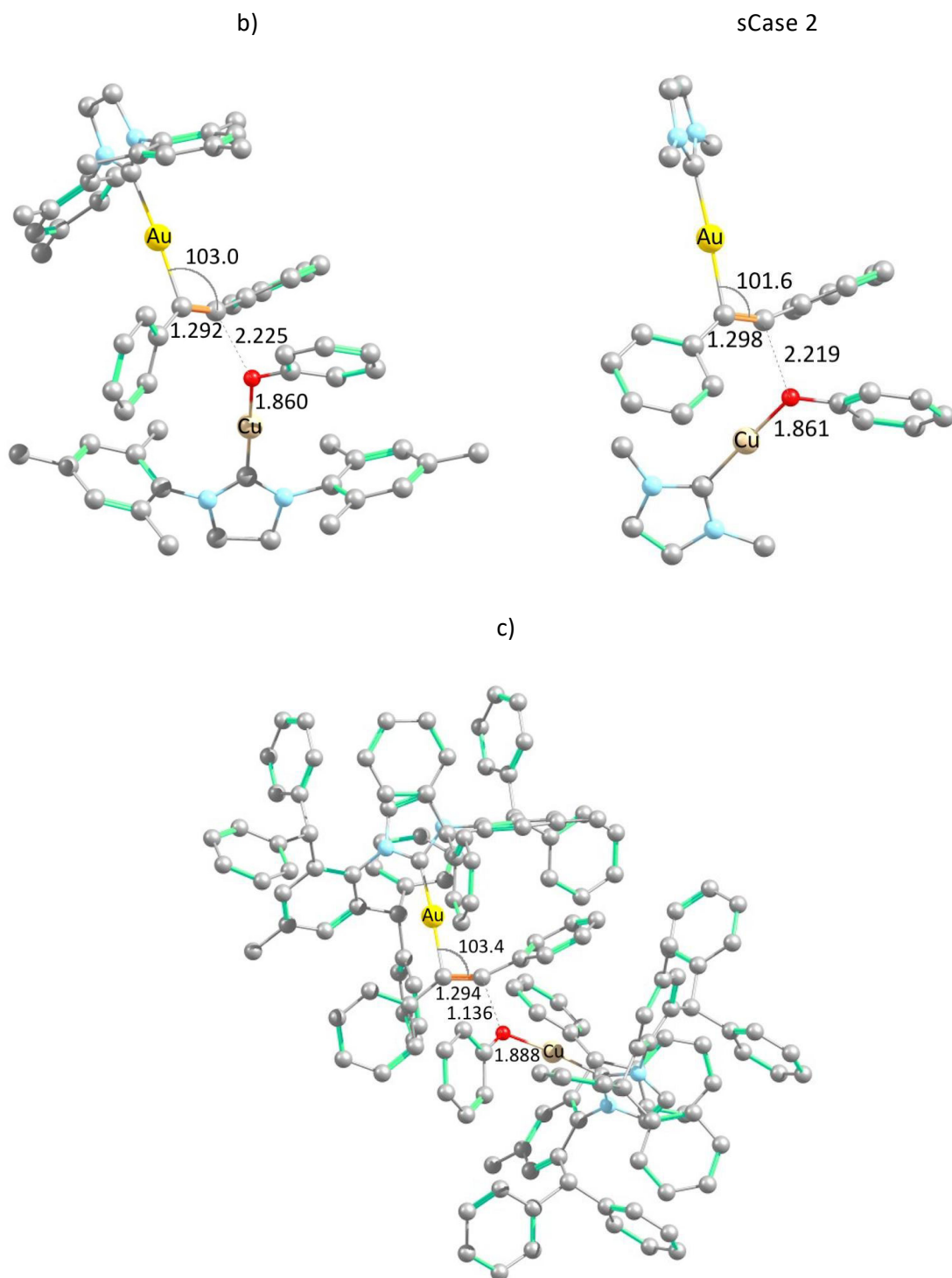


Figure 5.7.1. Molecular structures of the transition states proposed in Figures 5.6.1 and 5.6.2: Case 2, a) $[\text{Cu}(\text{SIMes})(\text{OPh})]/[\text{Au}(\text{SIMes})(\text{PhCCPh})]^+$, b) $[\text{Cu}(\text{IMes})(\text{OPh})]/[\text{Au}(\text{IMes})(\text{PhCCPh})]^+$, sCase 2, and c) $[\text{Cu}(\text{IPr}^*)(\text{OPh})]/[\text{Au}(\text{IPr}^*)(\text{PhCCPh})]^+$ (Hydrogen atoms were omitted for clarity, selected distances are in Å and angles in degrees).

Next, in order to figure out the electronic effects by the ligands, we computed NBO charges (see Table 5.7.2). The results reveal that the oxygen atom in the [Cu(IMes)(OPh)] and [Cu(SIMes)(OPh)] species has a similar nucleophilic character with values of -0.790 and -0.789 respectively. Obviously, these species are less nucleophilic than the [Cu(IPr*)(OPh)] compound which possesses a value of -0.801 . On the other hand, species that share a similar electrophilic character are the [Cu(SIMes)(PhCCPh)] and [Cu(IMe)(PhCCPh)] with a charge of -0.041 in each methinic carbon of the alkyne fragment. Thus, the electrophilic character of methinic carbons in NHC-gold-alkyne species increases as follows: [Au(IPr*)(PhCCPh)]⁺ > [Au(IPr)(PhCCPh)]⁺ > [Au(IMe)(PhCCPh)]⁺, [Au(SIMes)(PhCCPh)]⁺ > [Au(IMes)(PhCCPh)]⁺. Moreover, the analysis of the chemical hardness revealed why the [Cu(IMe)]/[Au(IMe)] system displays an energy barrier (13.6 kcal/mol) 1.1 kcal/mol higher than the [Cu(IMes)]/[Au(IMes)] (12.5 kcal/mol). This is because [Cu(IMe)(OPh)] compound is the second hardest in the NHC series.

Table 5.7.2. NBO charges and chemical hardness for the electrophile-nucleophile couples shown in Figure 5.6.1 and 5.6.2.

Species	NBO (C)	NBO (O)	Chemical hardness (η) in eV
[Cu(IPr*)(OPh)]	---	-0.810	2.01
[Cu(IMes)(OPh)]	---	-0.790	2.04
[Cu(SIMes)(OPh)]	---	-0.789	1.99
[Cu(IMe)(OPh)]	---	-0.757	2.26
[Au(IPr*)(PhCCPh)] ⁺	-0.038	---	2.75
[Au(IMes)(PhCCPh)] ⁺	-0.049	---	3.10
[Au(SIMes)(PhCCPh)] ⁺	-0.041	---	3.13
[Au(IMe)(PhCCPh)] ⁺	-0.041	---	3.02

Electronic data of the IPr* system reveal that copper phenoxide is a better nucleophile than the phenoxide species in IMe, IMes, SIMes and IPr systems, even though this is the second softest. In the case of the [Au(IPr*)]-alkyne species, this is the softest species with the highest nucleophilic character (NBO (O) charge of -0.038) with respect to the nucleophiles shown in Table 5.7.2. Thereby, due to promising results showed by the [M]-IPr* catalytic system, this will be considered for future experimental studies to improve the selectivity of the HPR.

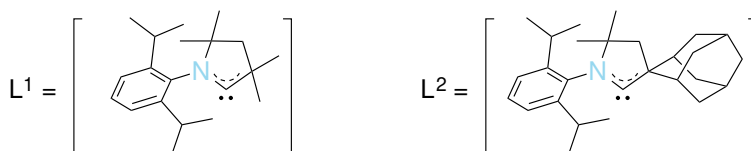
5.8. CAAC ligands as an alternative to NHC species.

In order to design a more efficient hydroalkoxylation reaction taking into account the metal effect studied in previous sections, we focused our efforts in the search of carbene ligands that could become in a good alternative to NHC ligands and allowed us to expand the hero-dual-assisted

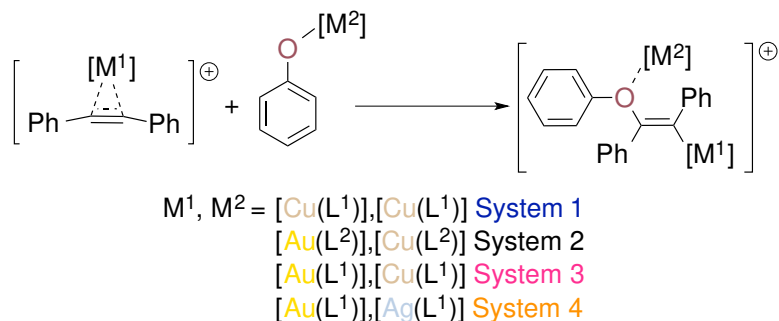
hydroalkoxylation field. Therefore, we proposed the non-symmetric type-CAAC ligands (Pyrrolidinidenes) shown in Scheme 5.8.1 due to their promising features mentioned in Chapter 1, section 1.3.

To study the metal and the ligand effect in hydroalkoxylation reaction (HAR) we proposed the possible nucleophile-electrophile couples shown in Scheme 5.8.2. However, the metal effect in the rate-determining step was studied only in the simple L^1 system. On the other hand, the most hindered ligand L^2 was used to perform the study of the rds only for the copper/gold combination, and so provide the sterical hindrance effect from type-CAAC ligands in the C-O bond formation.

The set of energy profiles for σ - and π -activated species proposed in Scheme 5.8.2 are shown in Figure 5.8.1. This set describes a quite similar behaviour regarding the previous studies. Our results indicate that the metal effect in the rate-determining step assisted by the metal- L^1 catalyst follows the same trend line than the results shown in sections 5.2 and 5.3.



Scheme 5.8.2. Proposed type-CAAC ligands.



Scheme 5.8.1. Possible starting species in hydrophenoxylation assisted by gold-, copper- and silver-CAAC catalysts.

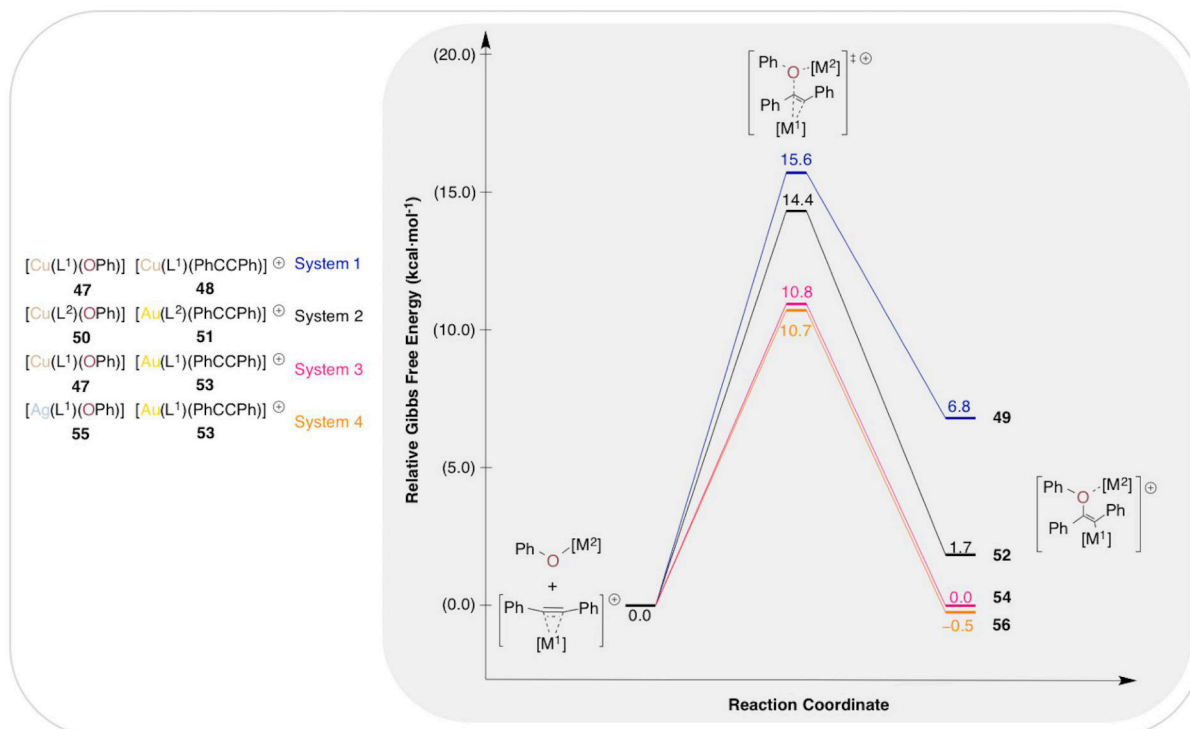


Figure 5.8.1. Comparative study of the rate-determining step for the nucleophile-electrophile couples: in black **50/51**, in pink **47/53**, in blue **47/48**, and in orange **55/53** (Gibbs free energies in solvent are given in kcal/mol).

Thus, these metal-L¹ systems increase in energy as follows: [Ag(L¹)(OPh)]/[Au(L¹)(PhCCPh)]⁺ < [Cu(L¹)(OPh)]/[Au(L¹)(PhCCPh)]⁺ << [Cu(L¹)(OPh)]/[Cu(L¹)(PhCCPh)]⁺. It is important to mention that $\Delta\Delta G^\ddagger$ between Systems 3 and 4 is relatively small (0.1 kcal/mol), so this means that both systems can improve the hydrophenoxylation process. In fact, the energy of the intermediates next to the C-O formation increases in the same way as the energy barriers do. On the other hand, the analysis of System 2 against 3 gave us information about the steric influence in the rds. Since the [Cu(L²)(OPh)]/[Au(L²)(PhCCPh)]⁺ couple displays an energy barrier 3.6 kcal/mol higher than the [Cu(L¹)(OPh)]/[Au(L¹)(PhCCPh)]⁺ pair for the intermediates next to the nucleophilic attack, the $\Delta\Delta G^\ddagger$ found is just 0.5 kcal/mol. This means that both systems seem to be kinetically and thermodynamically competitive, although structurally L² seems to be larger than L¹.

The optimized geometries of the transition states involved in Systems 1–4 are shown in Figure 5.8.1. As it can be noticed, M-C-C angles, C=C bond lengths, and C-O distances in the TSs, resemble each other. The overall bond lengths and angles display a difference no greater than 0.245 Å and 4.2 °, respectively.

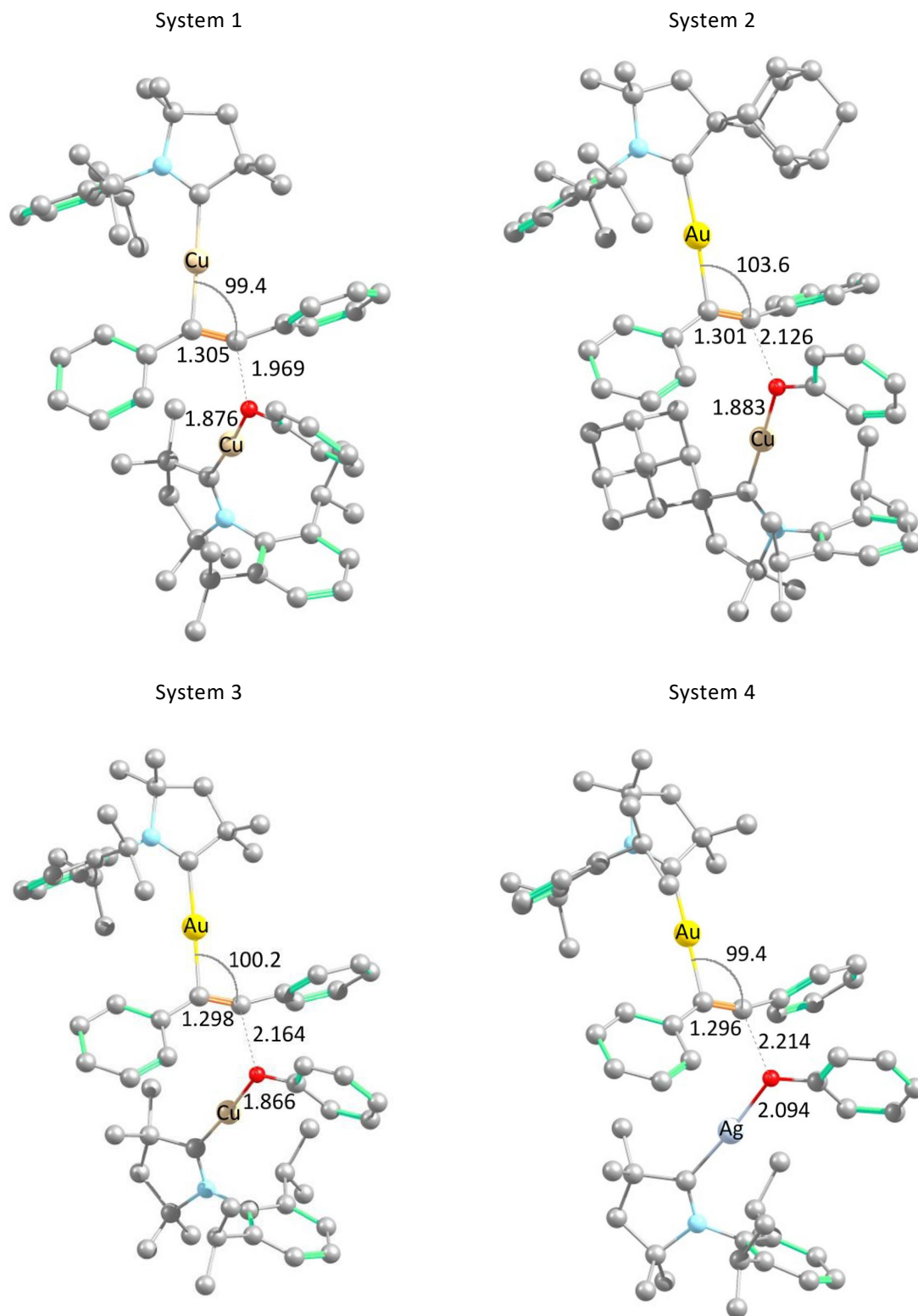


Figure 5.8.2. Molecular structures of the transition states involved in Systems 1–4 (Hydrogen atoms were omitted for a better view, selected distances and angles are given in Å and degrees, respectively).

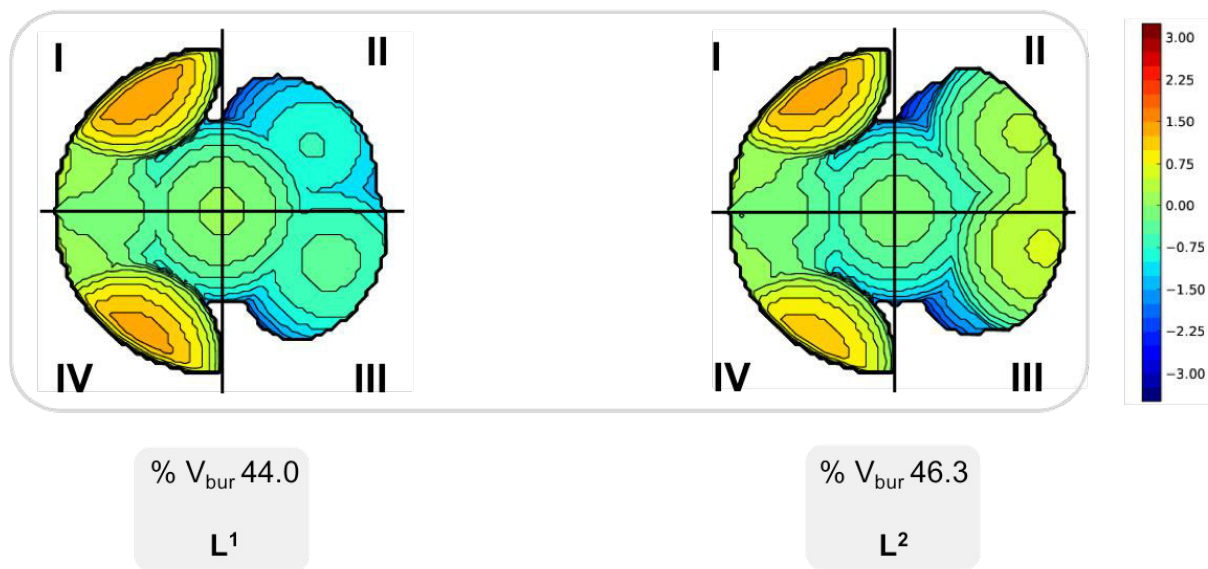


Figure 5.8.3. Topographic steric maps and percentage of volume buried (% V_{bur}) of L^1 and L^2 species (The maps were divided in four quadrants to provide a better explanation. The isocontour curves of the steric maps are given in Å).

On the other hand, to support how the sterical hindrance affects in the formation of the new C-O bond, we plotted the topographic steric maps of L^1 and L^2 in Figure 5.8.3. Moreover, we added their respective percentage of buried volume to facilitate the analysis. From Figure 5.8.3, the steric differences between each CAAC ligand are clearly distinguishable, since the quadrants I and IV are occupied by the aryl group in both graphs. Likewise, the methyl (L^1) and adamantyl (L^2) group are located in quadrants II and III, where we can see a clear difference. In the graph of L^1 this region is dominated by the blue tone. This means that methyl groups are far away from the metal. In the case of L^2 , we can conclude that the most part of adamantyl is closely attached to the metal since the yellow colour dominates in those quadrants, providing a less available region. As a conclusion of this section, due to our arguments and the % V_{bur} , we suggest that L^2 displays a higher steric character than L^1 .

5.9. Structural and electronic data analysis of intermediates, σ - and π -activated species in hetero-dual-assisted catalysis involving type-CAAC ligands.

Table 5.9.1 shows the MBOs and bond lengths of the C-O bond formed in the intermediates generated in Systems 1–4 (see Figure 5.8.1). On the one hand, the C-O bond length values display a negligible variation in all the species. On the other hand, the Mayer Bond Orders totally fit in the stability trend, so the most stable compound exhibits the largest MBO value (0.826), and the less stable displays the smallest one (0.757). In summary, the stability and the C-O bond strength of the intermediates increase as follow: $[\text{Cu}(\text{L}^1)(\text{OPh})(\text{PhCCPh})(\text{L}^1)\text{Cu}]^+$ (System 1) > $[\text{Cu}(\text{L}^2)(\text{OPh})(\text{PhCCPh})(\text{L}^2)\text{Au}]^+$ (System 2) > $[\text{Cu}(\text{L}^1)(\text{OPh})(\text{PhCCPh})(\text{L}^1)\text{Au}]^+$ (System 4) > $[\text{Ag}(\text{L}^1)(\text{OPh})(\text{PhCCPh})(\text{L}^1)\text{Au}]^+$ (System 4).

Table 5.9.1. Mayer bond orders and C-O bond length for the intermediates generated in Systems 1–4 (see Figure 5.8.1).

Species	MBO (C-O)	d (C-O) (Å)
$[\text{Cu}(\text{L}^1)(\text{OPh})(\text{PhCCPh})(\text{L}^1)\text{Cu}]^+$	0.757	1.484
$[\text{Cu}(\text{L}^2)(\text{OPh})(\text{PhCCPh})(\text{L}^2)\text{Au}]^+$	0.786	1.476
$[\text{Cu}(\text{L}^1)(\text{OPh})(\text{PhCCPh})(\text{L}^1)\text{Au}]^+$	0.790	1.476
$[\text{Ag}(\text{L}^1)(\text{OPh})(\text{PhCCPh})(\text{L}^1)\text{Au}]^+$	0.826	1.466

In addition, Table 5.9.2 shows the structural data for the studied metal-alkyne species. Mayer Bond Orders for metal-carbon bonds reveal that copper- L_1 catalyst interacts more strongly with the alkyne species than gold- L_1 and gold- L_2 compounds. This means that copper catalysts activate alkyne compounds efficiently. According to this, we should observe a low energy barrier, but instead we observed the opposite behavior. On the other hand, C-C bond length in π -compounds did not help us to clarify some aspects about their reactivity. Unfortunately, the alkynic moieties do not display any significant variation in C-C bond length.

Table 5.9.2. Structural data for [M]-alkyne species: C-C bond lengths and MBO indexes for metal-carbon (M-C) bonds.

Species	MBO (C-M)	d (C≡C) (Å)
$[\text{Au}(\text{L}^1)(\text{PhCCPh})]^+$	0.42	1.27
$[\text{Cu}(\text{L}^1)(\text{PhCCPh})]^+$	0.60, 0.52	1.26
$[\text{Au}(\text{L}^2)(\text{PhCCPh})]^+$	0.42, 0.45	1.27

Table 5.9.3. NBO charges and chemical hardness for the electrophile-nucleophile couples.

Species	NBO (C)	NBO (O)	Chemical hardness (η) in eV
[Au(L ¹)(PhCCPh)] ⁺	0.009, -0.096	---	3.07
[Cu(L ¹)(PhCCPh)] ⁺	-0.041, -0.113	---	2.99
[Au(L ²)(PhCCPh)] ⁺	0.007, -0.094	---	3.05
[Cu(L ¹)(OPh)]	---	-0.785	1.58
[Ag(L ¹)(OPh)]	---	-0.753	1.38
[Cu(L ²)(OPh)]	---	-0.783	1.55

To establish a clear conclusion about why the [Cu(L¹)(PhCCPh)]⁺/[Cu(L¹)(OPh)] couple displays a higher energy barrier, we need to analyze the NBO charges and chemical hardness (η) of the σ - and π -species studied in this section (see Table 5.9.3). As a first step, we need to look at the NBO charges of alkyne carbons in [Au]-alkyne compounds. These display a more electrophilic character than carbons attached to copper because their charges are more positive than copper's ones. On the other hand, the chemical hardness analysis reveals that the π -activated species exhibit a similar chemical hardness value. In addition, [Au]-alkyne species are still the best nucleophiles in the hetero-metal-catalyzed hydrophenoxylation reaction.

On the other hand, to determine the nucleophilic character of the metal-phenoxides, we need to analyze the oxygen charge and chemical hardness of these species. However, the analysis of the NBO charge in oxygen shows that [Ag(L¹)(OPh)] species is not better nucleophile than [Cu(L¹ or L²)(OPh)]. This is because of the oxygen in silver-phenoxide exhibits the most positive charge. In the case of chemical hardness analysis, it revealed that [Cu(L¹)(OPh)] and [Cu(L²)(OPh)] species are equally hard, but silver-phenoxide turned out to be the softest one. Once done this analysis, we can conclude that copper- and silver-phenoxide are capable to carry out the nucleophilic attack in a successful manner, as we observed in System 3 where the energy barrier and intermediate are energetically similar to System 4. In conclusion, the hetero-dual catalysis is the best synthetic strategy to successfully achieve the hydrophenoxylation process. Both copper- and silver-CAAC catalysts are good nucleophiles even when non-symmetric CAAC ligands replace NHCs.

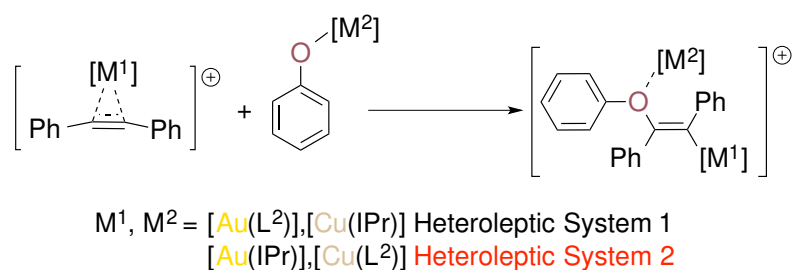
5.10. Hetero-dual and heteroleptic catalysis: in the way to find out a novel technique to catalyze the hydrophenoxylation process.

In this thesis, we studied the metal and the ligand effect in the rds. This was done through the exchange of metal cores and replacing NHC ligands by CAACs in pre-activated species. Fortunately, we obtained interesting results that could be experimentally tested. The well-studied behavior of the σ - and π -activated species allowed us to think about a hetero-dual system bearing the IPr and

L^2 ligands. Thus, now we have to think about the million dollar question: Which pair could be the best one: $[Au(L^2)(PhCCPh)]^+/[Cu(IPr)(OPh)]$ or $[Au(IPr)(PhCCPh)]^+/[Cu(L^2)(OPh)]$? Luckily, we can have a prediction according to the previous information and the last studies, which is that the second couple has the real chance to improve the addition of phenol to diphenyl acetylene. Thereby, to support our last assumption, we performed a computational study for both nucleophile-electrophile couples shown in Scheme 5.10.1.

Figure 5.10.1 shows the mechanistic study of the Heteroleptic Systems 1 and 2. The $[Au(IPr)(PhCCPh)]^+/[Cu(L^2)(OPh)]$ couple rocks down the energy barrier providing a barrier with only 7.3 kcal/mol. Furthermore, the intermediate next to the nucleophilic attack displayed a $\Delta\Delta G$ of 8.4 kcal/mol. This means that the nucleophilic attack assisted by $[Cu(L^2)]/[Au(IPr)]$ catalysts is kinetically and thermodynamically favoured over the previous couple catalysts. On the other hand, Heteroleptic System 1 displayed a low energy barrier regarding systems bearing IPr^*/IPr^* , IPr/IPr , $SIMes/SIMes$, and IMe/IMe ligand combinations, but equally competitive facing to the $IMes/IMes$ and L^1/L^1 systems. Thus, our prediction about Heteroleptic System 2 was right. With these awesome results, we dare to propose the $Cu-L^2/Au-IPr$ catalysis as the most efficient system.

The optimized structures of the transition states in Heteroleptic Systems 1 and 2 are shown in Figure 5.10.2. We observed in the geometries that the Au-C-C angles displayed similar values of 104.2 and 103.0 ° for the Systems 1 and 2, respectively. Moreover, the C=C bond length in both structures is quite similar also (1.304 and 1.291 Å, respectively). On the other hand, the C-O distance in the TSs is affected by the size of the ligand, so this distance in the TS of the Heteroleptic System 2 is 0.209 Å larger than the distance in the TS of the Heteroleptic System 1. Nevertheless, this interesting finding points out about the role of the steric effect in the rds.



Scheme 5.10.1. Electrophile-nucleophile couples in the hetero-dual and heteroleptic catalysis.

Results and discussion

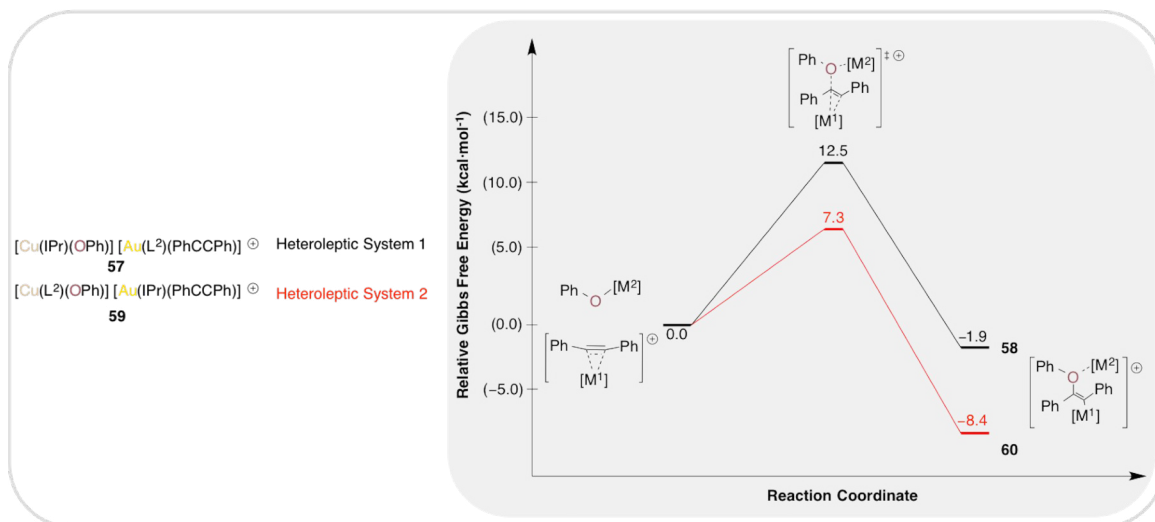


Figure 5.10.1. Energy profiles of the rate-determining step for the nucleophile-electrophile couples: in black **55**, in red **57** (Gibbs free energies in solvent are given in kcal/mol).

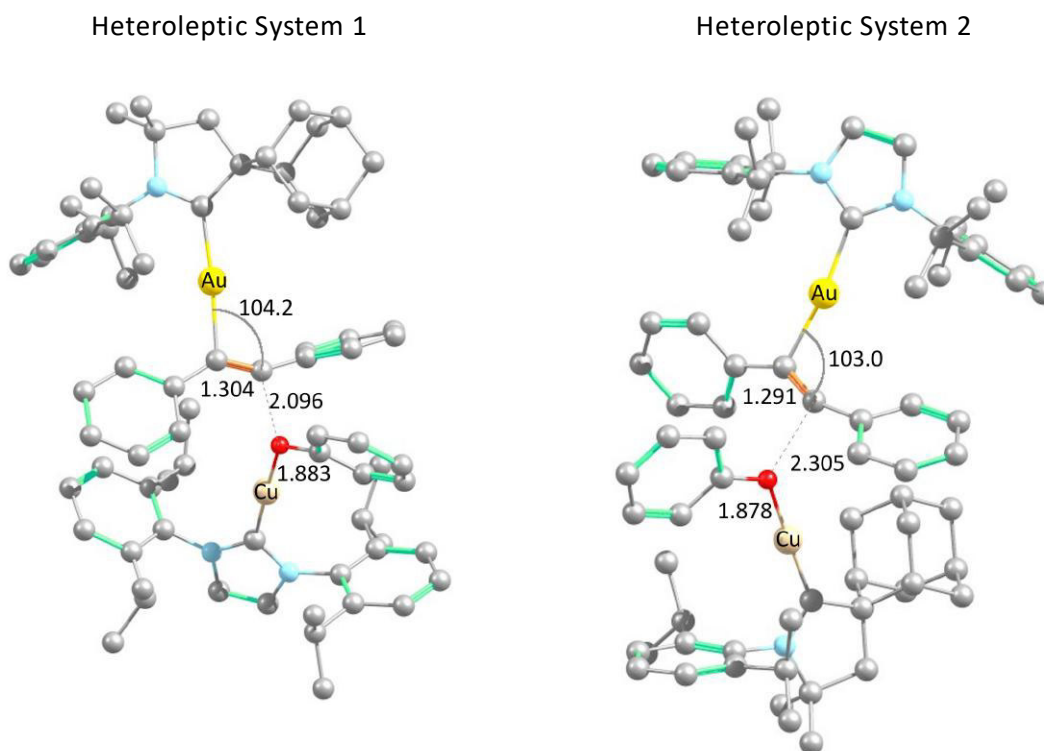


Figure 5.10.2. Molecular structures of the transition states in Heteroleptic Systems 1 and 2 (Hydrogen atoms were omitted for clarity, selected distances and angles are given in Å and degrees, respectively).

Table 5.10.1. Mayer bond orders and C-O bond lengths for the intermediates generated in the hetero-dual and heteroleptic cases shown in Figure 5.10.1.

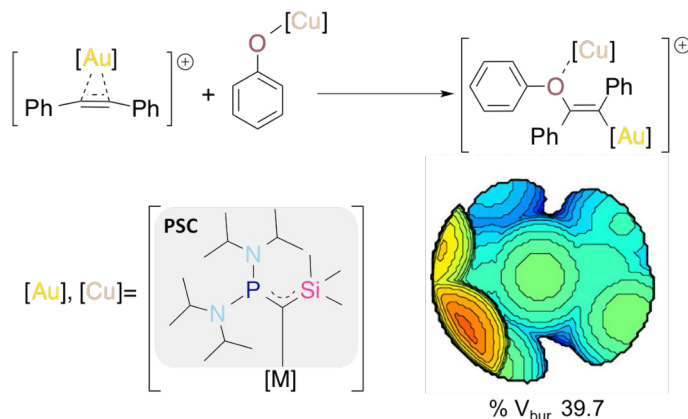
Species	MBO (C-O)	d (C-O) (Å)
[Cu(IPr)(OPh)(PhCCPh)(L ²)Au] ⁺	0.786	1.476
[Cu(L ²)(OPh)(PhCCPh)(IPr)Cu] ⁺	0.790	1.476

Finally, Table 5.10.1 shows the MBO values and C-O bond lengths of the intermediates involved in the Heteroleptic Systems 1 and 2. The C-O bond distance is the same for both species. Moreover, MBO analysis displayed a minor difference between each other, the most stable exhibited the largest value, and the less stable, the smallest one. As we can notice, the stability of the intermediates is totally related to MBO values, which is completely logical, as the most stable species must have the strongest bond (large MBO value).

In summary, this study has provided substantial evidence to support that CAAC-type ligands NHCs, but also the combination of both species in hetero-dual-assisted hydrophenoxylation reaction, can improve and become the most cost-efficient process. Moreover, our last results open the gate to a novel catalytic system capable to carry out the hetero-dual activation in an efficient manner, like improving a chemical process such as the hydroamination of unsaturated species, for instance.

5.11. In the searching of the perfect carbene ligand: Study of type *push-pull* carbenes in the hetero-dual-assisted hydrophenoxylation process.

Previously, we had to deal with *push-push* carbenes, but we asked ourselves, how does the nature of the ligand can affect to the nucleophilic attack? To answer this question, we proposed the study of the rds involving the non-cyclic *push-pull* carbene shown in Scheme 5.11.1. However, PSC species ([bis(diisopropylamine)phosphanyl](trimethylsilyl)carbene) are structurally and electronically different to NHCs and CAACs, for which the results obtained by using this push-pull carbene could be pretty exciting.



Scheme 5.11.1. Electrophile-nucleophile couple in the hetero-dual catalysis involving the PSC ligand instead of CAACs and NHCs.

The study of the rds in the HAP involving the PSC ligand is illustrated in Figure 5.11.1. After analyzing all the NHC and CAAC systems studied in previous sections, we observed that PSC ligand can serve as alternative ligand to the previous species. Since the **61/62** couple displayed a small energy barrier of only 11.8 kcal/mol, this result turns out the nucleophilic attack in the HAR assisted metal-PSC catalyst in a thermodynamically favored process. On the other hand, the NA does not seem to be totally favored in the kinetic sense, since the phenoxyated-alkyne species **63** is 2.6 kcal/mol higher in energy over the starting species, but this does not mean that the process will not proceed since the energy barrier is still low. The next question is, what does make special the metal-PSC species?

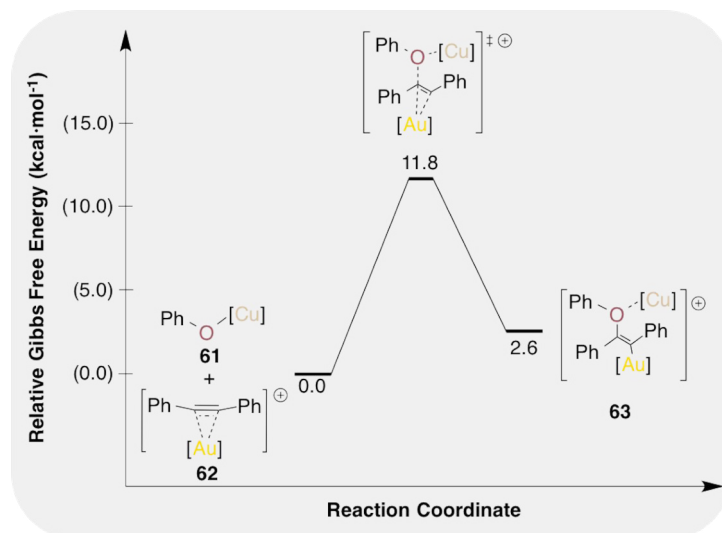
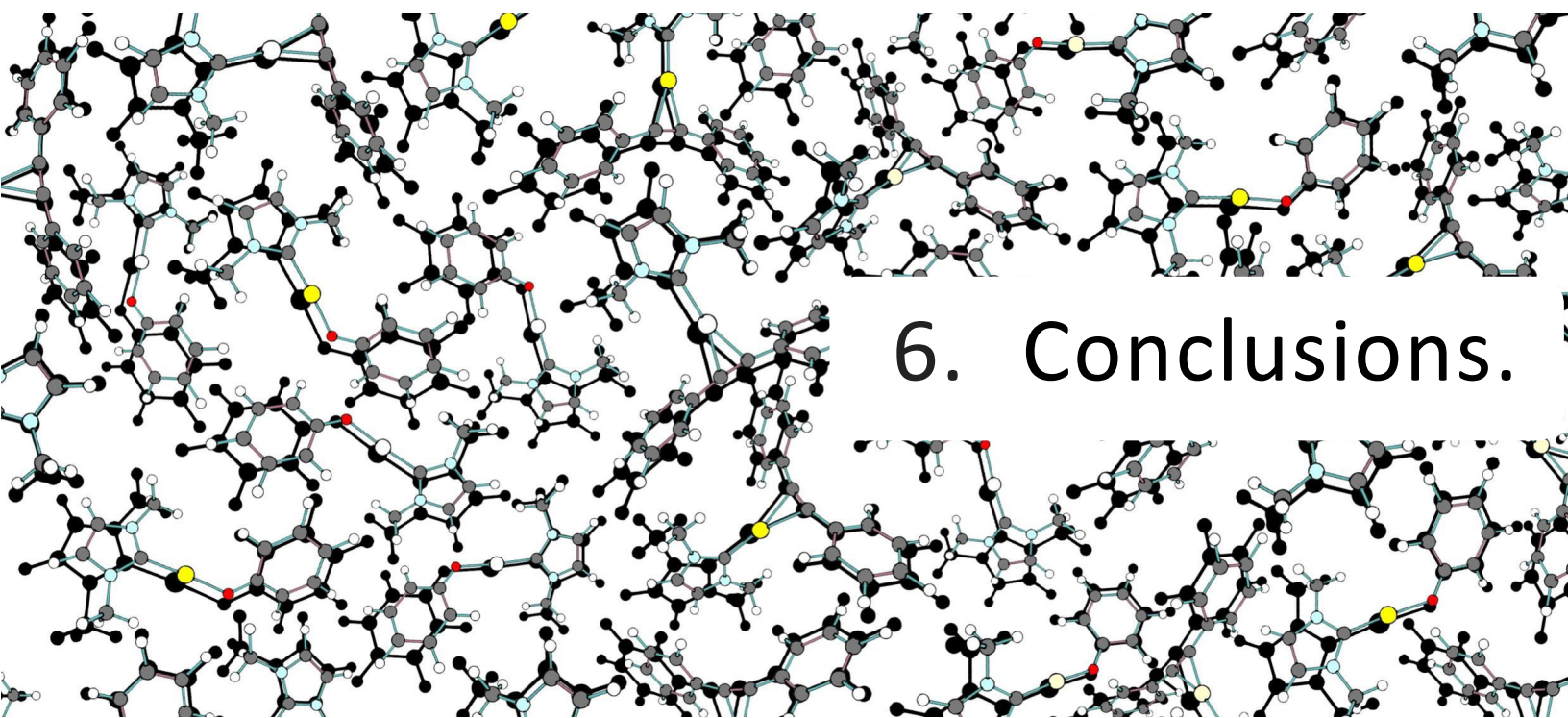


Figure 5.11.1. Energy profile of the rate-determining step for the nucleophile-electrophile couples bearing the PSC ligand in Scheme 5.11.1.

To answer the last question, we had to appeal to the electronic and structural analysis. Thus, the species **62** displayed a C≡C bond distance of 1.270 Å, which is a value quite similar to the previous values found in CAAC and NHC systems, but also the Mayer Bond Order for M-C bond (0.476, 0.487). Also, NBO analysis displayed charges with values of -0.043 and -0.047. This means that one carbon is more electrophilic than the other (the carbon with the less negative charge). It is worthy to be mentioned that the non-homogeneity in MBOs and NBOs is because the non-symmetric feature from the PSC ligand, however, this behavior was also observed in CAAC systems. On the other hand, the **62** species turned out to be softer (2.52 eV) than **5**, so that is why PSC would be a good ligand. In the case of species **61**, this one displayed a similar NBO charge (-0.784) in the oxygen atom to previous copper-phenoxides and the lowest chemical hardness (1.19 eV) regarding the copper-phenoxides in CAAC and NHC systems.



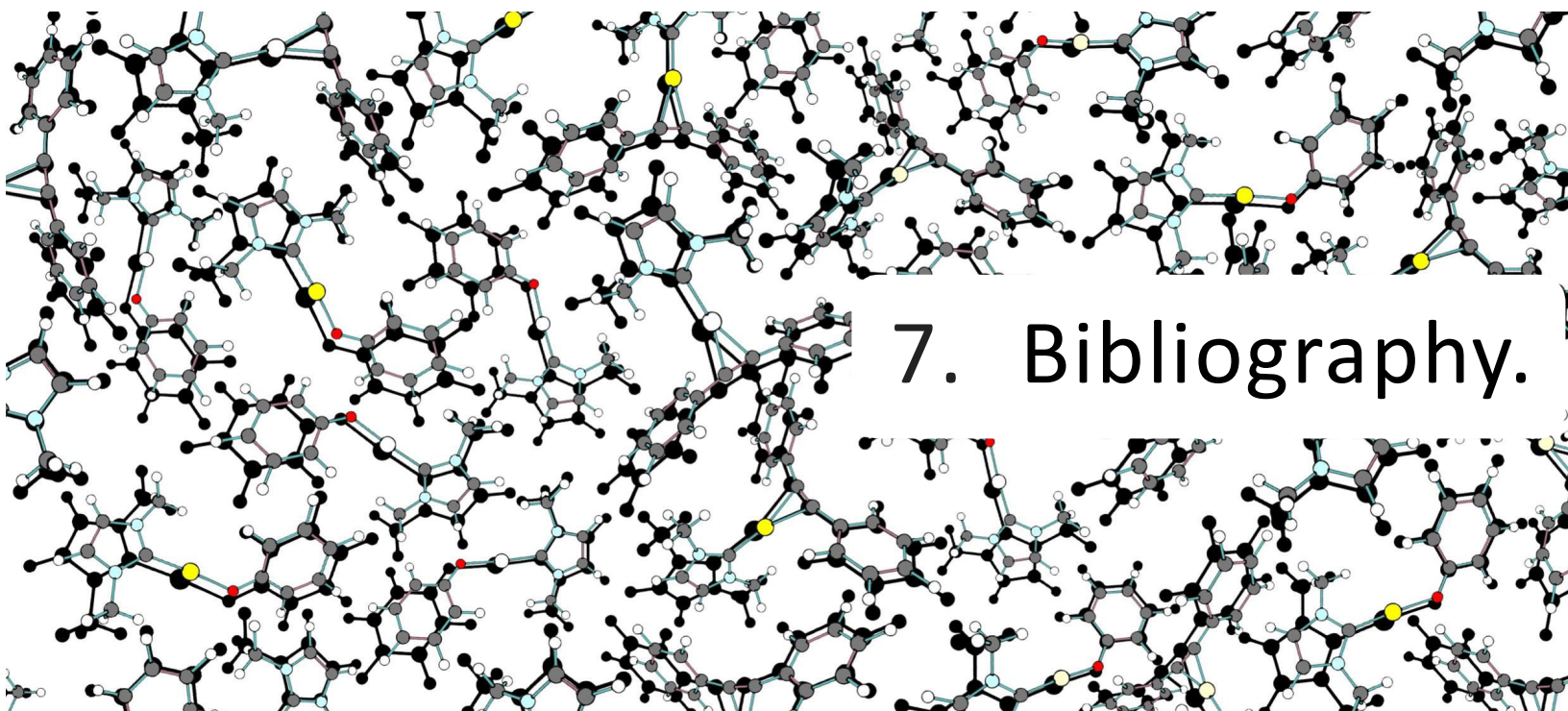
To support and explain the improvement of the hydrophenoxylation reaction assisted by gold-copper catalysis, we focused on the C-O bond formation that was proposed as rds by Poater *et al.* The computational studies performed in this work revealed that the [Au(IPr)]-OPh species exhibits less nucleophilic character and higher chemical hardness than the [Cu(IPr)]-OPh compound, which turned out to be the best nucleophile regarding to the gold-phenoxide compound. On the other hand, when the alkyne compound is attached to the gold-NHC catalyst, this acquires a higher electrophilic character than the alkynic fragment in the copper-alkyne species. This information allowed us to propose the copper-phenoxide and gold-alkyne species as the responsible compounds of the improvement observed in the experimental report. Moreover, these computational data provided us the information to compute the mechanism of the hetero-dual-assisted process, where the energy barrier for the rate-determining step is lower than the homo-dual mechanism reported. This turns out the heterobimetallic-assisted hydrophenoxylation reaction a cost-effective synthetic strategy to access to vinyl ether compounds.

Additionally, the rds was studied for hetero-metallic catalytic species bearing less hindered ligands to find out the role of steric effects in the C-O bond formation. Low sterically demanding systems involving IMes (12.5 kcal/mol) and SIMes (14.0 kcal/mol) ligands display lower energy barriers in the rds than the IPr system (15.2 kcal/mol). These results provide us valuable information to identify the nucleophilic attack as a steric-sensitive step. Moreover, exploring the reactivity of the metal, we performed the DFT studies for silver instead of copper and gold finding that the [Ag(NHC)(OPh)] species react more efficiently with the [Au(NHC)(PhCCPh)] compound than with the [Cu(NHC)(OPh)], improving the energy barrier of the Cu/Au case.

In the search of the best bimetallic catalysis, we focused our efforts in alternative ligands to NHCs. Thus, CAAC ligands turned out to be good candidates because the catalyst attached to them can catalyze the addition of amines to unsaturated hydrocarbons, and so, we proposed two non-symmetric CAAC ligands L^1 and L^2 , where the first one ($\%V_{bur} = 44.0$) is smaller than the second one ($\%V_{bur} = 46.3$). It is worth to mention that we only studied the metal effect in the rds for the hetero-dual catalysis involving L^1 . These results confirmed that [Cu(L^1)(OPh)] and [Ag(L^1)(OPh)] species are the best nucleophiles to react with the [Au(L^1)(PhCCPh)] moiety, even when these hetero-dual systems displayed energy barriers of only 10.8 and 10.7 kcal/mol, respectively. On the other hand, the analysis of the rds involving the large ligand L^2 in [Cu]/[Au] catalysis showed that the nucleophilic attack is quite sensitive to hindered species, as we observe an energy barrier 3.6 kcal/mol higher than the hetero-dual system that includes L^1 . In fact, the stability of the intermediates next to the nucleophilic attack was also affected by the steric hindrance, so the most stable species belongs to the system bearing L^1 .

Conclusions

Once we studied the NHC and CAAC ligands in the HRA, we appealed to perform the computational study of the rds by using Push-Pull-type carbenes instead of the Push-Push-type ones. The results obtained show that these kind of species, in conjunction with the metal core, can act well enough as catalyst of the HPR as the energy barrier (11.8 kcal/mol) of the rds turned out to be one of the lowest barriers. In addition, the DFT studies provided valuable information to support the hetero-bimetallic assistance of copper or silver and gold catalyst in the HRA. It also allowed us to amplify the hetero-dual catalysis through the introduction of the silver and copper phenoxide moiety as part of the best catalyst in this field. Moreover, the improvement of the rds can be achieved using CAAC-type and PSC ligands instead of NHCs.



7. Bibliography.

Bibliography

1. Kenly, S. J. "Encyclopaedia of Catalysis". *John Wiley and Sons, Inc.* (2010), 1–30.
2. Sabatier, P. *Ind. Eng. Chem.* 18(1926), 1005–1008.
3. American Chemical Society National Historic Chemical Landmarks. The Houdry Process for Catalytic Cracking. <http://www.acs.org/content/acs/en/education/whatischemistry/landmarks/houdry.html> (accessed May 23th, 2017).
4. Spitz, P. H. *Petrochemicals: "The Rise of an Industry"*. *John Wiley and Sons, Inc.* New York. (1988), 184–191.
5. Worthy, W. *Chem. Eng. News* 36 (Feb. 19, 1979).
6. Weirsselmel, K., and Arpe, H. J. "Industrial Organic Chemistry". Ed. 3rd (1997), 218.
7. <http://www.dupont.com/corporate-functions/our-company/dupont-history.html> (accessed May 24th, 2017).
8. Schröder, G. "Ullmann's Encyclopaedia of Industrial Chemistry". *John Wiley and Sons, Inc.* 28(2012), 481–485.
9. Okimoto, Y., Sakaguchi, S., and Ishii, Y. *J. Am. Chem. Soc.* 124(2002), 1590–1591.
10. Bosch, M., and Schlaf, M. *J. Org. Chem.* 68(2003), 5225–5227.
11. Nakamura, A.; Tokunaga, M. *Tetrahedron Lett.* 49(2008), 3729–3732.
12. Charbonnier, F., Moyano, A., and Green, A. *J. Org. Chem.* 52(1987), 2303–2306.
13. Sageot, O., Monteux, D., Langlois, Y. *Tetrahedron Lett.* 37(1996), 7019–7022.
14. Aloui, M., Chambers, D. J., Cumpstey, I., Fairbanks, A. J., Redgrave, A. J., and Seward, C. M. *P. Chem. Eur. J.* 8(2002), 2608–2621.
15. Crivello, J. V., and Kong, S. *J. Org. Chem.* 63(1998), 6745–6748.
16. Roche, C., Delair, P., and Greene, A. E. *Org. Lett.* 5(2003), 1741–1744.
17. Mizuno, K., Kimura, Y., and Otsuji, Y. *Synthesis* (1979), 688–689.
18. Hiersemann, M. *Synthesis* (2000), 1279–1290.
19. Park, H. G., Kim, D. H., Yoo, M. S., Park, M. K., and Jew, S. S. *Tetrahedron Lett.* 41(2000), 4579–4582.
20. Maeda, K., Shinokubo, H., Oshima, K., and Utimoto, K. *J. Org. Chem.* 61(1996), 2262–2263.
21. Sabitha, G., Reddy, M. M., Srinivas, D., and Yadav, J. S. *Tetrahedron Lett.* 40(1999), 165–166.
22. Kulkarni, M., Dhondge, A., Borhade, A., Gaikwad, D., Chavhan, S., Shaikh, Y., Nigdale, V., Desai, M., Birhade, D., and Shinde, M. *Eur. J. Org. Chem.* (2009), 3875–3877.
23. Surprenant, S., Chan, W. Y., and Berthelette, C. *Org. Lett.* 5(2003), 4851–4854.
24. Alcazar, E., Pletcher, J. M., and McDonald, F. E. *Org. Lett.* 6(2004), 3877–3880.
25. Danishefsky, S. J.; DeNinno, M. P.; and Chen, S. *J. Am. Chem. Soc.* 110(1988), 3929–3940.
26. Wan, Z., Jones, C. D., Koenig, T. M., Pu, Y. J., and Mitchell, D. *Tetrahedron Lett.* 44(2003), 8257–8259.
27. Shade, R. E., Hyde, A. M., Olsen, J.-C., and Merlic, C. A. *J. Am. Chem. Soc.* 132(2010), 1202–1203.
28. Arduengo, A. J., and Bertrand, G. *Chem. Rev.* 109(2009), 3209–3210.
29. Igau, A., Grutzmacher, H., Baceiredo, A., and Bertrand, G. *J. Am. Chem. Soc.* 110(1988), 6463–6466.
30. Arduengo, A. J., III, Harlow, R. L., and Kline, M. *J. Am. Chem. Soc.* 113(1991), 361–363.
31. Bourissou, D., Guerret, O., Gabbai, F. P., and Bertrand, G. *Chem. Rev.* 100(2000), 39–91.
32. Dröge, T., and Glorius, F. *Angew. Chem. Int. Ed.* 49(2010), 6940–6952.
33. Díez-González, S., Marion, N., and Nolan, S. P. *Chem. Rev.* 109(2009), 3612–3676.
34. Marion, N., Díez-González, S., and Nolan, S. P. *Angew. Chem. Int. Ed.* 46(2007), 2988–3000.
35. Dhudshia, B., and Thadani, A. N. *Chem. Commun.* (2006), 668–670.
36. César, V., Lugan, N., and Lavigne, G. *Eur. J. Inorg. Chem.* (2010), 361–365.
37. Blake, G. A., Moerdyk, J. P., and Bielawski, C. W. *Organomet.* 31(2012), 3373–3378.
38. Martin, D., Baceiredo, A., Gornitzka, H., Schöllner, W. W., and Bertrand, G. *Angew. Chem. Int. Ed.* 44(2005), 1700–1703.

Bibliography

39. Merceron, N., Miqueu, K., Baceiredo, A., and Bertrand, G. *J. Am. Chem. Soc.* 124(2002), 6806–6807.
40. Lavallo, V., Canac, Y., Donnadiou, B., Schoeller, W. W., and Bertrand, G. *Science* 312(2006), 722–724.
41. Alder, R. W., Butts, C. P., and Orpen, A. G. *J. Am. Chem. Soc.* 120(1998), 11526–11527.
42. Igau, A., Griitzmacher, H., Baceiredo, A., and Bertrand, G. *J. Am. Chem. Soc.* 110(1988) 6463–6466.
43. Lavallo, V., Mafhouz, J., Canac, Y., Donnadiou, B., Schoeller, W. W., and Bertrand, G. *J. Am. Chem. Soc.* 126(2004), 8670–8671.
44. Merceron-Saffon, N., Baceiredo, A., Gornitzka, H., and Bertrand, G. *Science* 301(2003), 1223–1225.
45. Soleilhavoup, M., Baceiredo, A., Treutler, O., Ahlrichs, R., Nieger, M., and Bertrand, G. *J. Am. Chem. Soc.* 114(1992), 10959–10961.
46. Kaur, H., Kauer, F. Z., Stevens, E. D., and Nolan, S. P. *Organomet.* 23(2004), 1157–1160.
47. Kuhl, S., Schneider, R., and Fort, Y. *Organomet.* 22(2003), 4184–4186.
48. Gnanamgari, D., Moores, A., Rajaseenlan, E., and Crabtree, R. H. *Organomet.* 26(2007), 1226–1230.
49. Kantchev, E. A. B., O'Brien, C. J., and Organ, M.G. *Angew. Chem. Int. Ed.* 46(2007), 2768–2813.
50. Fortman, G. C., and Nolan, S. P. *Chem. Soc. Rev.* 40(2011), 5151–5169.
51. Valente, C., Çalimsiz, S., Hoi, K. H., Mallik, D., Sayah, M., and Organ, M. G. *Angew. Chem. Int. Ed.* 51(2012), 3314–3332.
52. Samojs, C., Bieniek, M., and Grela, K. *Chem. Rev.* 109(2009), 3708–3742.
53. Vougioukalakis, G. C., and Grubs, R. H. *Chem. Rev.* 110(2010), 1746–1787.
54. Herrmann, W. A. *Angew. Chem. Int. Ed.* 41(2002), 1290–1309.
55. Melaimi, M., Jazzar, R., Soleilhavoup, M., and Bertrand, G. *Angew. Chem. Int. Ed.* 56(2017), 10046–10068.
56. Benitez, D., Shapiro, N. D. Tkatchouk, E., Wang, Y., Goddard III, W. A., and Toste, F. D. *Nat. Chem.* 1(2009), 482–486.
57. Gorin, D. J., and Toste, F. D. *Nature* 446(2007), 395–403.
58. McDonald, F. E. *Chem. Eur. J.* 5(1999), 3103–3106.
59. McDonald, F. E., and Reddy, K. S. J. *Organomet. Chem.* 617(2001), 444–452.
60. Wipf, P., and Graham, T. H. *J. Org. Chem.* 68(2003), 8798–8807.
61. Trost, B. M., and Rhee, Y. H. *J. Am. Chem. Soc.* 124(2002), 2528–2533.
62. Trost, B. M., Rudd, M. T., Costa, M. G., Lee, P. I., and Pomerantz, A. E. *Org. Lett.* 6(2004), 4235–4238.
63. Alonso, F., Beletskaya, I. P., and Yus, M. *Chem. Rev.* 104(2004), 3079–3159.
64. Nakamura, I., and Yamamoto, Y. *Chem. Rev.* 104(2004), 2127–2198.
65. Kataoka, Y., Matsumoto, O., and Tani, K. *Organomet.* 15(1996), 5246–5249.
66. Hartman, J. W., and Sperry, L. *Tetrahedron Lett.* 45(2004), 3787–3788.
67. Fukuda, Y., and Utimoto, K. *J. Org. Chem.* 56(1991), 3729–3731.
68. Teles, J. H., Brode, S., and Chabanas, M. *Angew. Chem. Int. Ed.* 37(1998), 1415–1418.
69. Antoniotti, S., Genin, E., Michelet, V., and Genêt, J. P. *J. Am. Chem. Soc.* 127(2005), 9976–9977.
70. Pale, P., and Chucho, J. *Tetrahedron Lett.* 28(1987), 6447–6448.
71. Kataoka, Y., Matsumoto, O., and Tani, K. *Chem. Lett.* (1996), 727–728.
72. Genin, E., Antoniotti, S., Michelet, V., and Genêt, J. P. *Angew. Chem. Int. Ed.* 44(2005), 4949–4953.
73. Nakagawa, H., Okimoto, Y., Sakaguchi, S., and Ishii, Y. *Tetrahedron Lett.* 44(2003), 103–106.
74. Masui, D., Kochi, T., Tang, Z., Ishii, Y., Mizobe, Y., and Hidai, M. *J. Organomet. Chem.* 620(2001), 69–79.
75. Messerle, B. A., and Vuong, K. Q. *Organomet.* 26(2007), 3031–3040.
76. Hindi, K. M., Panzner, M. J., Tessier, C. A., Cannon, C. L., and Youngs, W. J. *Chem. Rev.* 109(2009), 3859–3884.
77. Hopkinson, M. N., Richter, C., Schedler, M., and Glorius, F. *Nature* 506(2014), 487–488.
78. Brooner, R. E. M., and Widenhoefer, R. A. *Angew. Chem. Int. Ed.* 52(2013), 11714–11724.

Bibliography

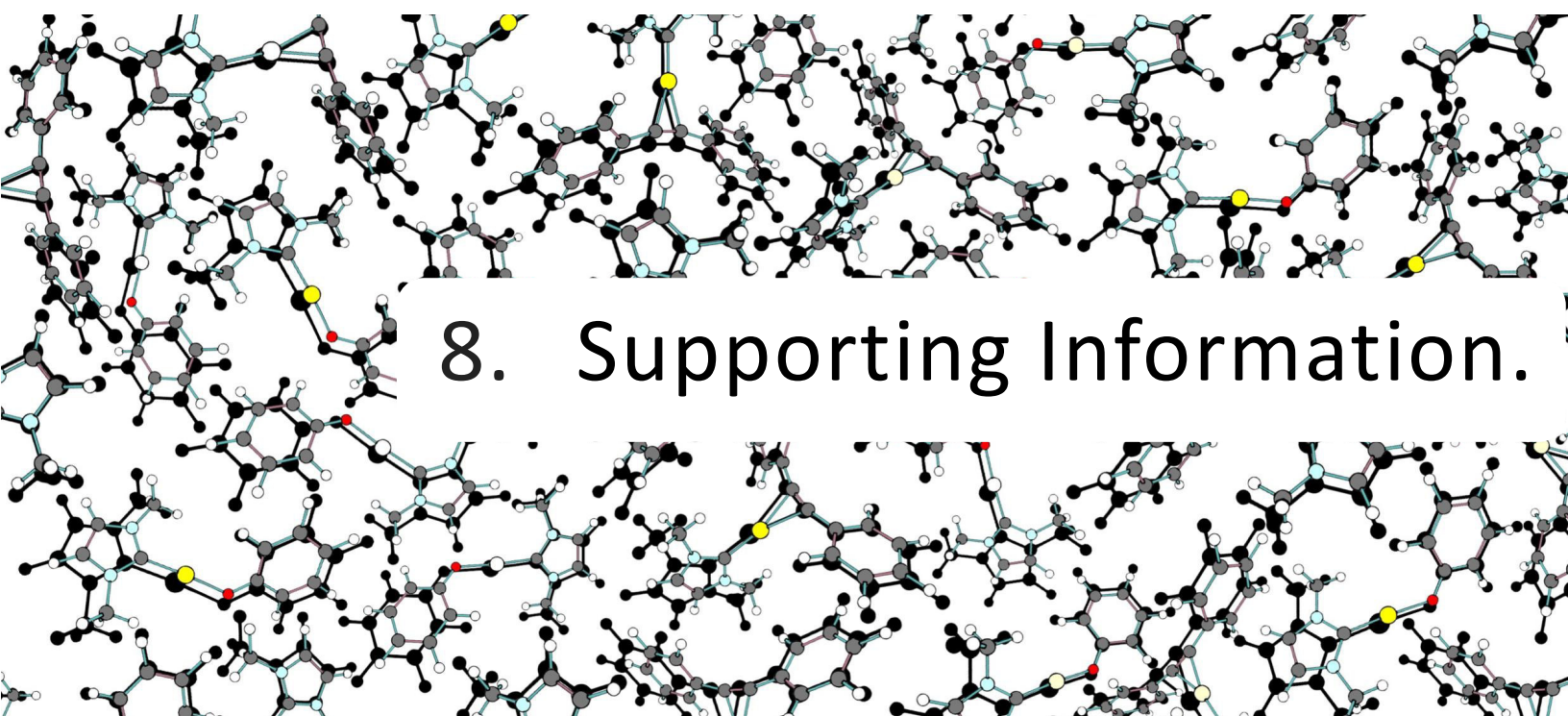
79. Gomez, S. A., Ramon, S. R., Songis, O., Slawin M. Z., Cazin, C. S. J., and Nolan S.P. *Organomet.* 30(2011), 5463–5460.
80. Trinchillo, M., Belanzoni, P., Belpassi, L., Biasiolo, L., Busico, V., D'Amora, A., D'Amore, L., Del Zotto, A., Tarantelli, F., Tuzi, A., and Zuccaccia, D. *Organomet.* 35(2016), 641–654.
81. Biasiolo, L., Del Zotto, A., and Zuccaccia, D. *Organomet.* 34(2015), 1759–1760.
82. Kuram, M. R., Bhanuchandra, M., and Sahoo A. K. *J. Org. Chem.* 75(2010), 2247–2258.
83. Kovács, G., Lledós, A., and Ujaque, G. *Organomet.* 29(2010), 3252–3260.
84. Zimmermann, B., Herwing, J., and Beller, M. *Angew. Chem. Int. Ed.* 38(1999), 2372–3275.
85. Yang, R., Zhang, Y., and Tsubaki, N. *Catal. Commun.* 6(2005), 275–279.
86. Das, R. K., Saha, B., Rahaman, S. M. W., and Bera, J. K. *Chem. Eur. J.* 16(2010), 14459–14468.
87. Proutiere, F., Aufiero, M., and Schönebeck, F. *Angew. Chem. Int. Ed.* 51(2012), 7226–7230.
88. Proutiere, F., Aufiero, M., and Schönebeck, F. *J. Am. Chem. Soc.* 134(2012), 606–612.
89. Hansmann, M. M., Pernpointner, M., Dröp, R., and Hashmi, A. S. K. *Chem. Eur.* 19(2013), 15290–15303.
90. Naumann, S., Scholten, P. B. V., Wilson, J. A., and Dove, A. P. *J. Am. Chem. Soc.* 137(2015), 14439–14445.
91. Xu, T., and Chen, E. Y.-X. *J. Polym. Sci. Part A: Polym. Chem.* 53(2015), 1895–1903.
92. Sammis, M. G., Danjo, H., and Jacobsen, N. E. *J. Am. Chem. Soc.* 126(2004), 9928–9929.
93. Rueping, M., Antonchick, A. P., and Brinkmann, C. *Angew. Chem. Int. Ed.* 119(2007), 7027–7030.
94. Du, J., Skubi, K. L., Schultz, D. M., and Yoon, T. P. *Science* 334(2014), 392–396.
95. Peters, R. “Cooperative catalysis: Designing Efficient Catalysis for Synthesis”. *John Wiley and Sons.* (2015), p.16.
96. Corey, E. J., Bakshi, R. K., and Shibata, S. *J. Am. Chem. Soc.* 109(1987), 5551–5553.
97. DiMauro, E. F., and Kozlowski, M. S. *Org. Lett.* 3(2001), 3053–3056.
98. DiMauro, E. F., and Kozlowski, M. S. *Org. Lett.* 4(2002), 3781–3784.
99. Wadamoto, M., Ozasa, N., Yanagisawa, A., and Yamamoto, H. *J. Org. Chem.* 68(2003), 5593–5601.
100. Denmark, S. E., and Chung, W.-J. *J. Org. Chem.* 73(2008), 4582–4595.
101. Kobayashi, S., Hamada, T., and Manabe, K. *J. Am. Chem. Soc.* 124(2002), 5640–5641.
102. *Ref. 95, p. 36.*
103. Ohkuma, T., Ooka, H., Hashiguchi, S., Ikariya, T., and Noyori, R. *J. Am. Chem. Soc.* 117(1995), 2675–2676.
104. Mikhailine, A. A., Maishan, M. I., Lough, A. J., and Morris, R. H. *J. Am. Chem. Soc.* 134(2012), 12266–12280.
105. Zuo, W., Lough, A. J., Li, Y. F., and Morris, R. H. *Science*, 342(2013), 1080–1083.
106. *Ref. 95, p. 68.*
107. Westerhausen, D., Herrmann, S., Hummel, W., and Steckhan, E. *Angew. Chem. Int. Ed.* 31(1992), 1496–1498.
108. Allen, J. V., and Williams, J. M. *J. Tetrahedron Lett.* 37(1996), 1859–1862.
109. Dinh, P. M., Howarth, J. A., Hudnott, A. R., Williams, J. M. J., and Harris, W. *Tetrahedron Lett.* 37(1996), 7623–7626.
110. Pàmies, O., and Bäckvall, J.-E. *Chem. Rev.* 103(2003), 3247–3261.
111. Denard, C. A., Huang, H., Bartlett, M. J., Lu, L., Tan, Y., Zhao, H., and Hartwig, J. F. *Angew. Chem. Int. Ed.* 126(2013), 475–479.
112. Simons, C., Hanefeld, U., Arends, I. W. C. E., Maschmeyer, T., and Sheldon, R. A. *Top. Catal.* 40(2006), 35–44.
113. Burns, N. Z., Witten, M. R., and Jacobsen, E. N. *J. Am. Chem. Soc.* 133(2011), 14578–14581.
114. Oliveira, M. T., Luparia, M., Audisio, D., and Maulide, N. *Angew. Chem. Int. Ed.* 52(2013), 13149–13152.

Bibliography

115. Hanna, L. E., and Jarvo, E. R. *Angew. Chem. Int. Ed.* 54(2015), 15618–15620.
116. Cheong, P. H., Morganelli, P., Luzung, M. R., Houk, K. N., and Toste, F. D. *J. Am. Chem. Soc.* 130(2008), 4517–4526.
117. Gaillard, S., Bosson, J., Ramon, R. S., Nun, P., Slawin, A. M. Z., and Nolan, S. P. *Chem. Eur. J.* 16(2010), 13729–13740.
118. Seidel, G., Lehmann, G. W., and Fürstner, A. *Angew. Chem. Int. Ed.* 49(2010), 8466–8470.
119. Brown, T. J., and Widenhöfer, R. A. *Organomet.* 30(2011), 6003–6009.
120. Oonishi, Y., Gómez-Suárez, A., Martin, A. R., and Nolan, S. P. *Angew. Chem. Int. Ed.* 52(2013), 9767–9771.
121. Veenboer, R. M. P., Dupuy, S., and Nolan, S. P. *ACS Catal.* 5(2015), 1330–1334.
122. Dupuy, S., Gasperini, D., and Nolan, S. P. *ACS Catal.*, 5(2015), 6918–6921.
123. Roithová, J., Janková, Š., Jašíková, L., Váňa, J., and Hybelbauerová, S. *Angew. Chem. Int. Ed.* 51(2012), 8378–8382.
124. Jašíková, L., Anania, M., Hybelbauerová, S., and Roithová, J. *J. Am. Chem. Soc.* 137(2015), 13647–13657.
125. Larsen, M. H., Houk, K. N., and Hashmi, A. S. K. *J. Am. Chem. Soc.*, 137(2015), 10668–10676.
126. Gómez-Suárez, A., Oonishi, Y., Martin, A. R., Vummaleti, S. V. C., Nelson, D. J., Cordes, D. B., Slawin, A. M. Z., Cavallo, L., Nolan, S. P., and Poater, A. *Chem. Eur. J.* 22(2016), 1125–1132.
127. Lazreg, F., Guidone, S., Gómez-Herrera, A., Nahra, F., and Cazin, S. J. C. *Dalton Trans.* 46(2017), 2439–2444.
128. Neese, F., *Coord. Chem. Rev.* 253(2009), 526–563.
129. Sholl, A., and Steckel, J. A. “Density Functional Theory: A Practical Introduction”. *John Wiley and Sons, Inc.* (2011). p. 1–7.
130. Parr, R.G. and Yang, W. “Density Functional Theory of Atoms and Molecules”. *Oxford University Press, Inc.* (1989). p. 47–51.
131. Sahní, V. “Quantal, Density Functional Theory”. *Springer* (2004), p. 100–103.
132. Bort, J. A., and Beltrán, J. “Química Teórica y Computacional”. *Universitat Jaume I* (2000), p. 124–128.
133. Koch, W., and Holthausen, M. C. “A Chemist’s Guide to Density Functional Theory”. 2nd ed. *Wiley-VCH*. (2001). p. 70–85.
134. Engel, E., and Dreizler, R. M. “Density Functional Theory: An advanced Course”. *Springer* (2011). p. 204–210.
135. Fiolhais, C., Nogueira, F., and Marques, M. “A Primer in Density Functional Theory”. *Springer* (2003). p. 50.
136. Mardirossian, N., and Head-Gordon, M. *Phys. Chem. Chem. Phys.* 16(2014), 9904–9924.
137. Slater, J. C. *Phys. Rev.* 36(1930), 57–64.
138. Boys, S.F. *Proc. Roy. Soc. A* 200(1950), 542–554.
139. Young, D. C. “Computational Chemistry: A Practical Guide for Applying Techniques to Real-World Problems”. *Wiley and Sons, Inc.* (2001), 78–90.
140. Ramachandran, K. I., Deepa, G., and Namboori, K. “Computational Chemistry and Molecular Modeling: Principles and Applications”. *Springer* (2008), 115–138.
141. Hehre, W. J., Stewart, R. F., and Pople, J. A. *J. Chem. Phys.* 51(1969), 2657–2664.
142. Binkley, J. S., Pople, J. A., and Hehre, W. J. *J. Am. Chem. Soc.* 102(1980), 939–947.
143. Binkley, J. S., Pople, J. A., and Hehre, W. J. *J. Am. Chem. Soc.* 102(1980), 939–947.
144. Ditchfield, R., Hehre, W. J., and Pople, J. A. *J. Chem. Phys.* 54(1971), 724.
145. Hehre, W. J., Ditchfield, R., and Pople, J. A. *J. Chem. Phys.*, 56(1972), 2257.
146. McLean, A. D. and Chandler, G. S. *J. Chem. Phys.* 72(1980), 5639–5648.

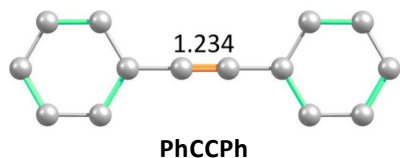
Bibliography

147. Dunning Jr., T. H. *J. Chem. Phys.* 90(1989), 1007–1023.
148. Kendall, R. A., Dunning Jr. T. H., and Harrison, R. J. *J. Chem. Phys.* 96(1992), 6796–6806.
149. Peterson, K. A., Woon, D. E., and Dunning Jr. T. H. *J. Chem. Phys.* 100(1994), 7410–7415.
150. Schäfer, A., Horn, H., and Ahlrichs, R. *J. Chem. Phys.* 97(1992), 2571–2577.
151. Schäfer, A., Huber, C., and Ahlrichs, R. *J. Chem. Phys.* 100(1994), 5829–5835.
152. Weigend, F., and Ahlrichs, R. *Phys. Chem. Chem. Phys.* 7(2005), 3297–3305.
153. Weigend, F. *Phys. Chem. Chem. Phys.* 8(2006), 1057–1065.
154. Lewards, E. G. “Computational Chemistry: Introduction to the Theory and Applications of Molecular and Quantum Mechanics”. 2nd ed. *Springer* (2011), 251,252.
155. Cramer, C. J. “Essentials of Computational Chemistry: Theories and Models”. 2nd ed. *John Wiley & Sons, Ltd* (2004), 178–180.
156. Hay, P. J. and Wadt, W. R. *J. Chem. Phys.* 82(1985), 270–283.
157. Wadt, W. R. and Hay, P. J. *J. Chem. Phys.* 82(1985), 284–298.
158. Hay, P. J. and Wadt, W. R. *J. Chem. Phys.* 82(1985), 299–310.
159. Stevens, W. J., Krauss, M., Basch, H., and Jasien, P. G. *Can. J. Chem.* 70(1992), 612–630.
160. Hurley, M. M., Pacios, L. F., Christiansen, P. A., Ross, R. B., and Ermler, W. C. *J. Chem. Phys.* 84(1986), 6840–6853.
161. Dolg, M., Wedig, U., Stoll, H., and Preuss, H. *J. Chem. Phys.* 86(1987), 866–872.
162. Leininger, T., Berning, A., Nicklass, A., Stoll, H., Werner, H.-J., and Flad, H.-J. *Chem. Phys.* 217(1997), 19–27.
163. Eyring, H. *J. Chem. Phys.* 3(1935), 107–115.
164. Evans, M. G. and Polanyi, M. *Trans. Faraday Soc.* 31(1935), 875–894.
165. Laidler, J. J. and King, M. C. *J. Phys. Chem.* 87(1993), 2657–2664.
166. Wright, M. R. “An Introduction to Chemical Kinetics”. *John Wiley & Sons, Ltd.* (2004), 122–144.
167. Yip, S. “Handbook of Materials Modeling”. *Springer* (2005), 1567–1581.
168. Perdew, J. P. *Phys. Rev. B* 34(1986), 7406–7406.
169. Häussermann, U., Dolg, M., Stoll, H., and Preuss, H. *Mol. Phys.* 78(1993), 1211–1224.
170. Küchle, W., Dolg, M., Stoll, H., and Preuss, H. *J. Chem. Phys.* 100(1994), 7535–7542.
171. Leninger, T., Nicklass, A., Stoll, H., Dolg, H., and Schwerdtfeger, P. *J. Chem. Phys.* 105(1996), 1052–1059.
172. Zhao, Y. and Truhlar, D. G. *Theor. Chem. Acc.* 120(2008), 215–241.
173. Marenich, A. V., Cramer, C. J., and Truhlar, D. G. *J. Phys. Chem. B.* 113(2009), 6378–6396.
174. Svensson, M., Humbel, S., Froese, R. D. J., Matsubara, T., Sieber, S., and Morokuma, K. *J. Phys. Chem.* 100(1996), 19357–19363.
175. Dapricha, S., Komáromia, I., Byuna, K. S., Morokuma, K., and Frisch, M. J. *J. Mol. Struc. (Theochem)* 462(1999), 1–21.
176. Stewart, J. J. P. *J. Mol. Model.* 13(2007), 1173–1213.
177. Falivene, L., Credendino, R., Poater, A., Petta, A., Serra, L., Oliva, R., Scarano, V., Cavallo, L. *Organomet.* 35(2016), 2286–2293.
178. Poater, A., Ragone, F., Giudice, S., Costabile, C., Dorta, R., Nolan, S. P., and Cavallo, L. *Organomet.* 27(2008), 2679–2681.
179. Poater, A., Cavallo, L. *Dalton Trans.* (2009), 8878–8883.
180. Jacobsen, H., Correa, A., Poater, A., Costabile, C., and Cavallo, L. *Coord. Chem. Rev.* 253(2009), 687–703.



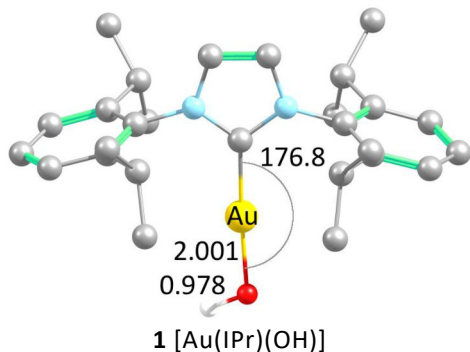
8. Supporting Information.

Table 8.1. Cartesian coordinates (xyz) of the optimized geometries for metal-NHC, -CAAC, and -PSC catalytic systems calculated at the BP86/SVP level (The hydrogen atoms that do not play a significant role in the mechanism were omitted to provide a better view. Bond distances and angles are given in Angstroms and degrees, respectively).



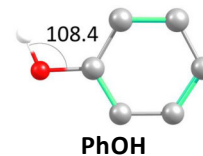
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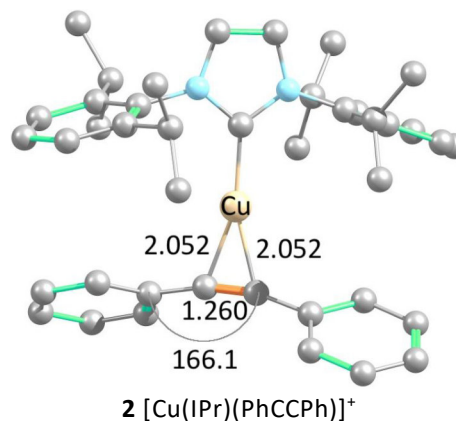
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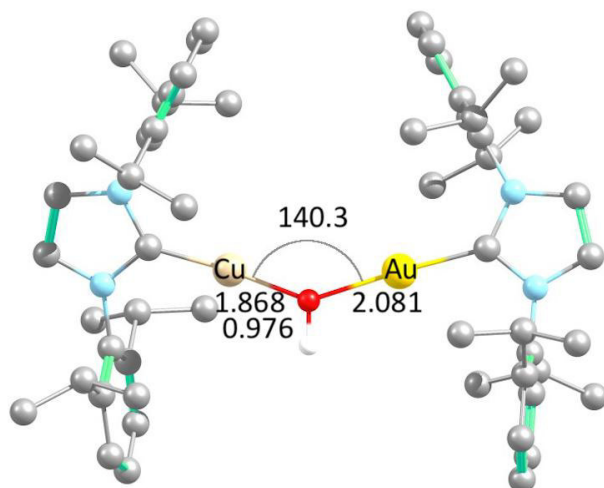
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Supporting Information

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1	3.219486000	-2.916839000	-2.899285000	1	0.749365000	-2.745466000	4.979886000
1	4.147555000	-3.722702000	-1.595906000	1	1.832342000	-3.563393000	3.806210000
1	1.637410000	4.192956000	0.644946000	1	2.490765000	-2.337431000	4.932532000
1	1.677883000	2.556291000	1.389765000	1	0.102139000	-0.278497000	4.654223000
1	3.198288000	3.492023000	1.181785000	1	1.816007000	0.227381000	4.576372000
1	2.525147000	4.534580000	-1.756855000	1	0.702345000	0.637417000	3.232159000
1	4.122856000	3.875995000	-1.300160000	1	3.339073000	-0.742075000	-3.475265000
1	3.221502000	3.154382000	-2.669868000	1	2.859734000	0.337300000	-2.120606000
1	-2.565894000	4.478622000	-1.929495000	1	4.564094000	-0.181255000	-2.299160000
1	-3.231307000	3.055142000	-2.798335000	1	3.930150000	-3.203250000	-3.031144000
1	-4.155035000	3.807665000	-1.460709000	1	5.179261000	-2.737791000	-1.837690000
1	-1.681875000	4.238923000	0.481124000	1	3.873247000	-3.866333000	-1.364743000
1	-3.234823000	3.537353000	1.038641000	29	-0.000088000	0.725615000	0.000230000
1	-1.705401000	2.632420000	1.291056000	6	-0.610880000	2.678822000	0.155353000
1	-1.643928000	-4.214183000	0.440522000	6	0.610452000	2.678831000	-0.154819000
1	-1.698151000	-2.629905000	1.290263000	6	-1.939252000	3.004420000	0.612088000
1	-3.214223000	-3.541984000	0.983947000	6	-2.108256000	3.657887000	1.863003000
1	-2.473545000	-4.408431000	-1.985960000	6	-3.076296000	2.717706000	-0.188454000
1	-4.079514000	-3.760504000	-1.541218000	6	-3.390485000	4.028733000	2.288955000
1	-3.131572000	-2.973538000	-2.841641000	1	-1.226041000	3.880476000	2.481912000
79	-0.018034000	-0.062176000	1.568881000	6	-4.352227000	3.098216000	0.249429000
1	0.758225000	-0.187207000	3.923464000	1	-2.946602000	2.205352000	-1.153768000
8	-0.150573000	-0.183463000	3.561940000	6	-4.512514000	3.752798000	1.484687000
				1	-3.515663000	4.544047000	3.253870000
				1	-5.229409000	2.884457000	-0.380229000
				1	-5.517011000	4.051925000	1.822578000
				6	1.938663000	3.004776000	-0.611817000
				6	3.076020000	2.717868000	0.188202000
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				6	4.351756000	3.098680000	-0.249993000

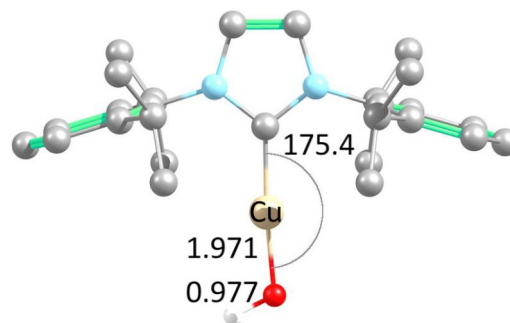
Supporting Information

**3** [Au(IPr)(OH)(IPr)Cu]⁺

E(scf)= -2727.48687624 a.u.

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8	0.301535000	-1.076293000	-0.344852000
1	0.272861000	-2.046375000	-0.447003000
29	2.060552000	-0.470389000	-0.178673000
6	-3.543426000	0.137036000	0.072780000
7	-4.631415000	-0.678621000	-0.113798000
6	-5.814389000	0.028349000	0.089356000
1	-6.794712000	-0.447159000	-0.012293000
6	-5.458974000	1.313177000	0.410512000
1	-6.064790000	2.193240000	0.647160000
7	-4.065717000	1.362721000	0.396854000
6	-4.574748000	-2.082741000	-0.476574000
6	-4.571935000	-2.426457000	-1.854463000
6	-4.536231000	-3.799529000	-2.174833000
1	-4.532435000	-4.106624000	-3.232614000
6	-4.509570000	-4.779712000	-1.172917000
1	-4.486024000	-5.845820000	-1.448577000
6	-4.518121000	-4.407319000	0.178560000
1	-4.500331000	-5.187388000	0.955928000
6	-4.552874000	-3.050496000	0.562386000
6	-4.596427000	-1.383477000	-2.972587000
1	-4.652642000	-0.379746000	-2.501076000
6	-3.293905000	-1.422805000	-3.800913000
1	-2.403498000	-1.267482000	-3.156470000
1	-3.301413000	-0.627943000	-4.575564000
1	-3.172362000	-2.395675000	-4.321979000
6	-5.843296000	-1.536751000	-3.870264000
1	-6.782358000	-1.481598000	-3.282016000
1	-5.843454000	-2.506852000	-4.410147000
1	-5.871705000	-0.732901000	-4.634974000
6	-4.551136000	-2.677266000	2.045460000
1	-4.635293000	-1.572485000	2.118570000
6	-5.761404000	-3.278406000	2.791434000
1	-5.770367000	-2.943200000	3.849422000
1	-5.730497000	-4.388108000	2.797026000
1	-6.722207000	-2.973361000	2.328173000
6	-3.217710000	-3.074685000	2.715249000
1	-3.204092000	-2.754080000	3.777813000
1	-2.355790000	-2.601060000	2.200448000
1	-3.064752000	-4.174298000	2.695454000
6	-3.298678000	2.559006000	0.686472000
6	-2.957085000	2.833174000	2.037282000

1	2.946727000	2.205136000	1.153369000
6	3.389187000	4.029888000	-2.288811000
1	1.224688000	3.881491000	-2.481042000
6	4.511534000	3.753750000	-1.485056000
1	5.229186000	2.884771000	0.379269000
1	3.513964000	4.545592000	-3.253569000
1	5.515879000	4.053105000	-1.823195000

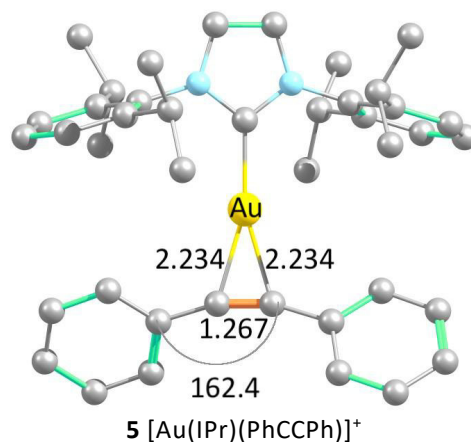
**4** [Cu(IPr)(OH)]

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6	0.698501000	-0.000388000	-2.264321000
6	-0.672241000	-0.000449000	-2.267863000
6	2.474200000	0.000095000	-0.488622000
6	-2.458140000	-0.000177000	-0.502630000
1	1.421937000	-0.000464000	-3.085561000
1	-1.391301000	-0.000583000	-3.092939000
6	3.127147000	-1.245098000	-0.287674000
6	4.475962000	-1.214219000	0.122665000
6	5.145856000	0.000518000	0.324694000
6	4.475394000	1.215037000	0.123279000
6	3.126572000	1.245484000	-0.287093000
6	2.409175000	-2.584224000	-0.456207000
1	5.009025000	-2.163039000	0.292992000
1	6.199352000	0.000679000	0.647049000
1	5.007996000	2.164030000	0.294098000
6	2.408081000	2.584383000	-0.455205000
6	-3.112123000	1.245040000	-0.305835000
6	-4.467381000	1.214315000	0.082245000
6	-5.141538000	-0.000026000	0.270554000
6	-4.467352000	-1.214439000	0.082818000
6	-3.112093000	-1.245318000	-0.305249000
6	-2.389865000	2.584323000	-0.450968000
1	-5.001174000	2.163336000	0.248861000
1	-6.199832000	0.000033000	0.576593000
1	-5.001123000	-2.163395000	0.249880000
6	-2.389855000	-2.584669000	-0.449843000
1	1.408035000	-2.375699000	-0.887623000
6	2.181778000	-3.256908000	0.915678000
6	3.143668000	-3.522778000	-1.435780000
1	1.406748000	2.375531000	-0.886007000
6	2.181259000	3.257123000	0.916732000
6	3.141771000	3.523041000	-1.435303000
1	-1.370913000	2.375822000	-0.838536000
6	-3.085017000	3.515993000	-1.465496000
6	-2.222602000	3.264436000	0.926310000
1	-1.370793000	-2.376316000	-0.837197000
6	-2.222969000	-3.264470000	0.927633000
6	-3.084821000	-3.516534000	-1.464323000
1	1.611246000	-4.202207000	0.797509000

Supporting Information

6	-2.241042000	4.021291000	2.291188000	1	3.145877000	-3.503917000	1.409306000
1	-1.958714000	4.269528000	3.326174000	1	1.609451000	-2.592216000	1.596460000
6	-1.888659000	4.893050000	1.251195000	1	2.565612000	-4.459397000	-1.581303000
1	-1.336183000	5.819174000	1.475331000	1	3.284219000	-3.049930000	-2.430005000
6	-2.244032000	4.594695000	-0.071448000	1	4.146896000	-3.812079000	-1.057278000
1	-1.964928000	5.291136000	-0.877812000	1	1.610345000	4.202218000	0.798781000
6	-2.961406000	3.422674000	-0.388753000	1	1.609514000	2.592314000	1.597887000
6	-3.310485000	1.890442000	3.188587000	1	3.145528000	3.504535000	1.409826000
1	-3.987085000	1.105589000	2.789814000	1	2.563457000	4.459549000	-1.580519000
6	-2.047894000	1.175106000	3.717991000	1	4.145194000	3.812502000	-1.057444000
1	-1.537442000	0.611346000	2.909060000	1	3.281776000	3.050156000	-2.429588000
1	-2.313927000	0.459410000	4.523767000	1	-2.507474000	4.456369000	-1.587557000
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1	-4.982397000	3.118853000	3.947064000	1	-1.640428000	4.205025000	0.828051000
1	-3.440346000	3.376590000	4.821294000	1	-3.206925000	3.523029000	1.371539000
1	-4.379968000	1.883724000	5.101223000	1	-1.691549000	2.601825000	1.641413000
6	-3.340427000	3.128044000	-1.840665000	1	-1.640828000	-4.205115000	0.829721000
1	-3.933758000	2.189622000	-1.853090000	1	-1.692033000	-2.601733000	1.642708000
6	-2.086275000	2.881775000	-2.706510000	1	-3.207407000	-3.522915000	1.372691000
1	-2.376742000	2.622376000	-3.745934000	1	-2.507329000	-4.456990000	-1.586006000
1	-1.474332000	2.049454000	-2.301012000	1	-4.106223000	-3.798769000	-1.131857000
1	-1.441468000	3.784219000	-2.754618000	1	-3.177245000	-3.040650000	-2.462772000
6	-4.231524000	4.239134000	-2.436103000	29	-0.018107000	0.000060000	1.770653000
1	-4.545098000	3.973816000	-3.467150000	1	0.689827000	0.000153000	3.983656000
1	-3.694622000	5.209161000	-2.493322000	8	-0.187128000	0.000107000	3.553983000
1	-5.147784000	4.399074000	-1.831282000				
6	3.859650000	-0.035357000	-0.040887000				
7	4.871410000	-0.912851000	0.272650000				
6	6.108283000	-0.272871000	0.277157000				
1	7.037335000	-0.805478000	0.502985000				
6	5.872098000	1.040683000	-0.041157000				
1	6.552921000	1.890346000	-0.152240000				
7	4.497413000	1.166775000	-0.231108000				
6	4.675930000	-2.322260000	0.551964000				
6	4.773147000	-3.245859000	-0.523219000				
6	4.579058000	-4.610087000	-0.222397000				
1	4.645174000	-5.355330000	-1.030596000				
6	4.307481000	-5.034195000	1.086100000				
1	4.163337000	-6.105524000	1.297336000				
6	4.226283000	-4.099168000	2.127506000				
1	4.018633000	-4.445838000	3.151996000				
6	4.410880000	-2.721206000	1.889317000				
6	5.057636000	-2.813809000	-1.962519000				
1	5.252251000	-1.720834000	-1.956125000				
6	3.827333000	-3.050792000	-2.865120000				
1	2.937302000	-2.509280000	-2.480880000				
1	3.569562000	-4.129135000	-2.925768000				
1	4.024852000	-2.695055000	-3.897788000				
6	6.318084000	-3.497937000	-2.533218000				
1	7.207731000	-3.313908000	-1.896530000				
1	6.540181000	-3.113076000	-3.550180000				
1	6.188222000	-4.597220000	-2.618077000				
6	4.312320000	-1.726418000	3.046400000				
1	4.548088000	-0.717665000	2.647237000				
6	5.342164000	-2.031238000	4.155159000				
1	6.377703000	-2.051457000	3.757656000				
1	5.149714000	-3.012339000	4.637772000				
1	5.295993000	-1.257745000	4.949690000				
6	2.875173000	-1.665587000	3.608260000				
1	2.145232000	-1.392023000	2.817374000				
1	2.804574000	-0.909064000	4.417538000				
1	2.562445000	-2.641868000	4.035133000				
6	3.839685000	2.410814000	-0.577660000				
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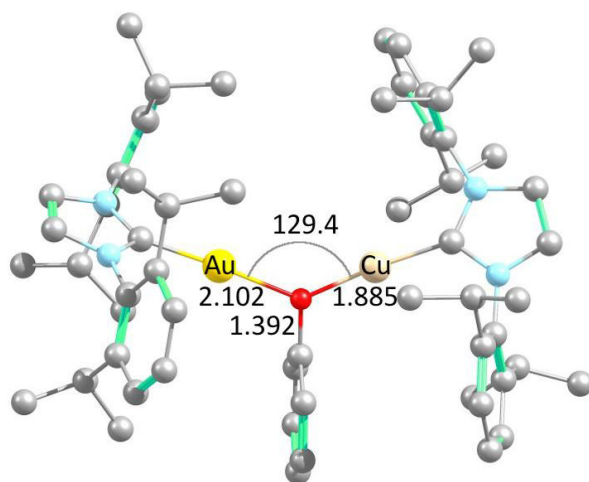


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6	-0.664001000	-3.572228000	-0.174731000
6	0.663145000	-3.572328000	0.175582000
6	-2.394380000	-1.803186000	-0.625150000
6	2.393930000	-1.803520000	0.625423000
1	-1.362662000	-4.394060000	-0.359750000
1	1.361630000	-4.394266000	0.360794000
6	-2.683262000	-1.520100000	-1.987159000
6	-4.001352000	-1.119871000	-2.292407000
6	-4.982177000	-1.024880000	-1.294619000
6	-4.664786000	-1.319708000	0.039052000
6	-3.362361000	-1.714021000	0.410830000
6	-1.646813000	-1.645097000	-3.104891000
1	-4.267083000	-0.893020000	-3.336814000
1	-6.008140000	-0.725938000	-1.561662000
1	-5.446328000	-1.246701000	0.811384000
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Supporting Information

1	2.543617000	5.213857000	0.892628000	6	4.001276000	-1.120175000	2.292306000
6	2.619515000	4.828122000	-1.239744000	6	4.982004000	-1.025678000	1.294372000
1	2.142347000	5.785519000	-1.502242000	6	4.664364000	-1.320721000	-0.039192000
6	3.006161000	3.939683000	-2.252929000	6	3.361793000	-1.714804000	-0.410704000
1	2.826096000	4.207825000	-3.305796000	6	1.646703000	-1.644575000	3.105216000
6	3.629432000	2.711153000	-1.949933000	1	4.267193000	-0.893117000	3.336621000
6	3.710178000	2.974848000	1.947035000	1	6.008072000	-0.726919000	1.561219000
1	4.165434000	1.964134000	2.005522000	1	5.445815000	-1.248082000	-0.811650000
6	2.391216000	2.924105000	2.747043000	6	3.049768000	-2.040768000	-1.872104000
1	1.682704000	2.187525000	2.315535000	1	-0.698155000	-2.001826000	-2.651329000
1	1.883987000	3.911523000	2.761619000	6	-1.353129000	-0.277222000	-3.757737000
1	2.588480000	2.636857000	3.800930000	6	-2.073158000	-2.693921000	-4.155422000
6	4.712197000	3.968012000	2.575328000	1	-1.963215000	-2.251289000	1.949602000
1	4.926073000	3.692711000	3.629134000	6	-3.344620000	-0.843480000	2.802232000
1	4.312673000	5.004042000	2.575736000	6	-3.799692000	-3.309508000	2.334535000
1	5.675237000	3.982950000	2.024725000	1	0.697820000	-2.000911000	2.651819000
6	4.040495000	1.763911000	-3.078023000	6	2.072741000	-2.693501000	4.155767000
1	4.585241000	0.910914000	-2.621487000	6	1.353734000	-0.276512000	3.757991000
6	5.006394000	2.438076000	-4.075711000	1	1.962284000	-2.251947000	-1.949180000
1	5.906182000	2.841025000	-3.567061000	6	3.344011000	-0.844731000	-2.802261000
1	4.522071000	3.278124000	-4.616487000	6	3.798382000	-3.310817000	-2.334140000
1	5.344711000	1.707490000	-4.839560000	1	-0.569547000	-0.377677000	-4.536956000
6	2.802442000	1.182962000	-3.795251000	1	-2.256336000	0.144807000	-4.246178000
1	2.135352000	0.651155000	-3.084552000	1	-0.996766000	0.460427000	-3.007851000
1	3.109237000	0.462866000	-4.582337000	1	-1.280636000	-2.819748000	-4.921948000
1	2.206390000	1.981301000	-4.285333000	1	-2.261931000	-3.684611000	-3.693240000

6 [Cu(IPr)(OPh)(IPr)Au]⁺

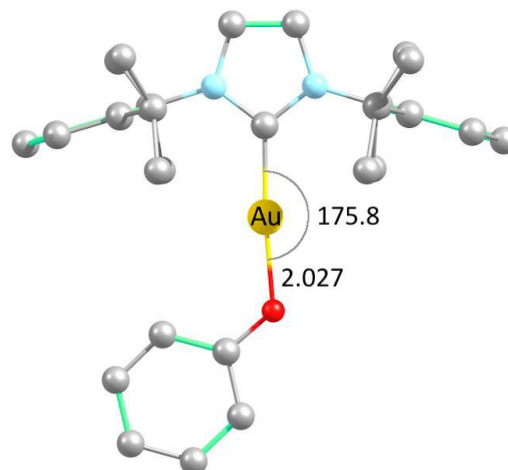
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29	1.983774000	-0.065933000	-0.274810000	6	0.628887000	2.757130000	-0.079354000
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Supporting Information

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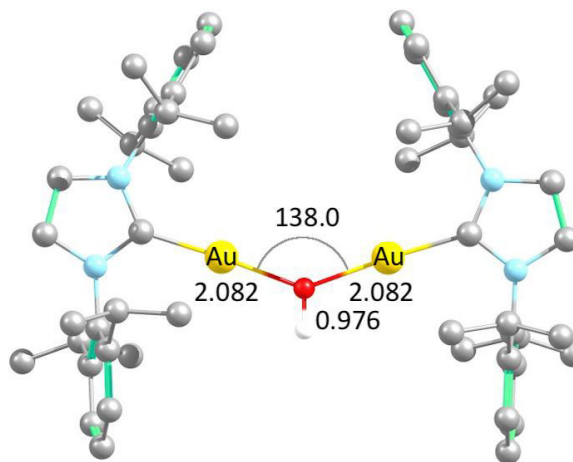
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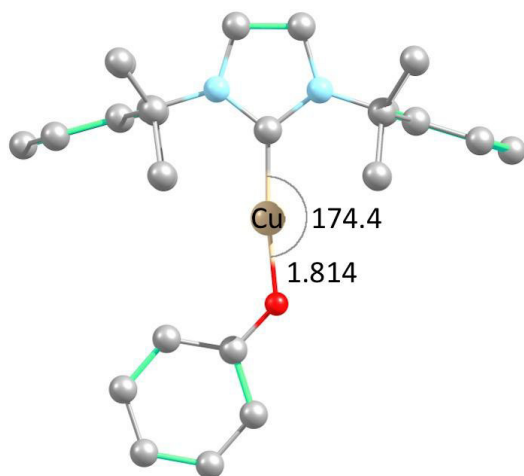
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Supporting Information



8 [Cu(IPr)(OPh)]

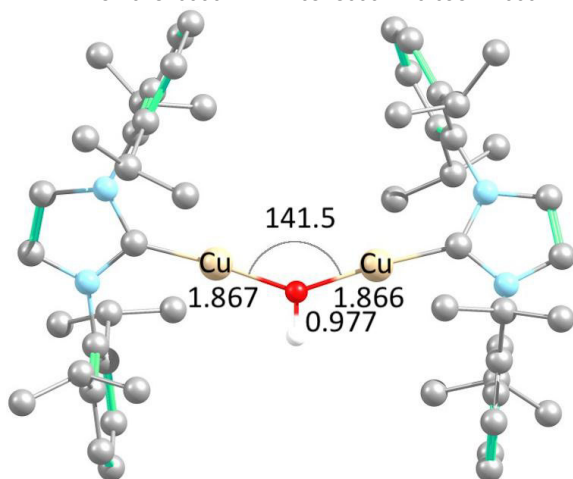
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Supporting Information

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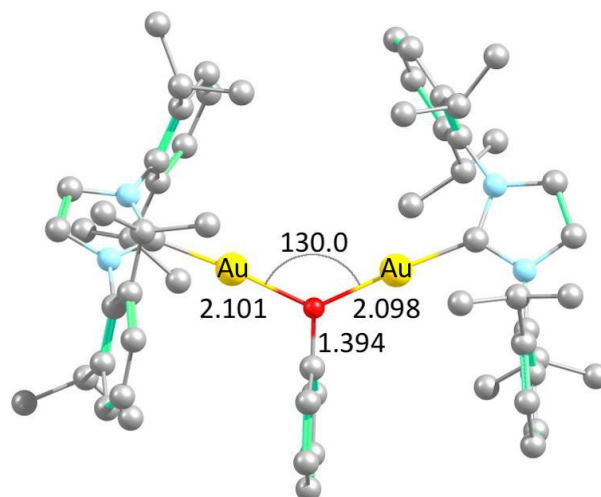
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Supporting Information

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11 [Au(IPr)(OPh)(IPr)Au]⁺

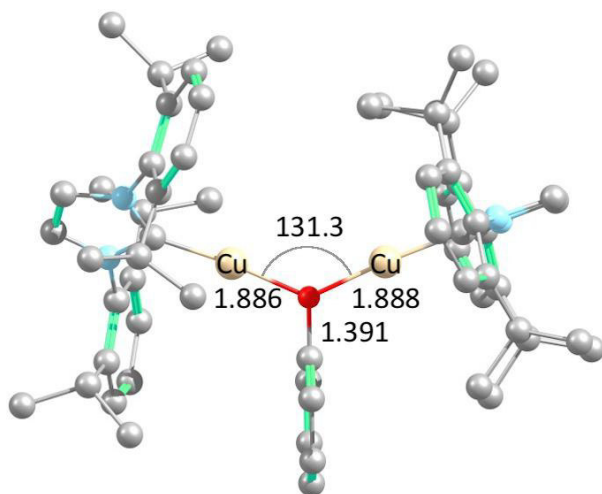
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Supporting Information

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6	4.797632000	2.197365000	-4.209722000	6	4.622442000	-1.956301000	2.701566000
1	5.703136000	2.621423000	-3.729217000	1	4.589196000	-0.852216000	2.586971000
1	4.322072000	3.005995000	-4.803174000	6	5.806200000	-2.282558000	3.638114000
1	5.125046000	1.414749000	-4.925126000	1	6.773059000	-1.946904000	3.209621000
6	2.575501000	0.997150000	-3.847727000	1	5.886880000	-3.373035000	3.830172000
1	1.903899000	0.519144000	-3.103772000	1	5.675385000	-1.781655000	4.619921000
1	2.868675000	0.227376000	-4.591839000	6	3.275757000	-2.388852000	3.320372000
1	1.989809000	1.774838000	-4.381622000	1	2.424137000	-2.113172000	2.664312000
				1	3.125428000	-1.899812000	4.305550000
				1	3.236776000	-3.486272000	3.484338000
				6	3.329390000	2.909211000	0.410989000
				6	2.888561000	3.376315000	1.677488000
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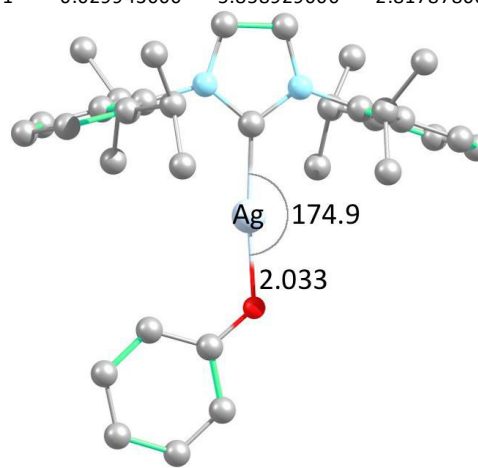
Supporting Information

**12** [Au(IPr)(OPh)(IPr)Au]⁺

E(scf)= -3019.94242715 a.u.

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6	-3.483112000	0.108331000	0.297895000
7	-4.274552000	-0.696992000	1.083050000
6	-5.544094000	-0.149106000	1.244957000
1	-6.318386000	-0.643843000	1.839396000
6	-5.556538000	1.030782000	0.544523000
1	-6.343674000	1.777724000	0.402130000
7	-4.294154000	1.170003000	-0.026532000
6	-3.859707000	-1.963794000	1.653582000
6	-4.090580000	-3.151437000	0.908897000
6	-3.695666000	-4.369948000	1.499693000
1	-3.860726000	-5.311605000	0.953184000
6	-3.101664000	-4.404497000	2.769010000
1	-2.803988000	-5.368886000	3.210035000
6	-2.893649000	-3.215507000	3.481918000
1	-2.433883000	-3.256673000	4.482060000
6	-3.270692000	-1.966670000	2.945802000
6	-4.762135000	-3.152874000	-0.465474000
1	-4.884181000	-2.096249000	-0.784215000
6	-3.894590000	-3.849550000	-1.534203000
1	-2.882478000	-3.399974000	-1.599837000
1	-4.372222000	-3.765040000	-2.532311000
1	-3.770598000	-4.932317000	-1.321975000
6	-6.172502000	-3.779468000	-0.390921000
1	-6.818444000	-3.255658000	0.343495000
1	-6.123828000	-4.847070000	-0.089729000
1	-6.673250000	-3.732883000	-1.380416000
6	-3.055264000	-0.690339000	3.760351000
1	-3.385529000	0.168396000	3.139045000
6	-3.914507000	-0.689898000	5.043553000
1	-3.789239000	0.264436000	5.596343000
1	-3.622982000	-1.513448000	5.728693000
1	-4.993055000	-0.812842000	4.814873000
6	-1.563075000	-0.466092000	4.082449000
1	-1.423671000	0.489721000	4.629168000
1	-0.952534000	-0.426800000	3.156568000
1	-1.155293000	-1.276447000	4.722439000
6	-3.903384000	2.286773000	-0.864547000
6	-3.328721000	3.428555000	-0.245999000
6	-2.965727000	4.502808000	-1.084111000

6	1.840414000	5.260365000	0.513745000
1	1.260199000	6.195698000	0.555012000
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1	2.053667000	5.325909000	-1.642294000
6	3.050523000	3.587199000	-0.804945000
6	3.203481000	2.651397000	2.986858000
1	3.810485000	1.754551000	2.742452000
6	1.916744000	2.148372000	3.675492000
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1	2.166160000	1.580444000	4.595975000
6	4.046569000	3.529962000	3.936411000
1	4.319338000	2.962719000	4.850547000
1	3.489197000	4.433528000	4.261281000
1	4.985644000	3.872206000	3.454854000
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6	4.286519000	4.145715000	-2.966895000
1	5.147273000	4.549203000	-2.394969000
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1	4.676500000	3.714857000	-3.912252000
6	2.333829000	2.500651000	-2.972093000
1	1.821639000	1.691445000	-2.409304000
1	2.683964000	2.081924000	-3.938691000
1	1.581550000	3.286249000	-3.195498000
6	0.008209000	-2.337613000	-1.100399000
6	0.107156000	-2.437201000	-2.503128000
6	-0.108112000	-3.501579000	-0.314850000
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6	-0.120732000	-4.762303000	-0.936262000
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1	0.168470000	-3.777120000	-4.210917000
1	-0.210629000	-5.669852000	-0.318243000
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**13** [Ag(IPr)(OPh)]

E(scf)= -1612.9774845 a.u.

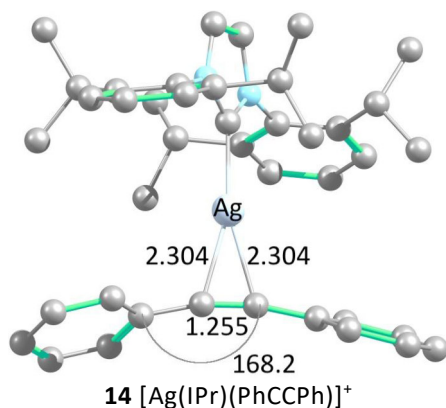
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7	0.230884000	-1.990734000	-0.000157000
6	1.269359000	-2.921643000	-0.000265000
1	1.081748000	-3.999746000	-0.000352000
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Supporting Information

1	-2.513214000	5.403792000	-0.641501000	1	3.484124000	-2.528212000	-0.000316000
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1	-3.927062000	3.282780000	-4.136306000	6	-3.188886000	-2.903355000	1.214647000
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1	-1.153691000	2.439698000	1.163738000	1	-3.731093000	-3.044302000	-2.163032000
1	-1.396323000	3.392373000	2.668179000	6	-1.830578000	-2.525962000	-1.246727000
1	-0.994579000	4.222505000	1.130309000	6	-1.132807000	-2.303992000	2.588916000
6	-3.682972000	4.780841000	1.889659000	1	-0.076446000	-2.034536000	2.380065000
1	-4.767374000	4.870166000	1.673695000	6	-1.762123000	-1.119329000	3.353821000
1	-3.189111000	5.702430000	1.516556000	1	-1.740656000	-0.189242000	2.749021000
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6	-4.804689000	0.991552000	-2.919140000	1	-2.820716000	-1.323339000	3.619940000
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1	-2.920812000	0.027492000	-3.544476000	1	-0.556546000	-3.418421000	4.389068000
1	-3.680266000	1.036337000	-4.820032000	6	-1.133001000	-2.303805000	-2.589108000
6	-6.182566000	1.361342000	-3.511579000	1	-0.076590000	-2.034501000	-2.380313000
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1	-6.087361000	2.100312000	-4.334720000	1	-0.556983000	-3.417966000	-4.389501000
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7	4.029256000	1.542197000	0.478791000	6	3.484072000	0.743304000	-1.246316000
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1	4.204590000	-5.840040000	-0.517040000	1	4.796552000	2.211749000	2.163157000
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6	4.092853000	-2.831876000	1.155752000	1	2.250221000	-0.595176000	-2.382609000
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6	4.055589000	-1.832694000	-3.648389000	1	1.812969000	0.909934000	-4.317236000
1	2.989468000	-1.696631000	-3.373795000	1	2.883311000	2.167169000	-3.622747000
1	4.166313000	-2.853965000	-4.069027000	6	4.118763000	-0.390105000	-3.432333000
1	4.296917000	-1.116661000	-4.461443000	1	4.643370000	-1.202638000	-2.887815000
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6	2.930132000	3.305668000	1.804588000	6	-4.357725000	4.784439000	0.000438000
6	2.303293000	4.568744000	1.837206000	1	-2.225378000	5.260333000	0.000411000
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Supporting Information

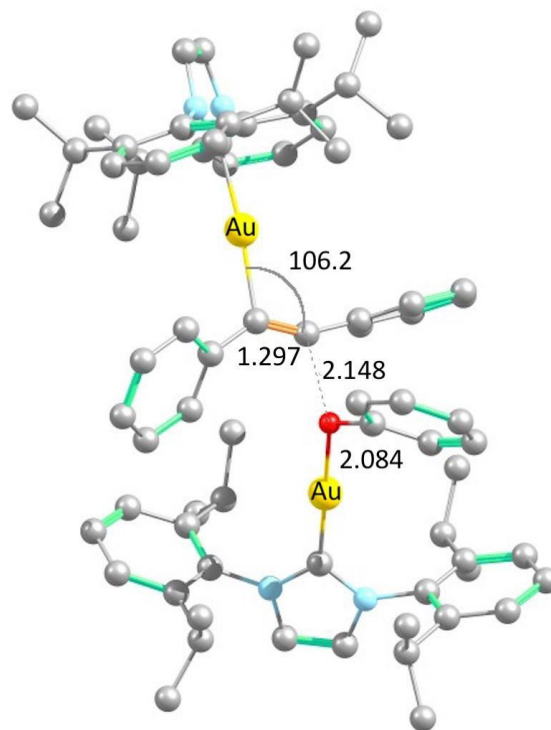
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6	3.135902000	3.534709000	-0.671869000
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1	1.824258000	3.678501000	-3.179790000
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6	-0.053491000	-1.139215000	-3.247714000
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6	-0.588597000	-3.497056000	-0.355228000
6	0.586981000	-3.497428000	0.354173000
6	-2.118721000	-1.727250000	-1.271036000
6	2.117770000	-1.728553000	1.270698000
1	-1.206441000	-4.319104000	-0.729953000
1	1.204479000	-4.319863000	0.728617000
6	-2.017428000	-1.463934000	-2.663146000
6	-3.192463000	-1.053669000	-3.327409000

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6	-5.338429000	3.772173000	0.000358000
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5+7-15 TS

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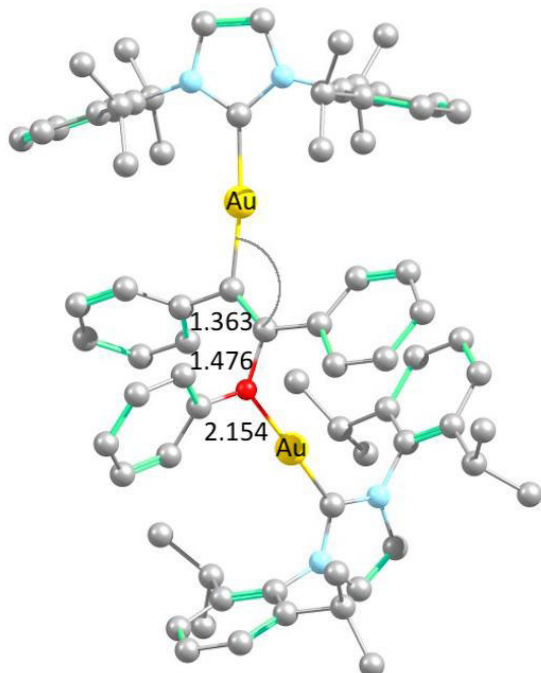
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6	-3.482068000	-3.538677000	4.039479000
6	-3.940032000	-4.077373000	2.829085000
6	-4.642098000	-3.286250000	1.896196000
6	-4.661614000	0.113979000	3.821968000
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Supporting Information

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Supporting Information

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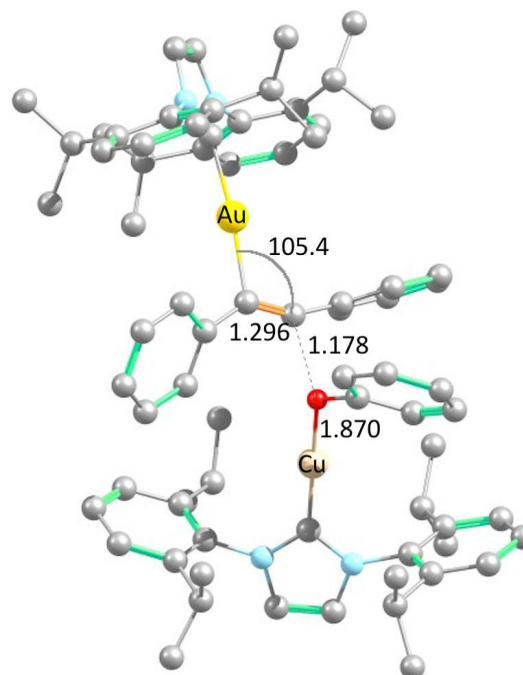
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Supporting Information

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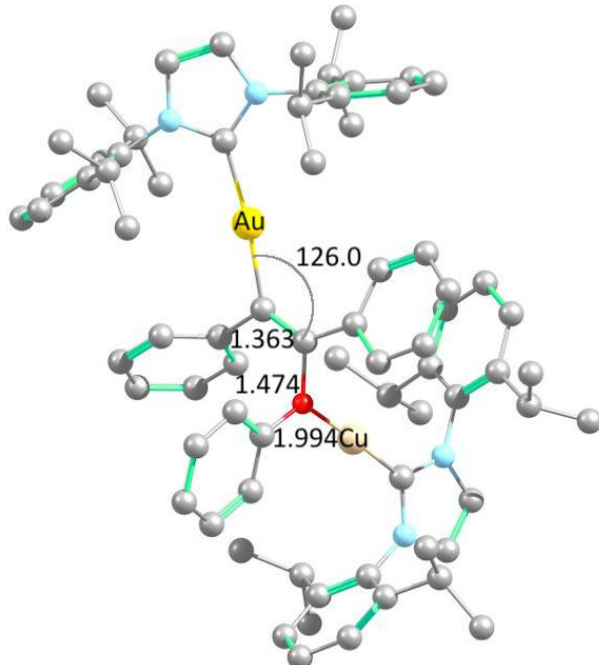
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Supporting Information

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Supporting Information

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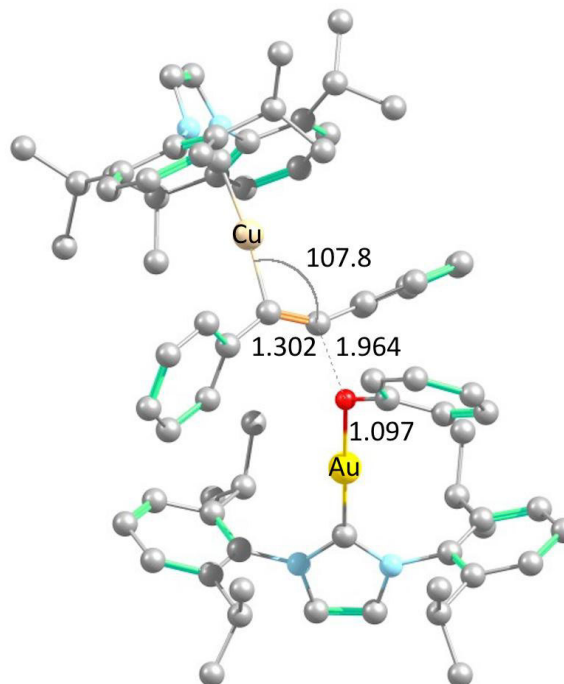
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1	2.283662000	5.067726000	3.657422000
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Supporting Information

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**2+7-17 TS**

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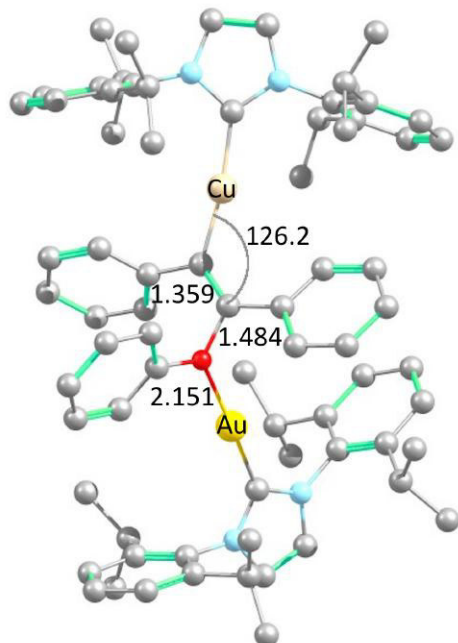
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Supporting Information

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Supporting Information

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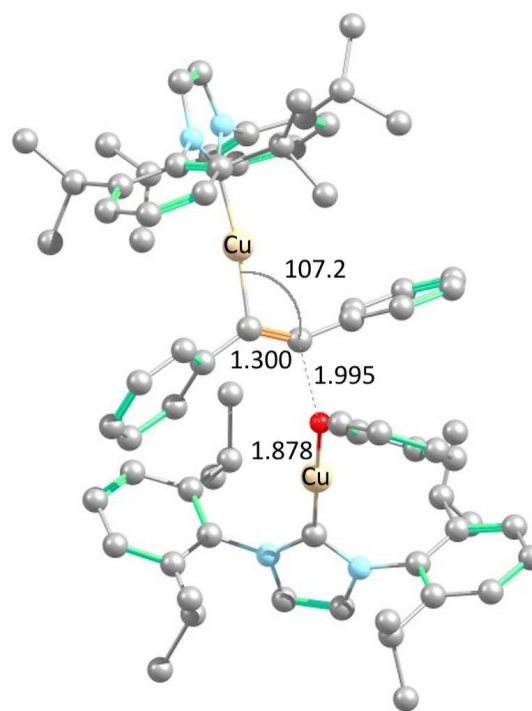
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Supporting Information

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**2+8-18 TS**

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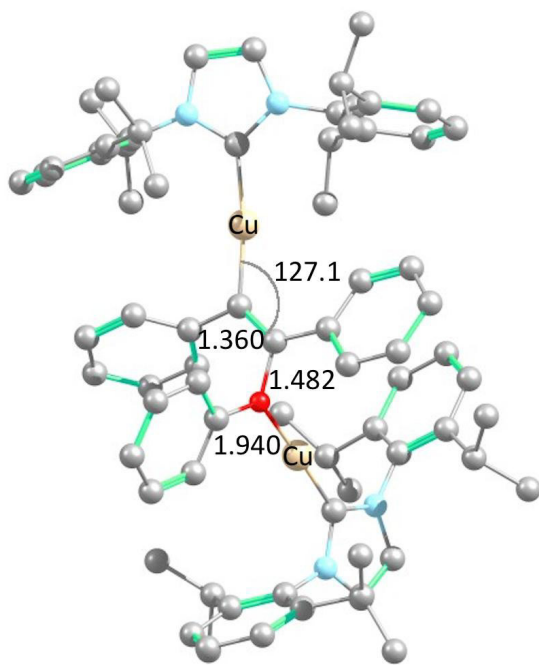
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Supporting Information

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Supporting Information

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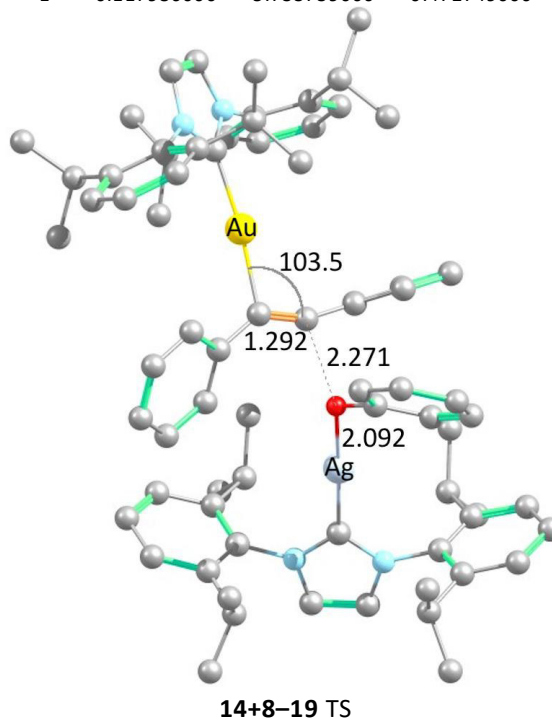
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1	6.266826000	1.072649000	-1.323696000
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Supporting Information

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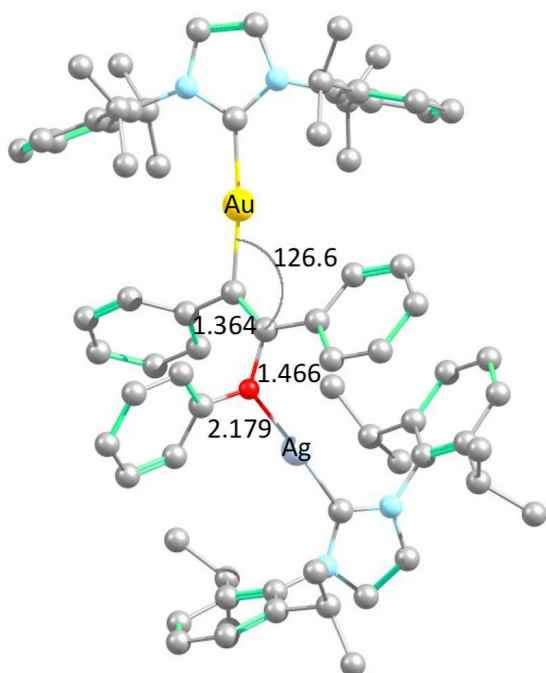
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Supporting Information

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Supporting Information

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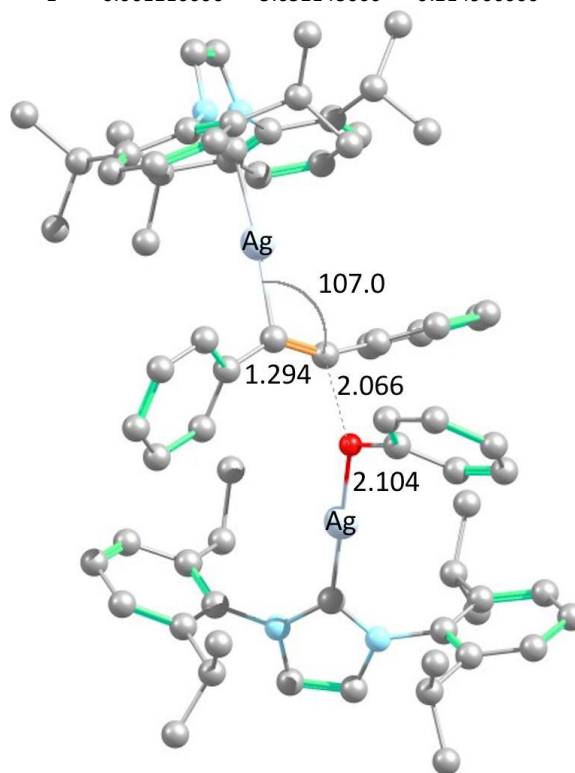
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Supporting Information

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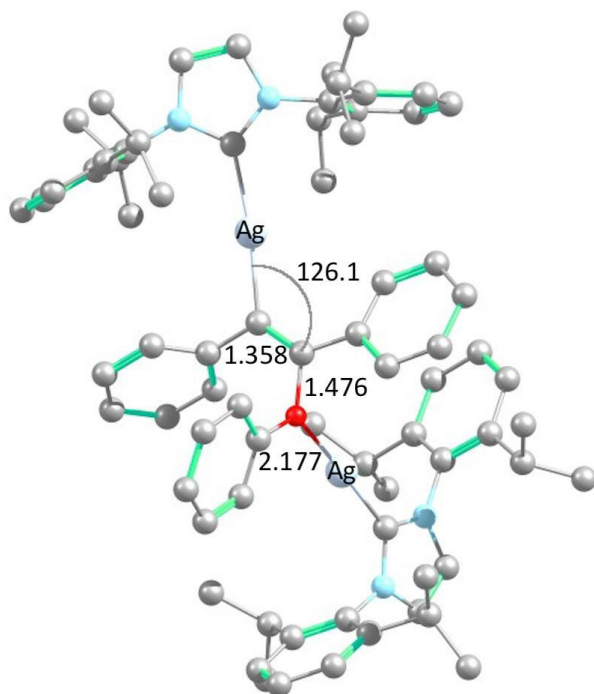
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6	-4.891444000	-2.267154000	1.890459000
6	-6.140944000	1.536394000	-1.004717000

Supporting Information

1	-7.067898000	-2.875833000	-3.108229000	1	-7.640791000	-1.814840000	1.866267000
6	-6.641304000	-0.252859000	-2.456172000	1	-8.361004000	0.347206000	0.209182000
6	-3.976471000	3.842048000	0.401517000	6	-4.378707000	-1.951851000	3.176838000
6	-3.041947000	4.852396000	0.710101000	6	-3.682657000	-2.970149000	3.860952000
6	-2.345334000	4.850695000	1.926053000	6	-3.511321000	-4.240677000	3.293506000
6	-2.567856000	3.835543000	2.867134000	6	-4.029230000	-4.520325000	2.021310000
6	-3.488827000	2.797100000	2.617787000	6	-4.732377000	-3.542826000	1.287244000
6	-4.763378000	3.902157000	-0.908755000	6	-4.564078000	-0.581521000	3.830081000
1	-2.860094000	5.658572000	-0.017300000	1	-3.273702000	-2.764085000	4.862757000
1	-1.623421000	5.653002000	2.145448000	1	-2.971091000	-5.022514000	3.850512000
1	-2.018638000	3.852053000	3.821100000	1	-3.886816000	-5.521808000	1.585859000
6	-3.765443000	1.739084000	3.687459000	6	-5.288998000	-3.882029000	-0.096207000
1	-5.777533000	-1.317112000	2.459695000	6	-6.202243000	1.286431000	-2.401857000
6	-5.022031000	-3.307208000	2.758203000	6	-6.164273000	2.406139000	-3.258985000
6	-7.441868000	-2.562168000	3.033130000	6	-6.077799000	3.709338000	-2.748882000
1	-6.346328000	0.639304000	-1.864965000	6	-6.023950000	3.922976000	-1.364300000
6	-5.623731000	-0.391583000	-3.607954000	6	-6.053773000	2.843939000	-0.456551000
6	-8.068051000	0.001230000	-2.991525000	6	-6.318841000	-0.120710000	-2.989141000
1	-5.306383000	2.940396000	-1.024847000	1	-6.210325000	2.253366000	-4.348760000
6	-5.823792000	5.025921000	-0.858020000	1	-6.057305000	4.568005000	-3.438483000
6	-3.846655000	4.054838000	-2.138953000	1	-5.960036000	4.951577000	-0.976122000
1	-4.326134000	0.910608000	3.204701000	6	-6.013954000	3.110007000	1.049065000
6	-2.475250000	1.132687000	4.274766000	1	-5.121374000	0.060593000	3.116332000
6	-4.663635000	2.316864000	4.805392000	6	-3.208181000	0.107697000	4.094446000
1	-4.834742000	-3.138709000	3.839090000	6	-5.408958000	-0.677938000	5.119010000
1	-5.311763000	-4.372371000	2.641025000	1	-5.780130000	-2.971180000	-0.497786000
1	-4.065917000	-3.155818000	2.216574000	6	-4.162093000	-4.258418000	-1.081361000
1	-7.279172000	-2.421595000	4.122049000	6	-6.363724000	-4.988237000	-0.018734000
1	-8.229754000	-1.850205000	2.711937000	1	-6.318672000	-0.840827000	-2.144234000
1	-7.839422000	-3.587827000	2.882079000	6	-7.650357000	-0.306086000	-3.748974000
1	-5.610529000	0.529273000	-4.227161000	6	-5.106234000	-0.467166000	-3.878946000
1	-4.596322000	-0.563859000	-3.224212000	1	-5.959383000	2.128034000	1.564109000
1	-5.875612000	-1.238323000	-4.279838000	6	-4.758270000	3.907643000	1.459294000
1	-8.089166000	0.909646000	-3.628835000	6	-7.306675000	3.807593000	1.527480000
1	-8.427193000	-0.848676000	-3.609032000	1	-3.363974000	1.122513000	4.516216000
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1	-4.447513000	4.015204000	-3.071272000	1	-4.901706000	-1.288089000	5.895722000
1	-3.311599000	5.027293000	-2.138134000	1	-4.579042000	-4.444813000	-2.093054000
1	-3.082819000	3.252131000	-2.186750000	1	-3.406064000	-3.450649000	-1.162088000
1	-2.723216000	0.310831000	4.977736000	1	-3.633190000	-5.181757000	-0.764902000
1	-1.817043000	0.720312000	3.483056000	1	-6.795497000	-5.182727000	-1.022581000
1	-1.887298000	1.880928000	4.845932000	1	-5.937823000	-5.944729000	0.350845000
1	-4.902183000	1.537277000	5.558735000	1	-7.194654000	-4.708429000	0.661201000
1	-4.157298000	3.152725000	5.332588000	1	-7.745391000	-1.348433000	-4.118306000
1	-5.621394000	2.708237000	4.405262000	1	-8.525125000	-0.092136000	-3.100926000
47	-3.137480000	-0.122517000	-0.290987000	1	-7.715435000	0.365862000	-4.630427000
6	-1.374645000	-2.145495000	-1.931980000	1	-5.183822000	-1.509453000	-4.252377000
6	-0.394383000	-2.457585000	-2.889241000	1	-5.043273000	0.198819000	-4.765046000
6	-2.449499000	-3.015252000	-1.686586000	1	-4.153561000	-0.373831000	-3.317167000
6	-0.506649000	-3.660393000	-3.608020000	1	-4.721951000	4.029257000	2.561993000
1	0.446390000	-1.770921000	-3.063931000	1	-3.827779000	3.397229000	1.136268000
6	-2.549342000	-4.211780000	-2.416175000	1	-4.754049000	4.925333000	1.015631000
1	-3.196784000	-2.760763000	-0.915749000	1	-7.289763000	3.947480000	2.628535000
6	-1.579083000	-4.540250000	-3.378951000	1	-7.421953000	4.810508000	1.065105000
1	0.257880000	-3.906489000	-4.361640000	1	-8.211197000	3.217436000	1.272875000
1	-3.390802000	-4.893517000	-2.218260000	47	-3.123728000	0.082668000	-0.152153000
1	-1.656525000	-5.480063000	-3.946592000	6	-0.427217000	-0.331049000	-0.838258000
8	-1.341677000	-0.934662000	-1.220324000	6	-1.153588000	0.732136000	-0.705721000
6	0.501139000	-1.942620000	0.628892000	6	4.922148000	0.247222000	0.745713000
6	-0.485338000	-1.825873000	1.641064000	7	6.058306000	-0.500736000	0.561558000
6	1.163672000	-3.187837000	0.493659000	7	5.237104000	1.100249000	1.773357000
6	-0.801833000	-2.910197000	2.476910000	6	7.058367000	-0.123647000	1.455162000
1	-0.987299000	-0.854564000	1.789304000	6	6.539325000	0.887916000	2.222224000

Supporting Information

6	0.829677000	-4.278517000	1.312659000
1	1.951170000	-3.294065000	-0.268759000
6	-0.152448000	-4.146698000	2.310758000
1	-1.555763000	-2.785269000	3.270881000
1	1.351896000	-5.238700000	1.175997000
1	-0.401912000	-4.998364000	2.963091000
6	-0.024755000	0.980793000	-1.904236000
6	-0.835491000	1.092793000	-3.065263000
6	0.810968000	2.077772000	-1.571070000
6	-0.786067000	2.240070000	-3.874215000
1	-1.495804000	0.260867000	-3.352107000
6	0.856783000	3.221413000	-2.380582000
1	1.427626000	2.019820000	-0.660057000
6	0.061537000	3.309711000	-3.538858000
1	-1.412252000	2.293242000	-4.779024000
1	1.518859000	4.053904000	-2.095635000
1	0.099101000	4.209377000	-4.173202000



20 [Ag(IPr)(PhO)(PhCCPh)(IPr)Ag]⁺ min

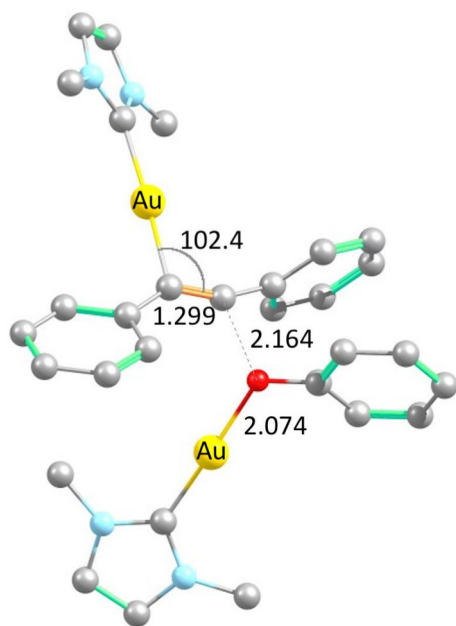
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6	7.047600000	1.146007000	0.422264000
6	7.202444000	-0.189720000	0.690463000
6	5.136617000	2.629864000	-0.213329000
6	5.686968000	-2.183227000	0.755747000
1	7.767481000	1.970378000	0.415137000
1	8.086004000	-0.775129000	0.963400000
6	4.576427000	3.422075000	0.824067000
6	4.065725000	4.687193000	0.466447000
6	4.124307000	5.147428000	-0.856879000
6	4.690431000	4.344755000	-1.857433000
6	5.209085000	3.066264000	-1.562842000
6	4.509585000	2.954767000	2.278628000
1	3.623480000	5.329143000	1.244523000

6	6.229564000	-1.528192000	-0.448722000
6	4.362198000	2.126341000	2.305522000
1	8.041689000	-0.603998000	1.462308000
1	6.974646000	1.473856000	3.037623000
6	6.680256000	-1.140549000	-1.739066000
6	6.865472000	-2.164894000	-2.690863000
6	6.618931000	-3.507544000	-2.372247000
6	6.179343000	-3.857870000	-1.087966000
6	5.974171000	-2.879157000	-0.093435000
6	6.996438000	0.309402000	-2.108319000
1	7.215041000	-1.902723000	-3.701661000
1	6.775058000	-4.289841000	-3.131710000
1	5.993362000	-4.916671000	-0.848910000
6	5.518447000	-3.294989000	1.305606000
6	3.514429000	1.800303000	3.396787000
6	2.687743000	2.825887000	3.900959000
6	2.711806000	4.115019000	3.350584000
6	3.569582000	4.408849000	2.281188000
6	4.418254000	3.424789000	1.731907000
6	3.480384000	0.410026000	4.032564000
1	2.015805000	2.610466000	4.746589000
1	2.059737000	4.900695000	3.763500000
1	3.588164000	5.428526000	1.864953000
6	5.354240000	3.782601000	0.576374000
1	6.671435000	0.952564000	-1.263612000
6	6.217276000	0.774716000	-3.355975000
6	8.517886000	0.513167000	-2.286249000
1	5.320554000	-2.369459000	1.886283000
6	4.200468000	-4.095980000	1.266921000
6	6.628479000	-4.075267000	2.044588000
1	4.189642000	-0.236091000	3.474559000
6	3.953132000	0.448621000	5.502162000
6	2.085016000	-0.236672000	3.905220000
1	5.920900000	2.868120000	0.302463000
6	4.569000000	4.220239000	-0.678123000
6	6.387350000	4.850427000	0.998054000
1	6.410997000	1.849754000	-3.551848000
1	6.522835000	0.216233000	-4.265463000
1	5.123377000	0.638158000	-3.230968000
1	8.746261000	1.577316000	-2.504257000
1	9.081971000	0.221512000	-1.376269000
1	8.909692000	-0.092861000	-3.130200000
1	3.860000000	-4.327029000	2.298047000
1	3.394577000	-3.530642000	0.755475000
1	4.322721000	-5.064066000	0.737070000
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1	6.866707000	-5.027659000	1.525826000
1	7.568504000	-3.489776000	2.112461000
1	3.976924000	-0.575074000	5.930821000
1	4.970983000	0.880311000	5.593476000
1	3.273911000	1.058702000	6.134128000
1	2.096075000	-1.267864000	4.315878000
1	1.314800000	0.336244000	4.463103000
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1	5.262831000	4.410571000	-1.523086000
1	3.845380000	3.441991000	-0.997528000
1	4.001705000	5.157993000	-0.500051000
1	7.093562000	5.057087000	0.167157000
1	5.897580000	5.810878000	1.263731000
1	6.980571000	4.524129000	1.877122000
47	3.188279000	0.138450000	-0.344715000
6	1.587038000	-0.151428000	-2.861393000
6	0.787114000	0.527636000	-3.817370000
6	2.498475000	-1.138846000	-3.317165000
6	0.911102000	0.230402000	-5.183149000
1	0.083263000	1.297134000	-3.465571000

Supporting Information

6	1.255711000	-3.212844000	0.579573000
6	-0.704634000	-2.858947000	2.554387000
1	-0.900975000	-0.835171000	1.781414000
6	0.926279000	-4.269609000	1.443180000
1	2.041435000	-3.351311000	-0.180086000
6	-0.053171000	-4.100068000	2.438596000
1	-1.459019000	-2.703425000	3.342660000
1	1.450593000	-5.233395000	1.344091000
1	-0.298469000	-4.924592000	3.126292000
6	0.087177000	0.831610000	-2.013283000
6	-0.702403000	0.890671000	-3.191904000
6	0.932763000	1.934389000	-1.727772000
6	-0.618656000	1.988055000	-4.065041000
1	-1.373545000	0.055294000	-3.440966000
6	1.013004000	3.029104000	-2.600105000
1	1.526064000	1.925292000	-0.799233000
6	0.241266000	3.061631000	-3.777162000
1	-1.229147000	1.999170000	-4.981996000
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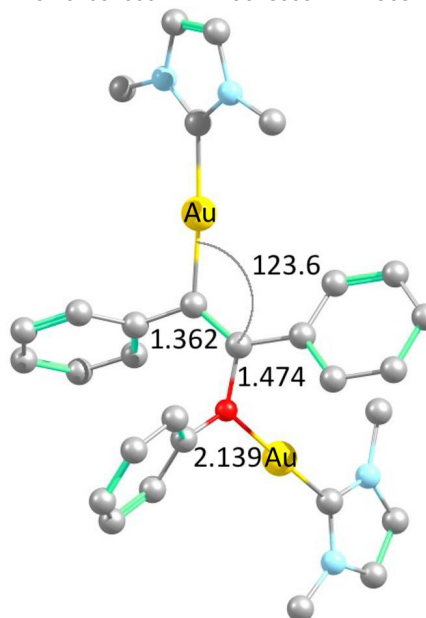
**21+22-23 TS**

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7	-5.496245000	0.117590000	-1.648182000
6	-7.136710000	-0.781096000	-0.458859000
6	-6.865836000	-0.117080000	-1.628630000
6	-5.778909000	-1.586660000	1.505659000
6	-4.796499000	0.804536000	-2.732579000
1	-8.082413000	-1.151462000	-0.049626000
1	-7.529301000	0.203838000	-2.438443000
79	-2.934634000	-0.332885000	-0.006335000
6	-0.461751000	0.751989000	0.277961000
6	-0.921272000	-0.403011000	0.657056000
6	3.996588000	-1.537833000	-1.069221000
7	3.716975000	-2.835579000	-1.408867000
7	5.277126000	-1.320167000	-1.506826000
6	4.803677000	-3.416927000	-2.051152000

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1	-1.834093000	-0.949904000	-2.333381000
6	-2.932192000	1.046421000	2.257296000
1	-1.833664000	0.949856000	2.334296000
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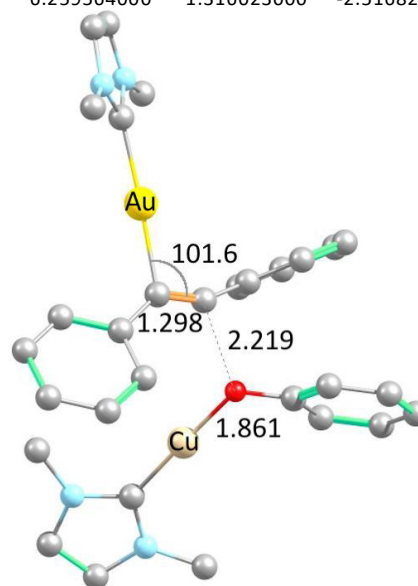
**23 [Au(IME)(PhO)(PhCCPh)(IME)Au]⁺ min**

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7	5.881038000	-0.381034000	-1.307500000
6	6.988550000	-1.626387000	0.152944000
6	7.121770000	-0.941280000	-1.028589000
6	5.113357000	-2.024627000	1.791006000
6	5.591027000	0.432856000	-2.486725000
1	7.717349000	-2.206076000	0.728967000
1	7.988629000	-0.809690000	-1.684505000
79	3.006266000	-0.113003000	-0.228314000
6	0.073648000	-0.010040000	0.557862000
6	1.073183000	0.603871000	-0.134456000
6	-4.535898000	-1.089196000	-0.895122000
7	-5.848681000	-0.750404000	-0.711115000
7	-4.548754000	-2.168770000	-1.735518000
6	-6.672815000	-1.606855000	-1.430441000
6	-5.854483000	-2.499148000	-2.075714000
6	-6.334814000	0.348343000	0.124198000
6	-3.366087000	-2.877781000	-2.226511000
1	-7.763804000	-1.514600000	-1.421296000
1	-6.092615000	-3.335825000	-2.740632000
79	-2.947220000	-0.211944000	-0.108457000
6	-1.258535000	1.876200000	1.515595000
6	-0.383808000	2.053585000	2.598249000
6	-2.234485000	2.831813000	1.195436000
6	-0.507238000	3.215282000	3.380359000
1	0.386329000	1.300132000	2.818904000
6	-2.349070000	3.983721000	1.992554000
1	-2.878951000	2.679265000	0.314739000
6	-1.487880000	4.179151000	3.086323000
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Supporting Information

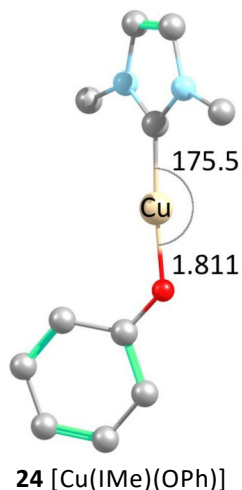
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6	6.020323000	-0.070428000	-1.352686000	8	-1.205996000	0.700436000	0.735127000
1	4.790591000	-4.453094000	-2.404587000	6	0.836784000	1.891811000	-0.846980000
1	6.799094000	-2.504030000	-2.527494000	6	-0.142471000	1.989414000	-1.868762000
79	2.813720000	-0.259626000	-0.122455000	6	1.624988000	3.038087000	-0.573566000
6	1.950232000	2.252388000	1.311205000	6	-0.329350000	3.185205000	-2.581639000
6	1.509794000	2.787518000	2.548582000	1	-0.744668000	1.101330000	-2.122617000
6	2.754388000	3.057982000	0.467068000	6	1.421439000	4.239764000	-1.270472000
6	1.891223000	4.080943000	2.937465000	1	2.401916000	2.977054000	0.205391000
1	0.880091000	2.164174000	3.202477000	6	0.445635000	4.319564000	-2.280431000
6	3.132004000	4.350108000	0.866451000	1	-1.084237000	3.230173000	-3.383414000
1	3.076549000	2.650489000	-0.505622000	1	2.037516000	5.120483000	-1.028419000
6	2.704927000	4.869222000	2.102319000	1	0.296563000	5.258200000	-2.836873000
1	1.553892000	4.475980000	3.909213000	6	0.008657000	-1.345929000	1.186979000
1	3.764881000	4.960011000	0.201827000	6	-0.800546000	-1.581638000	2.330693000
1	3.004743000	5.881759000	2.413351000	6	0.733138000	-2.442061000	0.648264000
8	1.573144000	0.990085000	0.974020000	6	-0.855356000	-2.851574000	2.928168000
6	-0.457947000	-1.569622000	1.430627000	1	-1.376351000	-0.753700000	2.772227000
6	-0.966896000	-2.861177000	1.137185000	6	0.677435000	-3.708175000	1.250157000
6	0.469502000	-1.435245000	2.495882000	1	1.333228000	-2.286021000	-0.262357000
6	-0.552629000	-3.983441000	1.872484000	6	-0.114356000	-3.920588000	2.394688000
1	-1.696776000	-2.972810000	0.318790000	1	-1.478812000	-3.003602000	3.823442000
6	0.867420000	-2.558511000	3.237727000	1	1.245914000	-4.543686000	0.810885000
1	0.872666000	-0.439919000	2.725266000	1	-0.159653000	-4.916446000	2.862794000
6	0.363292000	-3.835787000	2.929717000	1	-5.464475000	0.846299000	0.589751000
1	-0.958965000	-4.977656000	1.627234000	1	-6.999267000	-0.043198000	0.919330000
1	1.579314000	-2.433006000	4.069037000	1	-6.889578000	1.081185000	-0.494233000
1	0.676616000	-4.712216000	3.518730000	1	-2.477504000	-2.495801000	-1.691023000
6	-0.533944000	2.003851000	-0.420614000	1	-3.240177000	-2.708632000	-3.314409000
6	-0.146897000	2.081895000	-1.787683000	1	-3.469894000	-3.962451000	-2.029731000
6	-0.954103000	3.185611000	0.247764000	1	4.029271000	-1.805832000	1.811274000
6	-0.208545000	3.303707000	-2.469081000	1	5.595538000	-1.565069000	2.677102000
1	0.196742000	1.169113000	-2.298236000	1	5.268012000	-3.121422000	1.817441000
6	-1.007220000	4.405031000	-0.443498000	1	4.540144000	0.772034000	-2.422559000
1	-1.248118000	3.129620000	1.305747000	1	5.728423000	-0.163377000	-3.410896000
6	-0.638664000	4.466752000	-1.799050000	1	6.259564000	1.316023000	-2.516820000
1	0.084416000	3.354777000	-3.529565000				
1	-1.336276000	5.315094000	0.081369000				
1	-0.681144000	5.426740000	-2.337344000				
1	5.382535000	0.647736000	-0.804949000				
1	6.278060000	0.348692000	-2.345632000				
1	6.948750000	-0.247189000	-0.774584000				
1	1.821341000	-2.870958000	-0.511532000				
1	2.649131000	-4.469646000	-0.597465000				
1	1.926866000	-3.745096000	-2.089313000				
1	-4.705389000	-1.597124000	1.771469000				
1	-6.154166000	-2.627801000	1.455082000				
1	-6.341571000	-1.029414000	2.280772000				
1	-4.906095000	0.238963000	-3.679263000				
1	-3.725100000	0.872551000	-2.468471000				
1	-5.204927000	1.825910000	-2.864712000				



$E(\text{scf}) = -1788.21511888 \text{ a.u.}$

$\nu_{\text{min}} = -99.3138 \text{ cm}^{-1}$

Supporting Information

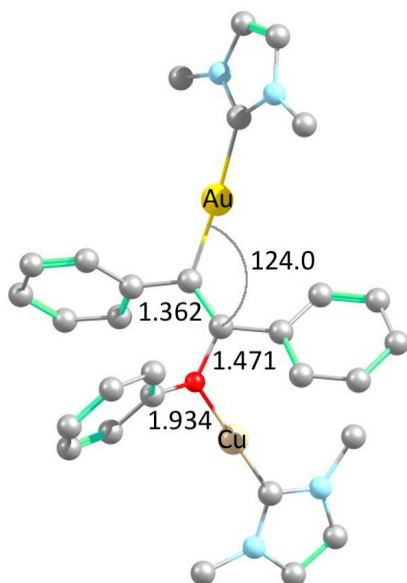


$E(\text{scf}) = -808.781095257 \text{ a.u.}$

29	0.343120000	-0.458284000	-0.166935000
8	-1.356909000	-1.057440000	-0.340989000
6	2.128755000	0.024218000	-0.037543000
7	2.683010000	1.271971000	-0.209025000
6	4.059441000	1.243424000	-0.018913000
1	4.686409000	2.136633000	-0.108682000
6	4.388961000	-0.055205000	0.278906000
1	5.359144000	-0.513528000	0.497305000
7	3.203598000	-0.780589000	0.263967000
6	1.917490000	2.468547000	-0.543460000
6	3.105278000	-2.212818000	0.524810000
6	-2.522629000	-0.454966000	-0.107066000
6	-3.729600000	-1.085651000	-0.528565000
6	-2.640330000	0.798635000	0.560890000
6	-4.976537000	-0.486992000	-0.298930000
1	-3.650533000	-2.056373000	-1.043408000
6	-3.893381000	1.389130000	0.785661000
1	-1.715220000	1.292581000	0.908089000
6	-5.075342000	0.755349000	0.358136000
1	-5.891331000	-1.000443000	-0.640510000
1	-3.947525000	2.360003000	1.307105000
1	-6.057643000	1.220580000	0.535952000
1	0.857096000	2.175714000	-0.664654000
1	2.282848000	2.910982000	-1.492146000
1	1.995565000	3.221814000	0.266685000
1	3.533963000	-2.456146000	1.517848000
1	3.638685000	-2.791477000	-0.256644000
1	2.034427000	-2.492266000	0.513939000

6	-4.557671000	-0.254469000	-0.418803000
7	-5.561396000	-0.784347000	0.347481000
7	-5.190125000	0.303559000	-1.497418000
6	-6.799587000	-0.559600000	-0.241200000
6	-6.565482000	0.127388000	-1.405628000
6	-5.371323000	-1.483378000	1.618289000
6	-4.522935000	0.994021000	-2.600016000
1	-7.736380000	-0.901478000	0.211048000
1	-7.258440000	0.501125000	-2.166628000
79	-2.564343000	-0.306330000	-0.015905000
6	-0.053195000	0.667381000	0.208019000
6	-0.522702000	-0.497327000	0.534564000
6	4.258847000	-1.559678000	-1.035741000
7	3.981182000	-2.838782000	-1.448530000
7	5.563258000	-1.353317000	-1.413373000
6	5.082530000	-3.413513000	-2.070208000
6	6.083268000	-2.474497000	-2.047178000
6	2.697171000	-3.510765000	-1.264696000
6	6.314959000	-0.124769000	-1.168049000
1	5.068658000	-4.432306000	-2.471356000
1	7.111171000	-2.516900000	-2.422318000
29	3.144009000	-0.361046000	-0.146957000
6	2.496974000	2.042863000	1.195568000
6	2.147691000	2.545123000	2.476665000
6	3.275504000	2.861975000	0.336300000
6	2.591891000	3.810297000	2.890504000
1	1.537219000	1.914998000	3.142460000
6	3.716029000	4.125894000	0.759996000
1	3.521584000	2.486609000	-0.671237000
6	3.379153000	4.607701000	2.038489000
1	2.323977000	4.177299000	3.894430000
1	4.325876000	4.744219000	0.081580000
1	3.727614000	5.598346000	2.368766000
8	2.073842000	0.811420000	0.825196000
6	-0.061694000	-1.728225000	1.200901000
6	-0.642536000	-2.978042000	0.863753000
6	0.941227000	-1.696819000	2.204744000
6	-0.225754000	-4.160122000	1.496768000
1	-1.429344000	-3.009351000	0.092591000
6	1.342803000	-2.880638000	2.844153000
1	1.395143000	-0.731870000	2.468371000
6	0.766364000	-4.115613000	2.492970000
1	-0.688539000	-5.120559000	1.219318000
1	2.113207000	-2.836147000	3.630383000
1	1.082581000	-5.039686000	3.002171000
6	-0.088481000	1.969815000	-0.386634000
6	0.264243000	2.140097000	-1.755076000
6	-0.436944000	3.111873000	0.385269000
6	0.240108000	3.413690000	-2.335652000
1	0.551300000	1.257196000	-2.346753000
6	-0.453821000	4.383462000	-0.206580000
1	-0.705930000	2.983909000	1.443616000
6	-0.119039000	4.536942000	-1.563489000
1	0.506367000	3.536951000	-3.397194000
1	-0.727090000	5.262111000	0.397764000
1	-0.132243000	5.537725000	-2.023200000
1	5.651918000	0.593004000	-0.649160000
1	6.655159000	0.318754000	-2.125153000
1	7.195133000	-0.330796000	-0.526763000
1	2.042140000	-2.863827000	-0.651482000
1	2.841578000	-4.473820000	-0.736953000
1	2.212658000	-3.698739000	-2.244104000
1	-4.286628000	-1.539758000	1.826752000
1	-5.786278000	-2.508725000	1.556196000
1	-5.872644000	-0.931987000	2.438336000
1	-4.719515000	0.469439000	-3.556108000

Supporting Information

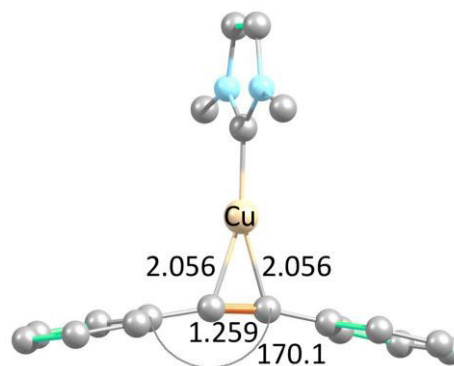


25 [Cu(Ime)(Pho)(PhCCPh)(Ime)Au]⁺ min

E(scf) = -1788.23510142 a.u.

6	4.533795000	-0.724952000	-0.205667000
7	5.193291000	-1.503357000	0.709546000
7	5.479569000	-0.422603000	-1.150746000
6	6.522072000	-1.683347000	0.343784000
6	6.702490000	-1.000829000	-0.832906000
6	4.591267000	-2.053955000	1.921870000
6	5.239264000	0.395510000	-2.338327000
1	7.223801000	-2.273163000	0.942700000
1	7.591552000	-0.881926000	-1.460943000
79	2.575818000	-0.110118000	-0.172900000
6	-0.414085000	-0.006150000	0.383647000
6	0.653898000	0.641129000	-0.159616000
6	-4.728527000	-1.158991000	-0.834487000
7	-6.026262000	-0.728051000	-0.935796000
7	-4.744519000	-2.436227000	-1.332677000
6	-6.833945000	-1.714130000	-1.486907000
6	-6.023364000	-2.793120000	-1.738711000
6	-6.507200000	0.586701000	-0.516107000
6	-3.573209000	-3.305638000	-1.440910000
1	-7.907578000	-1.573774000	-1.650477000
1	-6.253794000	-3.774247000	-2.166999000
29	-3.251529000	-0.244297000	-0.163967000
6	-1.812096000	1.834099000	1.331551000
6	-1.089978000	1.923609000	2.531085000
6	-2.709711000	2.837941000	0.936489000
6	-1.289177000	3.045459000	3.355017000
1	-0.377062000	1.133714000	2.809770000
6	-2.902369000	3.949055000	1.775247000
1	-3.224216000	2.756742000	-0.033925000
6	-2.194909000	4.055817000	2.985598000
1	-0.728844000	3.124631000	4.299697000
1	-3.599323000	4.744619000	1.468841000
1	-2.343369000	4.930266000	3.637188000
8	-1.699442000	0.699029000	0.499315000
6	0.499272000	1.989107000	-0.777278000
6	-0.382944000	2.187461000	-1.870541000
6	1.273456000	3.093040000	-0.340037000
6	-0.488005000	3.440082000	-2.497161000

1	-3.435413000	0.998359000	-2.401623000
1	-4.884759000	2.038723000	-2.672191000



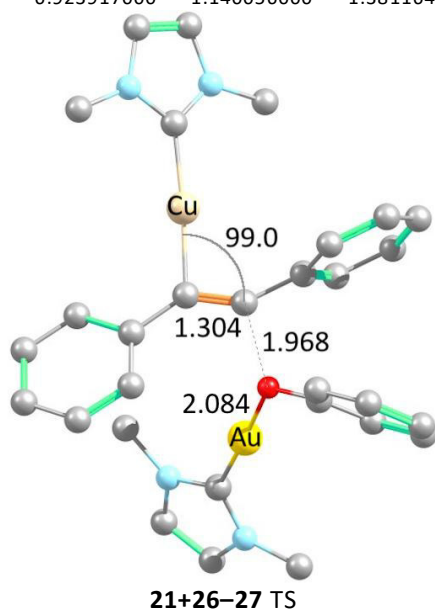
26 [Cu(Ime)(PhCCPh)]⁺

E(scf) = -1041.00301361 a.u.

6	0.036525000	2.347450000	-0.000062000
7	0.051838000	3.184387000	-1.085156000
7	0.051237000	3.184238000	1.085144000
6	0.075589000	4.512682000	-0.686808000
6	0.075211000	4.512590000	0.686998000
6	0.044623000	2.747411000	-2.480941000
6	0.043094000	2.746966000	2.480842000
1	0.090808000	5.343582000	-1.400202000
1	0.089984000	5.343379000	1.400531000
29	0.004348000	0.446694000	-0.000373000
6	0.604739000	-1.519976000	0.000009000
6	-0.653806000	-1.501177000	-0.000177000
6	2.020021000	-1.787632000	0.000212000
6	2.721210000	-1.930589000	1.228222000
6	2.721172000	-1.931601000	-1.227738000
6	4.092436000	-2.217733000	1.220032000
1	2.177323000	-1.828247000	2.179630000
6	4.092378000	-2.218738000	-1.219388000
1	2.177195000	-1.830019000	-2.179174000
6	4.780417000	-2.360486000	0.000375000
1	4.629343000	-2.336325000	2.173820000
1	4.629263000	-2.338115000	-2.173090000
1	5.857806000	-2.587491000	0.000443000
6	-2.076227000	-1.728471000	-0.000116000
6	-2.781194000	-1.851195000	1.227904000
6	-2.781266000	-1.851911000	-1.228037000
6	-4.160139000	-2.098816000	1.219746000
1	-2.234602000	-1.764617000	2.179326000
6	-4.160205000	-2.099535000	-1.219652000
1	-2.234719000	-1.765853000	-2.179534000
6	-4.852006000	-2.221476000	0.000106000
1	-4.700189000	-2.201996000	2.173551000
1	-4.700328000	-2.203270000	-2.173355000
1	-5.935516000	-2.417189000	0.000189000
1	0.023285000	1.641498000	2.502034000
1	-0.854173000	3.136323000	3.001148000
1	0.953514000	3.103960000	3.001501000
1	0.955311000	3.104669000	-3.000948000
1	-0.852401000	3.136711000	-3.001711000
1	0.025042000	1.641942000	-2.502399000

Supporting Information

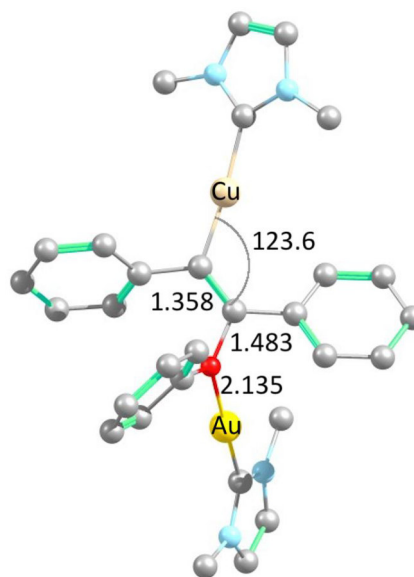
1	-0.970576000	1.334679000	-2.248182000
6	1.150494000	4.350312000	-0.952577000
1	1.975043000	2.953229000	0.497979000
6	0.272243000	4.530108000	-2.036536000
1	-1.165493000	3.564862000	-3.357436000
1	1.753449000	5.196130000	-0.585465000
1	0.187713000	5.512918000	-2.526294000
6	-0.553847000	-1.395157000	0.872561000
6	-1.462499000	-1.720374000	1.917394000
6	0.187804000	-2.454725000	0.285458000
6	-1.600517000	-3.043135000	2.371780000
1	-2.040314000	-0.921732000	2.409129000
6	0.048857000	-3.773413000	0.744845000
1	0.871397000	-2.224781000	-0.547321000
6	-0.844540000	-4.076356000	1.790382000
1	-2.297226000	-3.263650000	3.196018000
1	0.635370000	-4.577191000	0.271478000
1	-0.952235000	-5.112523000	2.147740000
1	4.192518000	0.751713000	-2.306441000
1	5.395463000	-0.203141000	-3.257939000
1	5.922476000	1.267809000	-2.347525000
1	3.514736000	-1.800467000	1.918952000
1	5.067151000	-1.616839000	2.822550000
1	4.710047000	-3.155432000	1.942932000
1	-2.725961000	-2.832982000	-0.908802000
1	-3.299221000	-3.456317000	-2.504380000
1	-3.785478000	-4.286882000	-0.973817000
1	-5.655943000	1.154810000	-0.096928000
1	-7.288360000	0.481297000	0.262726000
1	-6.923917000	1.140056000	-1.381164000



$E(\text{scf}) = -1788.20398027 \text{ a.u.}$

$\nu_{\text{min}} = -203.6824 \text{ cm}^{-1}$

6	-4.849025000	-0.780211000	-0.520571000
7	-5.867279000	-1.472556000	0.084969000
7	-5.427387000	-0.228649000	-1.635532000
6	-7.049875000	-1.356453000	-0.634216000
6	-6.771187000	-0.569337000	-1.723830000
6	-5.732375000	-2.225953000	1.330024000
6	-4.723629000	0.598547000	-2.613085000
1	-7.983661000	-1.832971000	-0.317612000



27 [Au(IMe)(PhCCPh)(IMe)Cu]⁺ min

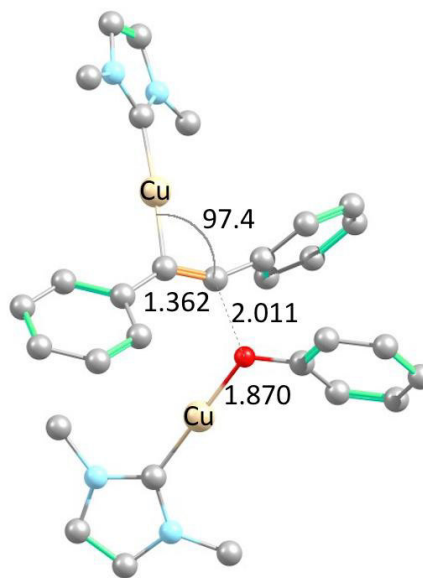
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6	5.121091000	-0.757258000	-0.458188000
7	5.880468000	-1.469057000	0.436930000
7	5.976283000	-0.509950000	-1.503537000
6	7.172438000	-1.660233000	-0.036957000
6	7.232448000	-1.053823000	-1.267176000
6	5.400696000	-1.940705000	1.733452000
6	5.611473000	0.226635000	-2.711596000
1	7.936723000	-2.202365000	0.529834000
1	8.058345000	-0.967948000	-1.981207000
29	3.306408000	-0.193788000	-0.290441000
6	0.539932000	-0.042552000	0.558779000
6	1.540066000	0.536581000	-0.155160000
6	-4.083810000	-1.051037000	-0.905607000
7	-5.392382000	-0.693018000	-0.727564000
7	-4.108844000	-2.128252000	-1.748909000
6	-6.225692000	-1.535087000	-1.453288000
6	-5.417679000	-2.438139000	-2.096552000
6	-5.866209000	0.411587000	0.107128000
6	-2.934708000	-2.854974000	-2.234099000
1	-7.315176000	-1.426131000	-1.449707000
1	-5.665061000	-3.269534000	-2.764708000
79	-2.486504000	-0.198404000	-0.109096000
6	-0.771267000	1.867565000	1.510480000
6	0.108343000	2.041323000	2.590075000
6	-1.729454000	2.838516000	1.181807000
6	0.009606000	3.214430000	3.358384000
1	0.861278000	1.273483000	2.820193000
6	-1.820085000	4.001794000	1.965245000
1	-2.379476000	2.687117000	0.304936000
6	-0.952518000	4.193798000	3.054643000
1	0.693681000	3.357667000	4.209406000
1	-2.566213000	4.769871000	1.708590000
1	-1.022174000	5.108502000	3.662709000
8	-0.740085000	0.683163000	0.745652000
6	1.348560000	1.823628000	-0.875327000
6	0.366801000	1.960930000	-1.891722000
6	2.193703000	2.935037000	-0.621631000
6	0.233039000	3.157561000	-2.614957000
1	-0.282168000	1.102016000	-2.130611000

Supporting Information

1	-7.414949000	-0.228606000	-2.541591000
29	-3.047053000	-0.633552000	0.066444000
6	-0.885660000	0.597453000	0.388941000
6	-1.227241000	-0.605062000	0.761179000
6	3.602595000	-1.295110000	-1.103554000
7	3.398774000	-2.594089000	-1.488560000
7	4.887626000	-1.004872000	-1.479352000
6	4.537953000	-3.105369000	-2.098514000
6	5.476067000	-2.104610000	-2.091979000
6	2.160803000	-3.348287000	-1.293812000
6	5.563601000	0.273614000	-1.261509000
1	4.589237000	-4.130494000	-2.479570000
1	6.505397000	-2.086855000	-2.464721000
79	2.317031000	-0.106062000	-0.177430000
6	1.230347000	2.355008000	1.248943000
6	0.730138000	2.842036000	2.479352000
6	1.991769000	3.212869000	0.422684000
6	1.013214000	4.157103000	2.881475000
1	0.134306000	2.171315000	3.117683000
6	2.275623000	4.524455000	0.838065000
1	2.357427000	2.833109000	-0.545689000
6	1.789182000	5.003265000	2.067695000
1	0.629615000	4.522149000	3.847625000
1	2.878381000	5.180650000	0.189998000
1	2.012799000	6.031616000	2.390594000
8	0.960203000	1.060059000	0.890674000
6	-0.634203000	-1.716482000	1.520169000
6	-1.047131000	-3.048133000	1.254656000
6	0.327054000	-1.504131000	2.543735000
6	-0.510033000	-4.130047000	1.970709000
1	-1.801327000	-3.223018000	0.469155000
6	0.848588000	-2.586940000	3.268741000
1	0.654956000	-0.478180000	2.760792000
6	0.438103000	-3.903018000	2.984687000
1	-0.844308000	-5.155506000	1.745846000
1	1.584311000	-2.399906000	4.067168000
1	0.849005000	-4.748104000	3.559246000
6	-1.286180000	1.806753000	-0.311766000
6	-0.880608000	2.026014000	-1.655456000
6	-2.060044000	2.800224000	0.342941000
6	-1.265206000	3.193520000	-2.330014000
1	-0.263538000	1.265054000	-2.158353000
6	-2.439658000	3.966772000	-0.339364000
1	-2.363884000	2.640742000	1.388345000
6	-2.045790000	4.165726000	-1.674545000
1	-0.950035000	3.351426000	-3.373565000
1	-3.041226000	4.729879000	0.178678000
1	-2.340447000	5.084947000	-2.204937000
1	4.870621000	0.947463000	-0.724703000
1	5.843299000	0.730274000	-2.231621000
1	6.473877000	0.123991000	-0.648037000
1	1.468029000	-2.741936000	-0.680680000
1	2.375955000	-4.295859000	-0.762796000
1	1.688431000	-3.571399000	-2.271403000
1	-4.684353000	-2.145414000	1.675209000
1	-5.980248000	-3.293530000	1.165257000
1	-6.403172000	-1.811082000	2.108632000
1	-4.663393000	0.078644000	-3.590480000
1	-3.700661000	0.793758000	-2.240052000
1	-5.248255000	1.565192000	-2.745073000

6	2.042369000	4.138988000	-1.327792000
1	2.972110000	2.846231000	0.154013000
6	1.063707000	4.256608000	-2.331437000
1	-0.527098000	3.232233000	-3.409672000
1	2.701543000	4.991432000	-1.097964000
1	0.955095000	5.196156000	-2.895579000
6	0.480225000	-1.365270000	1.214131000
6	-0.356591000	-1.606230000	2.336074000
6	1.261366000	-2.446412000	0.725754000
6	-0.386070000	-2.865563000	2.958511000
1	-0.973660000	-0.790187000	2.742241000
6	1.233275000	-3.700477000	1.353108000
1	1.881955000	-2.286557000	-0.172351000
6	0.410311000	-3.917965000	2.475018000
1	-1.033512000	-3.021427000	3.835971000
1	1.845292000	-4.523894000	0.950995000
1	0.384336000	-4.904827000	2.963058000
1	-4.991500000	0.891380000	0.583428000
1	-6.545872000	0.029496000	0.893939000
1	-6.400980000	1.157161000	-0.513751000
1	-2.041872000	-2.478893000	-1.701486000
1	-2.806858000	-2.695649000	-3.323245000
1	-3.050888000	-3.936916000	-2.029022000
1	4.319300000	-1.719430000	1.806994000
1	5.934277000	-1.425350000	2.557470000
1	5.555138000	-3.034040000	1.827119000
1	4.577588000	0.601804000	-2.591662000
1	5.659706000	-0.433822000	-3.600716000
1	6.293928000	1.087281000	-2.858130000



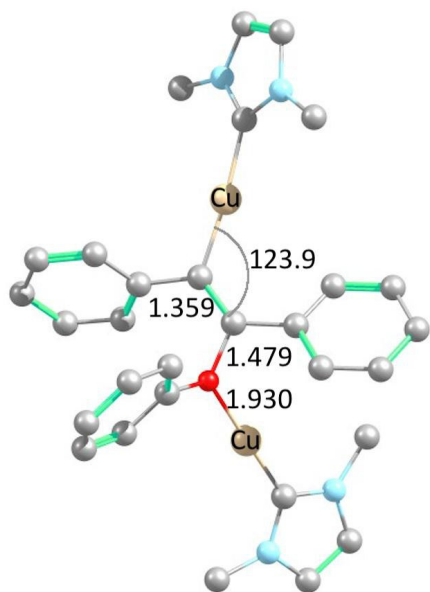
24+26-28 TS

$E(\text{scf}) = -1849.78880792 \text{ a.u.}$

$\nu_{\text{min}} = -187.8175 \text{ cm}^{-1}$

6	-4.527883000	-0.660959000	-0.432600000
7	-5.545682000	-1.317315000	0.212211000
7	-5.136547000	-0.052990000	-1.501047000
6	-6.757793000	-1.124590000	-0.438018000
6	-6.498572000	-0.324572000	-1.523029000
6	-5.383076000	-2.107582000	1.430866000
6	-4.444932000	0.760671000	-2.498511000
1	-7.696253000	-1.561847000	-0.081134000

Supporting Information

**28** [Cu(IMe)(PhCCPh)(IMe)Cu]⁺ min

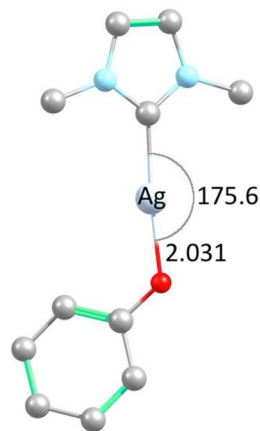
E(scf)= -1849.80186794 a.u.

6	4.685193000	-0.812157000	-0.305219000
7	5.374494000	-1.572772000	0.606096000
7	5.604388000	-0.552128000	-1.291255000
6	6.686902000	-1.780575000	0.200053000
6	6.831802000	-1.135144000	-1.002964000
6	4.808952000	-2.073646000	1.856108000
6	5.325853000	0.232959000	-2.491838000
1	7.404517000	-2.360542000	0.789951000
1	7.699248000	-1.046606000	-1.665543000
29	2.879056000	-0.204473000	-0.223706000
6	0.047418000	-0.031509000	0.389088000
6	1.128429000	0.572046000	-0.170558000
6	-4.274359000	-1.094346000	-0.857243000
7	-5.560338000	-0.639548000	-0.997154000
7	-4.305811000	-2.381269000	-1.329518000
6	-6.375717000	-1.620295000	-1.546441000
6	-5.582270000	-2.720525000	-1.757521000
6	-6.023183000	0.693219000	-0.615808000
6	-3.150636000	-3.276227000	-1.393930000
1	-7.442258000	-1.461667000	-1.737415000
1	-5.823288000	-3.705531000	-2.170828000
29	-2.793321000	-0.198668000	-0.170047000
6	-1.309936000	1.844530000	1.338718000
6	-0.568808000	1.930531000	2.527082000
6	-2.192276000	2.864116000	0.948562000
6	-0.732261000	3.063482000	3.343519000
1	0.129595000	1.127044000	2.803616000
6	-2.350191000	3.986002000	1.780038000
1	-2.723552000	2.785215000	-0.013117000
6	-1.622486000	4.089084000	2.978641000
1	-0.156730000	3.139281000	4.279326000
1	-3.035892000	4.792605000	1.477069000
1	-1.743612000	4.971964000	3.624480000
8	-1.230336000	0.701693000	0.516701000
6	1.039072000	1.920917000	-0.790433000
6	0.149407000	2.175871000	-1.867409000
6	1.896549000	2.973979000	-0.379284000
6	0.117911000	3.429218000	-2.500396000

1	-7.167265000	0.068769000	-2.295942000
29	-2.690464000	-0.618352000	0.053377000
6	-0.496961000	0.512126000	0.311254000
6	-0.830516000	-0.703596000	0.635154000
6	3.864779000	-1.232294000	-1.104271000
7	3.694249000	-2.519061000	-1.550044000
7	5.162062000	-0.924272000	-1.431930000
6	4.854596000	-2.999470000	-2.143528000
6	5.783111000	-1.991549000	-2.067776000
6	2.456177000	-3.285134000	-1.427017000
6	5.815632000	0.349009000	-1.136866000
1	4.928184000	-4.007818000	-2.564075000
1	6.823476000	-1.951788000	-2.407178000
29	2.629761000	-0.144172000	-0.232900000
6	1.741178000	2.188523000	1.133800000
6	1.365747000	2.610392000	2.432332000
6	2.436571000	3.090373000	0.292163000
6	1.706723000	3.895692000	2.882486000
1	0.819917000	1.909361000	3.082903000
6	2.778692000	4.371933000	0.754244000
1	2.700510000	2.767047000	-0.728532000
6	2.416973000	4.781218000	2.050469000
1	1.419865000	4.207577000	3.899595000
1	3.327144000	5.060414000	0.091455000
1	2.685236000	5.786300000	2.410550000
8	1.427912000	0.926695000	0.718103000
6	-0.226986000	-1.875290000	1.284540000
6	-0.721730000	-3.173915000	0.996355000
6	0.831487000	-1.753010000	2.224268000
6	-0.170992000	-4.311100000	1.608695000
1	-1.550183000	-3.278513000	0.276068000
6	1.369072000	-2.891739000	2.844879000
1	1.216517000	-0.751487000	2.461280000
6	0.875877000	-4.174009000	2.538375000
1	-0.569908000	-5.309513000	1.368475000
1	2.181621000	-2.775555000	3.579748000
1	1.299295000	-5.063186000	3.031524000
6	-0.890990000	1.776373000	-0.281888000
6	-0.594550000	2.055271000	-1.643367000
6	-1.545879000	2.767321000	0.495880000
6	-0.972289000	3.278678000	-2.214329000
1	-0.067457000	1.296248000	-2.242260000
6	-1.918537000	3.990142000	-0.083855000
1	-1.765307000	2.561796000	1.554209000
6	-1.635714000	4.248110000	-1.436846000
1	-0.742661000	3.482816000	-3.272087000
1	-2.428166000	4.750312000	0.528464000
1	-1.925018000	5.211025000	-1.886423000
1	5.083998000	1.011717000	-0.637503000
1	6.164395000	0.830405000	-2.072255000
1	6.680300000	0.192778000	-0.461329000
1	1.742877000	-2.711512000	-0.805778000
1	2.656239000	-4.256167000	-0.933445000
1	2.009895000	-3.466390000	-2.425713000
1	-4.317559000	-2.077947000	1.726916000
1	-5.682589000	-3.159731000	1.253086000
1	-5.998498000	-1.686109000	2.250496000
1	-4.437240000	0.248106000	-3.481661000
1	-3.403279000	0.922325000	-2.162946000
1	-4.944868000	1.743542000	-2.602662000

Supporting Information

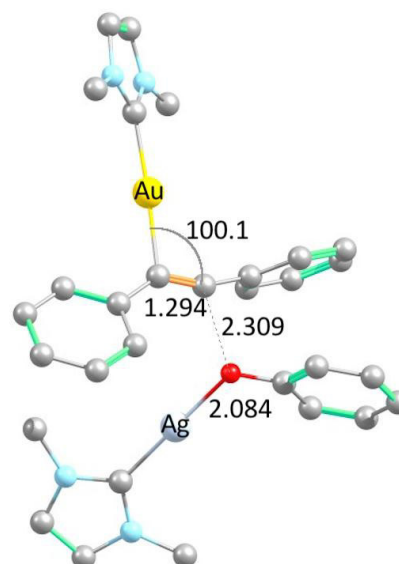
1	-0.504481000	1.364235000	-2.226575000
6	1.846685000	4.233776000	-0.996945000
1	2.603636000	2.793084000	0.446943000
6	0.960121000	4.467756000	-2.063775000
1	-0.569208000	3.596122000	-3.345883000
1	2.513278000	5.038491000	-0.647617000
1	0.932307000	5.451352000	-2.558339000
6	-0.107478000	-1.411599000	0.895700000
6	-1.032706000	-1.729665000	1.927368000
6	0.658072000	-2.473245000	0.343013000
6	-1.163734000	-3.046473000	2.401767000
1	-1.628821000	-0.929068000	2.393176000
6	0.527683000	-3.785182000	0.822575000
1	1.350964000	-2.247582000	-0.485190000
6	-0.383676000	-4.080617000	1.855251000
1	-1.874516000	-3.261310000	3.215491000
1	1.132108000	-4.590332000	0.374661000
1	-0.486783000	-5.111611000	2.228404000
1	4.292291000	0.621509000	-2.421139000
1	5.418122000	-0.396727000	-3.399555000
1	6.028883000	1.086319000	-2.565862000
1	3.729891000	-1.830362000	1.871422000
1	5.301833000	-1.595429000	2.726573000
1	4.935594000	-3.172442000	1.923919000
1	-2.307562000	-2.812276000	-0.847774000
1	-2.853032000	-3.450016000	-2.447495000
1	-3.395301000	-4.245092000	-0.916943000
1	-5.168363000	1.254420000	-0.194759000
1	-6.819602000	0.620557000	0.151232000
1	-6.414013000	1.234254000	-1.500474000



29 [Ag(IMe)(OPh)]

E(scf)= -758.380828526 a.u.

6	-2.244612000	0.097657000	-0.009554000
7	-3.314390000	-0.696597000	0.317814000
7	-2.789997000	1.342348000	-0.196198000
6	-4.497338000	0.034126000	0.333832000
6	-4.165054000	1.325270000	0.009693000
6	-3.226184000	-2.125938000	0.603759000
6	-2.026618000	2.534305000	-0.556348000
1	-5.466690000	-0.416712000	0.570742000
1	-4.787695000	2.220516000	-0.089419000
47	-0.280189000	-0.443893000	-0.165278000
6	2.737173000	-0.440471000	-0.113686000
6	2.758353000	0.839807000	0.515208000
6	3.998790000	-1.015793000	-0.453833000
6	3.965356000	1.505440000	0.780023000



22+29-30 TS

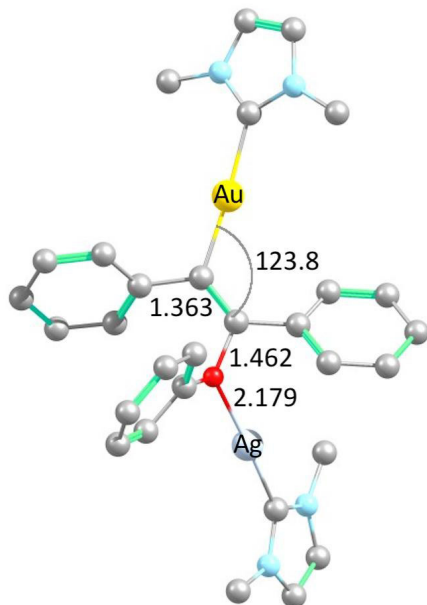
E(scf)= -1737.81706946 a.u.

 $\nu_{\min} = -74.7509 \text{ cm}^{-1}$

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7	-5.724883000	-0.997699000	0.273913000
7	-5.361680000	0.114224000	-1.558433000
6	-6.957068000	-0.834792000	-0.346859000
6	-6.728142000	-0.132310000	-1.503044000
6	-5.532129000	-1.693906000	1.545860000
6	-4.702919000	0.845119000	-2.639914000
1	-7.886572000	-1.226066000	0.079662000
1	-7.419330000	0.208859000	-2.280767000
79	-2.747669000	-0.365883000	-0.013343000
6	-0.322086000	0.735315000	0.241944000
6	-0.709289000	-0.451210000	0.585100000
6	4.317263000	-1.629557000	-1.012280000
7	4.054537000	-2.934016000	-1.335132000
7	5.603303000	-1.419046000	-1.434656000
6	5.152051000	-3.525574000	-1.949932000
6	6.132174000	-2.567470000	-2.012014000
6	2.788846000	-3.621178000	-1.084018000
6	6.338570000	-0.163688000	-1.291508000
1	5.149462000	-4.567868000	-2.285685000
1	7.151423000	-2.612090000	-2.409871000
47	3.076953000	-0.284859000	-0.089039000
6	2.224841000	2.303160000	1.203943000
6	1.849076000	2.921424000	2.429445000
6	2.977486000	3.067934000	0.270987000
6	2.240065000	4.238140000	2.715868000
1	1.264668000	2.333665000	3.154887000
6	3.361379000	4.384953000	0.565947000
1	3.251793000	2.602921000	-0.691713000
6	2.997176000	4.979464000	1.789121000
1	1.953909000	4.690841000	3.679095000
1	3.951323000	4.956429000	-0.169001000
1	3.303929000	6.011406000	2.019144000
8	1.851690000	1.032816000	0.962996000
6	-0.192442000	-1.638849000	1.284803000
6	-0.709749000	-2.924977000	0.984256000
6	0.806214000	-1.525040000	2.287301000
6	-0.236140000	-4.064688000	1.654050000

Supporting Information

1	1.791527000	1.295446000	0.798874000
6	5.198276000	-0.342502000	-0.184483000
1	3.998317000	-2.005562000	-0.937499000
6	5.199412000	0.924271000	0.433303000
1	3.940848000	2.494516000	1.268694000
1	6.154859000	-0.816357000	-0.463509000
1	6.145583000	1.447792000	0.642147000
8	1.623500000	-1.115140000	-0.387754000
1	-3.632595000	-2.343235000	1.611817000
1	-2.160164000	-2.419845000	0.570699000
1	-3.787877000	-2.709679000	-0.153245000
1	-2.419748000	2.974767000	-1.494362000
1	-0.972027000	2.236389000	-0.708107000
1	-2.078078000	3.288740000	0.254483000

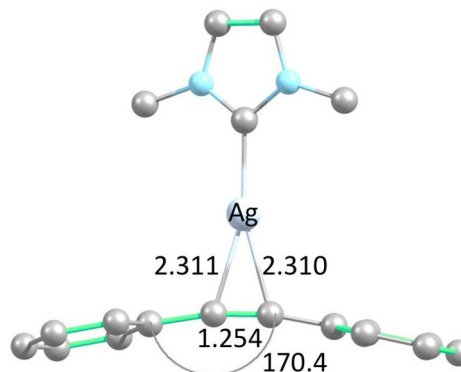


30 [Ag(Ime)(OPh)(PhCCPh)(Ime)Au]⁺ min

E(scf)= -1737.84091803 a.u.

6	4.714163000	-0.897988000	-0.188974000
7	5.327828000	-1.687504000	0.748564000
7	5.681223000	-0.663653000	-1.132099000
6	6.649098000	-1.940093000	0.398785000
6	6.871918000	-1.293590000	-0.790876000
6	4.690037000	-2.180414000	1.967419000
6	5.490891000	0.139010000	-2.339014000
1	7.316280000	-2.550207000	1.016555000
1	7.770571000	-1.232390000	-1.413515000
79	2.790803000	-0.180894000	-0.181743000
6	-0.178510000	0.112266000	0.406944000
6	0.911355000	0.670800000	-0.192097000
6	-4.887663000	-1.181695000	-0.816127000
7	-6.194131000	-0.806344000	-0.661876000
7	-4.936353000	-2.347425000	-1.530066000
6	-7.045608000	-1.719975000	-1.271533000
6	-6.250213000	-2.693720000	-1.821152000
6	-6.652149000	0.387306000	0.048052000
6	-3.772281000	-3.125798000	-1.953491000
1	-8.134917000	-1.607990000	-1.261582000
1	-6.511048000	-3.595028000	-2.385781000
47	-3.206816000	-0.215717000	-0.135977000
6	-1.501672000	2.033832000	1.282278000

1	-1.492227000	-3.018506000	0.213676000
6	1.264960000	-2.667753000	2.962273000
1	1.208028000	-0.528221000	2.518702000
6	0.750634000	-3.939999000	2.649055000
1	-0.650197000	-5.055124000	1.406567000
1	2.031145000	-2.561178000	3.746754000
1	1.110778000	-4.831166000	3.187019000
6	-0.371990000	2.022480000	-0.372663000
6	-0.024482000	2.173471000	-1.746007000
6	-0.733545000	3.174675000	0.380010000
6	-0.068076000	3.435617000	-2.348836000
1	0.271227000	1.283965000	-2.323354000
6	-0.769967000	4.434328000	-0.235458000
1	-0.999906000	3.062264000	1.440545000
6	-0.441277000	4.567652000	-1.595863000
1	0.194094000	3.543597000	-3.413049000
1	-1.053043000	5.320074000	0.353669000
1	-0.469875000	5.559628000	-2.073508000
1	5.685510000	0.568198000	-0.780788000
1	6.623250000	0.232625000	-2.286544000
1	7.251597000	-0.320036000	-0.683455000
1	2.150035000	-2.975540000	-0.452809000
1	2.974172000	-4.573128000	-0.549526000
1	2.265870000	-3.831684000	-2.038644000
1	-4.455050000	-1.672225000	1.795945000
1	-5.867338000	-2.746518000	1.460802000
1	-6.103856000	-1.188975000	2.349468000
1	-4.858195000	0.323356000	-3.605051000
1	-3.620641000	0.893720000	-2.419729000
1	-5.107435000	1.874325000	-2.708448000



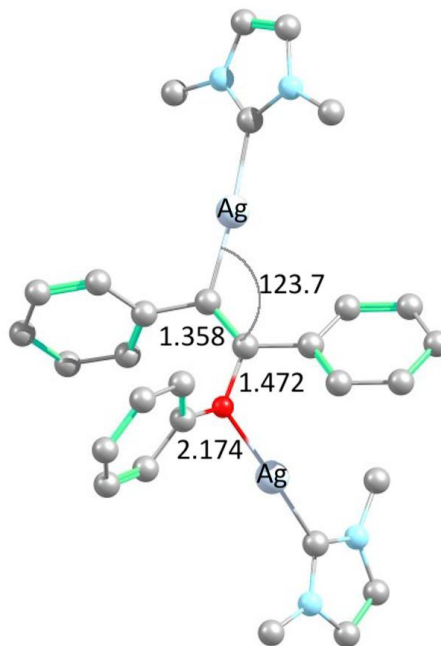
31 [Ag(Ime)(PhCCPh)]⁺

E(scf)= -990.60857688 a.u.

6	-0.158906000	-2.561434000	0.003948000
7	-1.206049000	-3.328951000	0.434199000
7	0.779843000	-3.455769000	-0.431706000
6	-0.927856000	-4.680227000	0.270447000
6	0.328150000	-4.760455000	-0.276656000
6	-2.456463000	-2.818217000	0.996359000
1	-1.635977000	-5.466575000	0.552663000
1	0.928261000	-5.630349000	-0.564066000
47	-0.025477000	-0.485959000	0.007639000
6	0.732561000	1.696298000	0.044534000
6	-0.516394000	1.772038000	-0.036894000
6	2.161930000	1.853758000	0.110880000
6	2.916684000	2.020150000	-1.082338000
6	2.824507000	1.876596000	1.368099000
6	4.302837000	2.212604000	-1.010501000
1	2.403193000	2.011905000	-2.055867000

Supporting Information

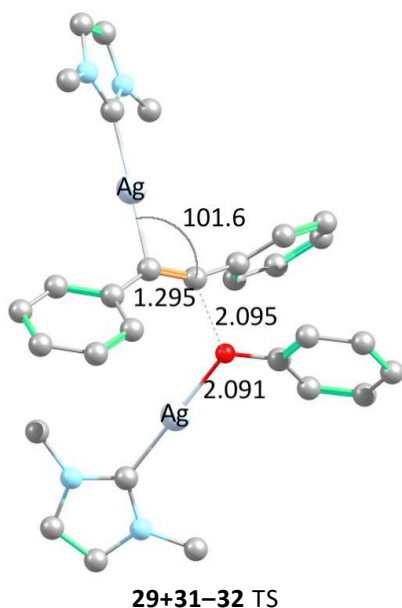
6	-0.652848000	2.234150000	2.382122000	6	4.211142000	2.070394000	1.423127000
6	-2.497195000	2.967050000	0.949066000	1	2.240525000	1.754102000	2.292933000
6	-0.821730000	3.390203000	3.164561000	6	4.952370000	2.237174000	0.238128000
1	0.132734000	1.500245000	2.614655000	1	4.881515000	2.351229000	-1.936837000
6	-2.656367000	4.114269000	1.744613000	1	4.718522000	2.096448000	2.399839000
1	-3.122925000	2.801634000	0.056741000	1	6.041445000	2.391412000	0.288195000
6	-1.820646000	4.329892000	2.854679000	6	-1.916799000	2.096189000	-0.111240000
1	-0.161082000	3.552630000	4.030574000	6	-2.568756000	2.173621000	-1.371898000
1	-3.430845000	4.851878000	1.482320000	6	-2.649958000	2.371527000	1.075186000
1	-1.943087000	5.232135000	3.472874000	6	-3.923197000	2.526018000	-1.437265000
8	-1.425700000	0.869372000	0.496754000	1	-2.000174000	1.967455000	-2.291488000
6	0.817171000	1.993979000	-0.872134000	6	-4.004158000	2.722274000	0.992994000
6	-0.103855000	2.209441000	-1.929428000	1	-2.143578000	2.320888000	2.051157000
6	1.691104000	3.056559000	-0.528819000	6	-4.643114000	2.799237000	-0.258925000
6	-0.152518000	3.437829000	-2.608525000	1	-4.421352000	2.593217000	-2.416752000
1	-0.769257000	1.387154000	-2.238728000	1	-4.565363000	2.944446000	1.913816000
6	1.625726000	4.292014000	-1.192404000	1	-5.706661000	3.078335000	-0.316788000
1	2.425513000	2.901457000	0.278104000	1	-2.578095000	-3.165190000	2.041584000
6	0.705510000	4.488721000	-2.237813000	1	-3.317494000	-3.164611000	0.391541000
1	-0.864026000	3.574698000	-3.438988000	1	-2.427747000	-1.713058000	0.982128000
1	2.306619000	5.106051000	-0.896567000	6	2.086309000	-3.107742000	-0.990404000
1	0.664168000	5.453096000	-2.768081000	1	2.202809000	-2.008633000	-0.963591000
6	-0.363816000	-1.236512000	0.986541000	1	2.161240000	-3.455910000	-2.039647000
6	-1.240818000	-1.444454000	2.087237000	1	2.894478000	-3.570799000	-0.390779000
6	0.295830000	-2.369538000	0.440781000				
6	-1.424853000	-2.725957000	2.634487000				
1	-1.747791000	-0.583694000	2.552209000				
6	0.110559000	-3.646498000	0.992342000				
1	0.952011000	-2.230312000	-0.433041000				
6	-0.749386000	-3.833058000	2.091902000				
1	-2.092912000	-2.855665000	3.500705000				
1	0.632985000	-4.509842000	0.549687000				
1	-0.893749000	-4.836970000	2.521143000				
1	-5.771825000	0.905484000	0.471164000				
1	-7.335620000	0.103764000	0.872514000				
1	-7.178518000	1.071181000	-0.647075000				
1	-2.871473000	-2.715400000	-1.460585000				
1	-3.646400000	-3.067809000	-3.053181000				
1	-3.895390000	-4.184242000	-1.652268000				
1	3.625325000	-1.881880000	1.945503000				
1	5.174346000	-1.740808000	2.862424000				
1	4.761597000	-3.285000000	2.017828000				
1	4.461441000	0.543494000	-2.326223000				
1	5.628784000	-0.485698000	-3.244099000				
1	6.213613000	0.978716000	-2.358866000				

32 [Ag(IMe)(OPh)(PhCCPh)(IMe)Ag]⁺ min

E(scf)= -1749.01376803 a.u.

6	5.031834000	-0.941136000	-0.232356000
7	5.661879000	-1.735792000	0.688793000
7	5.993104000	-0.684276000	-1.174463000
6	6.985126000	-1.969375000	0.331587000
6	7.194520000	-1.303713000	-0.849966000
6	5.037782000	-2.253570000	1.904201000
6	5.788996000	0.131341000	-2.370134000
1	7.662684000	-2.580164000	0.937503000
1	8.089507000	-1.223203000	-1.475890000
47	3.062865000	-0.225684000	-0.206851000
6	0.067502000	0.096755000	0.390233000
6	1.152093000	0.652239000	-0.209010000

Supporting Information



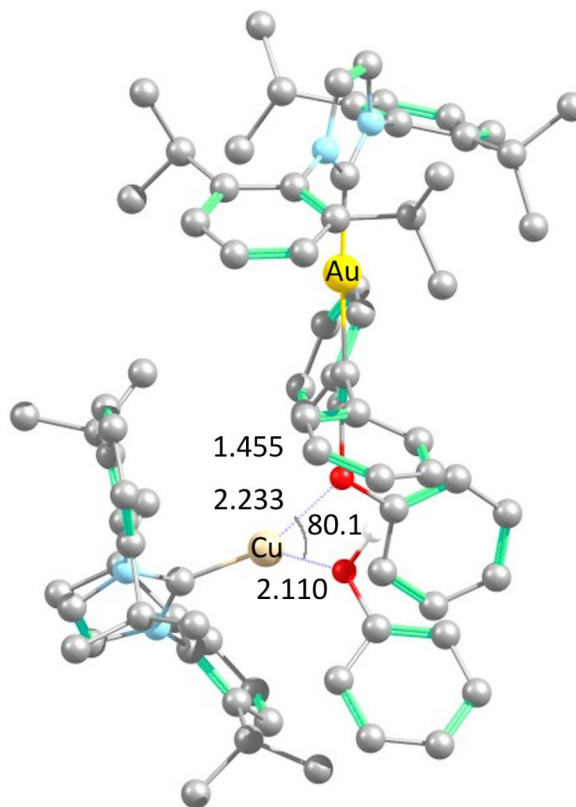
$E(\text{scf}) = -1748.99816204 \text{ a.u.}$

$\nu_{\text{min}} = -147.7747 \text{ cm}^{-1}$

6	-4.956733000	-0.639918000	-0.444127000
7	-5.938928000	-1.286825000	0.256946000
7	-5.607236000	-0.072450000	-1.506760000
6	-7.177135000	-1.126821000	-0.353915000
6	-6.967196000	-0.357648000	-1.470679000
6	-5.728693000	-2.045659000	1.488871000
6	-4.968563000	0.732555000	-2.546258000
1	-8.095854000	-1.565812000	0.049221000
1	-7.667350000	0.004680000	-2.230786000
47	-2.923652000	-0.536261000	0.021002000
6	-0.504200000	0.695445000	0.274821000
6	-0.853389000	-0.505929000	0.610829000
6	4.141783000	-1.482441000	-1.043840000
7	3.941590000	-2.794626000	-1.379756000
7	5.432643000	-1.219905000	-1.418701000
6	5.082704000	-3.340122000	-1.956390000
6	6.026261000	-2.344338000	-1.980024000
6	2.695356000	-3.531803000	-1.177660000
6	6.112896000	0.062679000	-1.246670000
1	5.132809000	-4.380144000	-2.295415000
1	7.060057000	-2.347372000	-2.341145000
47	2.811712000	-0.196116000	-0.164321000
6	1.820975000	2.338229000	1.169193000
6	1.410561000	2.865125000	2.421616000
6	2.580434000	3.165413000	0.302280000
6	1.777384000	4.165935000	2.800398000
1	0.817088000	2.227078000	3.095252000
6	2.945624000	4.464138000	0.691708000
1	2.877985000	2.767316000	-0.682855000
6	2.547969000	4.972451000	1.942028000
1	1.463167000	4.553056000	3.783185000
1	3.543418000	5.088452000	0.008068000
1	2.836312000	5.990563000	2.245639000
8	1.479829000	1.069713000	0.833462000
6	-0.282082000	-1.667091000	1.308062000
6	-0.706303000	-2.980548000	0.977291000
6	0.680127000	-1.512100000	2.341797000
6	-0.179372000	-4.099880000	1.641937000
6	-4.659850000	-1.181893000	-0.817683000
7	-5.965064000	-0.806266000	-0.653387000
7	-4.714290000	-2.344509000	-1.536401000
6	-6.821266000	-1.716484000	-1.261509000
6	-6.030294000	-2.688471000	-1.820536000
6	-6.417403000	0.384392000	0.065166000
6	-3.553592000	-3.121811000	-1.970633000
1	-7.910387000	-1.603634000	-1.244009000
1	-6.295552000	-3.587065000	-2.387417000
47	-2.975018000	-0.219310000	-0.143954000
6	-1.264090000	2.019466000	1.269965000
6	-0.412426000	2.224726000	2.367125000
6	-2.256317000	2.955582000	0.933537000
6	-0.574695000	3.386419000	3.142396000
1	0.370330000	1.488869000	2.603057000
6	-2.409367000	4.108520000	1.721883000
1	-2.884689000	2.787241000	0.043519000
6	-1.570436000	4.328247000	2.828723000
1	0.088419000	3.551795000	4.006014000
1	-3.181527000	4.847446000	1.456377000
1	-1.687882000	5.235025000	3.441241000
8	-1.193036000	0.850475000	0.494188000
6	1.075404000	1.976911000	-0.877986000
6	0.159803000	2.214146000	-1.937167000
6	1.962090000	3.028030000	-0.527436000
6	0.130708000	3.447038000	-2.609152000
1	-0.517892000	1.404100000	-2.252238000
6	1.913764000	4.268999000	-1.181533000
1	2.693657000	2.859899000	0.280134000
6	1.000390000	4.485048000	-2.229440000
1	-0.577229000	3.598472000	-3.440265000
1	2.603790000	5.072310000	-0.877291000
1	0.973677000	5.453124000	-2.753762000
6	-0.113997000	-1.254174000	0.969267000
6	-0.984564000	-1.471177000	2.072486000
6	0.554420000	-2.381019000	0.421988000
6	-1.153121000	-2.754548000	2.620937000
1	-1.499772000	-0.615655000	2.537855000
6	0.385089000	-3.660142000	0.973623000
1	1.203050000	-2.235884000	-0.456953000
6	-0.468513000	-3.855125000	2.076742000
1	-1.816872000	-2.890793000	3.489508000
1	0.913911000	-4.518306000	0.528374000
1	-0.601051000	-4.860269000	2.506859000
1	-5.533706000	0.901066000	0.483077000
1	-7.094008000	0.097373000	0.894089000
1	-6.949581000	1.070968000	-0.622830000
1	-2.649668000	-2.714702000	-1.480748000
1	-3.433937000	-3.058226000	-3.070721000
1	-3.676011000	-4.181706000	-1.674216000
1	3.966508000	-1.979113000	1.890232000
1	5.514279000	-1.813458000	2.803244000
1	5.131455000	-3.356956000	1.944434000
1	4.758148000	0.531683000	-2.347301000
1	5.922740000	-0.480667000	-3.284569000
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Supporting Information

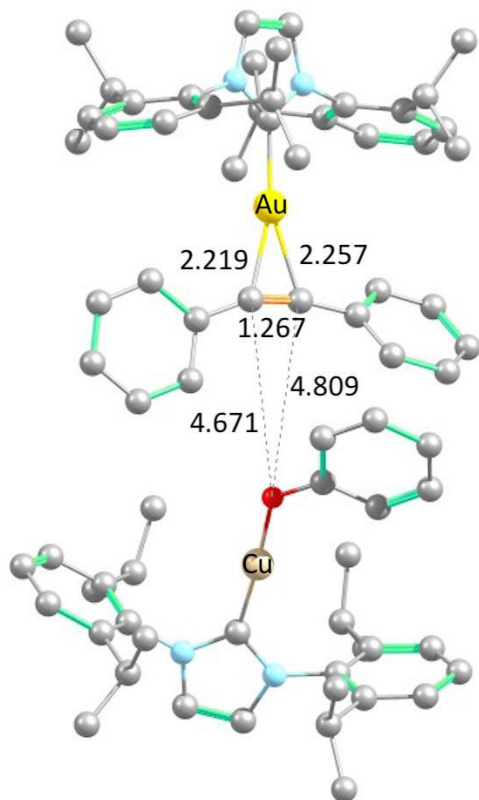
1	-1.462009000	-3.113134000	0.185228000
6	1.192043000	-2.633709000	3.013315000
1	1.012996000	-0.498270000	2.604207000
6	0.769889000	-3.930977000	2.666328000
1	-0.524054000	-5.109946000	1.368404000
1	1.927890000	-2.491588000	3.820926000
1	1.170994000	-4.806397000	3.201031000
6	-0.759655000	1.957721000	-0.376328000
6	-0.474795000	2.115640000	-1.760044000
6	-1.260363000	3.067156000	0.354690000
6	-0.710596000	3.342028000	-2.395568000
1	-0.070352000	1.260492000	-2.323453000
6	-1.489635000	4.292387000	-0.290133000
1	-1.476810000	2.952536000	1.426786000
6	-1.218451000	4.432744000	-1.662479000
1	-0.492554000	3.452846000	-3.469535000
1	-1.879570000	5.145968000	0.285750000
1	-1.397709000	5.397031000	-2.163560000
1	5.414878000	0.766994000	-0.757250000
1	6.416283000	0.473536000	-2.230191000
1	7.009659000	-0.060713000	-0.607670000
1	2.008659000	-2.914959000	-0.568203000
1	2.898195000	-4.478058000	-0.639527000
1	2.216869000	-3.758204000	-2.151797000
1	-4.654062000	-2.005989000	1.746925000
1	-6.030003000	-3.102548000	1.346724000
1	-6.317209000	-1.605262000	2.318100000
1	-5.104749000	0.258666000	-3.538774000
1	-3.888212000	0.803623000	-2.321319000
1	-5.401780000	1.752244000	-2.564054000



16-33+34 TS

$E(\text{scf}) = -3804.67831484 \text{ a.u.}$

$\nu_{\text{min}} = -17.8468 \text{ cm}^{-1}$



5+8 [Cu(Ime)(OPh)]+[(PhCCPh)(Ime)Au]⁺ min

$E(\text{scf}) = -3497.41953708 \text{ a.u.}$

6	4.779312000	0.211035000	-0.088526000
7	5.820348000	-0.687337000	-0.101851000
7	5.388874000	1.433585000	-0.255797000
6	7.043671000	-0.041030000	-0.270153000
6	6.771204000	1.297999000	-0.367400000
6	5.711736000	-2.127225000	0.027193000
6	4.714887000	2.715062000	-0.318982000
1	7.988290000	-0.592379000	-0.305172000
1	7.429428000	2.161578000	-0.503781000
6	5.643571000	-2.905368000	-1.159177000
6	5.597148000	-4.306865000	-1.008949000
6	5.616334000	-4.902676000	0.260688000
6	5.684534000	-4.106507000	1.412531000
6	5.744075000	-2.699640000	1.326257000
6	5.595275000	-2.279370000	-2.553980000
1	5.547842000	-4.943616000	-1.905978000
1	5.583643000	-5.999807000	0.353485000
1	5.704586000	-4.587836000	2.402844000
6	5.839612000	-1.858328000	2.599838000
6	4.481217000	3.421545000	0.889855000
6	3.858367000	4.683060000	0.789237000
6	3.499832000	5.219661000	-0.455086000
6	3.758158000	4.503785000	-1.632846000
6	4.373224000	3.235152000	-1.595375000
6	4.903409000	2.884277000	2.257389000
1	3.660395000	5.260438000	1.705908000
1	3.025662000	6.212621000	-0.508218000
1	3.486996000	4.943501000	-2.605853000

Supporting Information

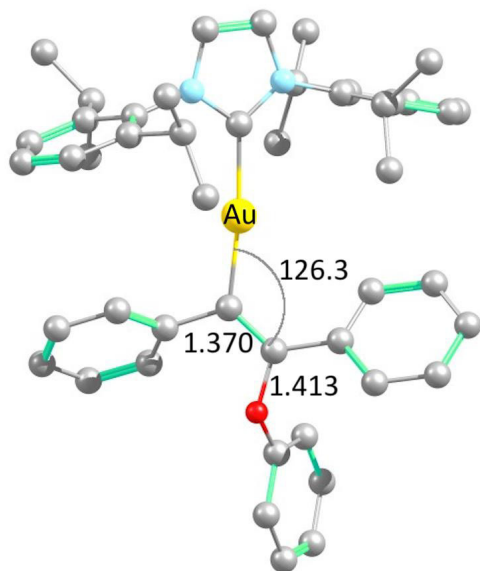
6	-5.60427000	0.06156100	0.11918700	6	4.67909400	2.49362500	-2.89751700
7	-6.42912400	-0.89127900	0.65294500	1	5.83141200	-1.19961400	-2.44728200
7	-6.43661100	1.05017700	-0.33335600	6	4.17272100	-2.37714300	-3.14804000
6	-7.76197800	-0.50576000	0.53182900	6	6.64941400	-2.88024700	-3.50661000
6	-7.76638600	0.71798500	-0.08862500	1	5.98331400	-0.80048500	2.29557000
6	-5.99526300	-2.12664400	1.28060100	6	4.52528500	-1.92054200	3.40802300
6	-6.00559400	2.29188600	-0.95079200	6	7.05590400	-2.25543000	3.46287300
1	-8.57992400	-1.13452400	0.89672800	1	5.33995700	1.87582500	2.10263200
1	-8.58905400	1.37935000	-0.37739200	6	6.00163800	3.76781400	2.88952200
6	-5.71835300	-2.11259400	2.67386700	6	3.69824600	2.71571200	3.20481700
6	-5.33346300	-3.33497000	3.26359600	1	5.09564000	1.50014500	-2.63104600
6	-5.23944000	-4.51007500	2.50441100	6	3.40371700	2.23632800	-3.72531900
6	-5.52122800	-4.48902800	1.13124500	6	5.75005700	3.23641500	-3.72648400
6	-5.90628500	-3.29756400	0.48201300	1	4.13091900	-1.88115600	-4.14047900
6	-5.83718400	-0.85473600	3.53609400	1	3.86591300	-3.43529600	-3.28603700
1	-5.11375000	-3.36702000	4.34228600	1	3.42456300	-1.89480200	-2.48538800
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6	-6.22867600	-3.31080300	-1.01299300	1	6.44827200	-3.94946700	-3.72762300
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6	-5.85092200	3.43552000	-0.12059400	1	6.96392500	-3.29026000	3.85419600
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1	-5.33084800	5.54518800	-0.14146700	1	5.63167100	4.79482000	3.09315500
6	-6.13232200	3.41551000	1.38348600	1	4.02448000	2.27047800	4.16793500
1	-6.13772200	-0.01477000	2.87474300	1	3.21845300	3.68966900	3.43603200
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1	-4.01030600	3.39547800	1.99572500	6	-0.70875000	3.02416200	-2.94212800
1	-4.75408600	5.02660500	2.01251400	6	-0.81605800	4.27846000	-2.32660000
1	-7.65712800	4.12797400	2.79619800	6	-1.98435800	4.62588300	-1.63433800
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79	-3.58368200	0.00594000	-0.03234300	1	0.20984300	2.76745800	-3.49125300

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6	-1.456861000	-0.742361000	-0.145640000	1	0.017646000	4.994953000	-2.391678000
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6	9.704720000	-1.500802000	-2.241810000	1	-5.017677000	5.040510000	1.076733000
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6	4.287545000	-2.903307000	2.312774000	1	-3.584824000	5.844476000	0.390343000
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1	5.089440000	1.514654000	5.685857000	6	-3.526589000	0.595031000	4.453637000
1	6.349556000	2.581140000	4.982233000	6	-4.808034000	2.001287000	2.919222000
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Supporting Information

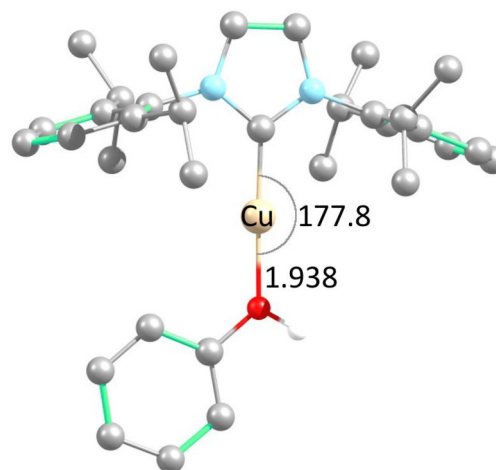
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**33** [Au(IMe)(PhCCPh)(OPh)] min

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**34** [Cu(IMe)(OHPh)]⁺

E(scf)= -1663.77639538 a.u.

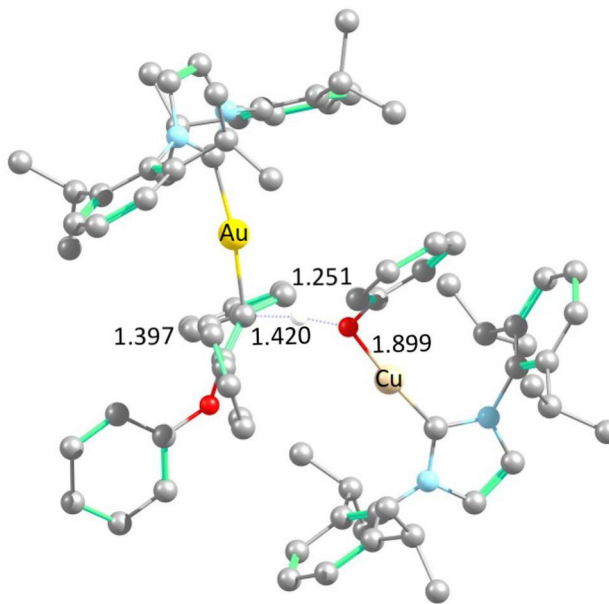
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6	3.459431000	-2.432416000	1.213780000
6	4.149166000	-2.540795000	-0.002206000

Supporting Information

6	4.131605000	1.390388000	0.468766000	6	3.459189000	-2.429632000	-1.217808000
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6	0.825914000	5.173782000	1.389935000	6	-2.282729000	1.200228000	-3.404019000
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Supporting Information

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6	-1.127602000	-3.291540000	-0.448901000
6	-2.885862000	-2.758652000	1.132968000
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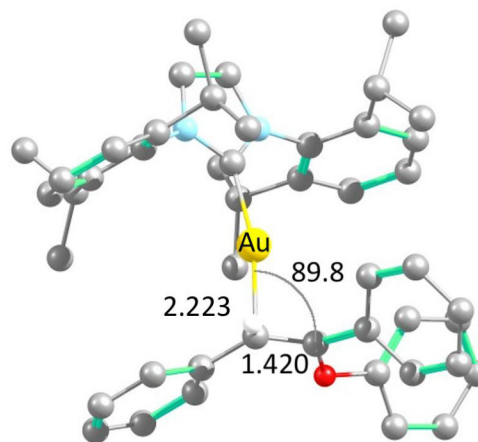


33+34-35 TS

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35 [Au(IMe)(PhHC=CPh)(OPh)]⁺ min

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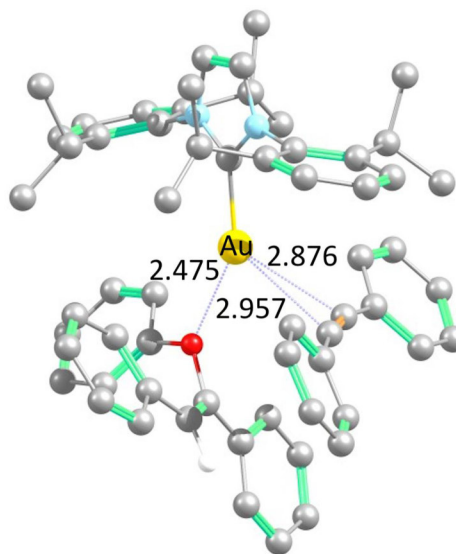
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Supporting Information

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6	4.571695000	-3.778420000	0.622329000	1	-0.889597000	2.172225000	-5.366375000
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6	-1.164154000	5.116827000	0.623636000				

Supporting Information

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1	-0.434569000	8.444394000	1.102053000
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6	-3.454182000	-0.623360000	4.586471000
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35-36 TS

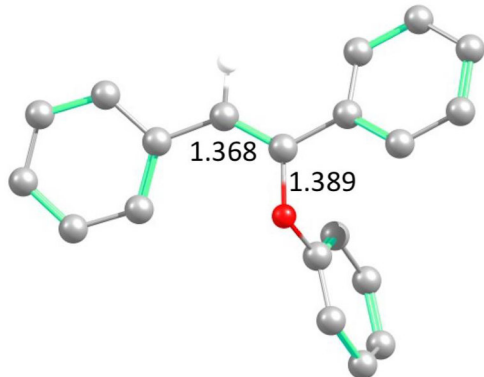
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Supporting Information

1	-6.736556000	-0.525140000	-4.990373000	6	3.063125000	1.558348000	4.355220000
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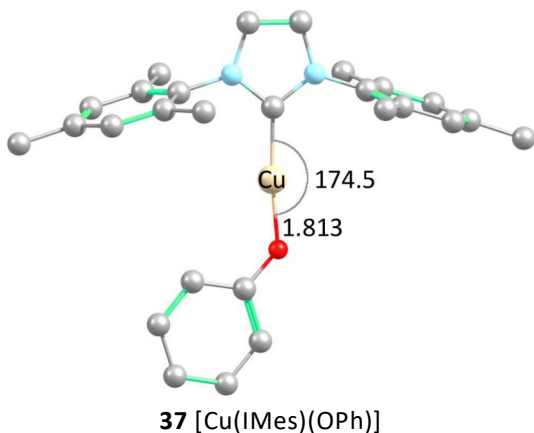


36 Product

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Supporting Information

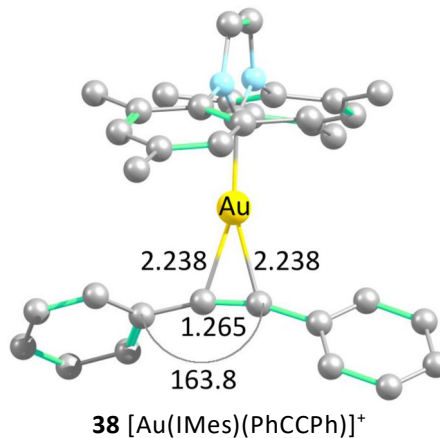
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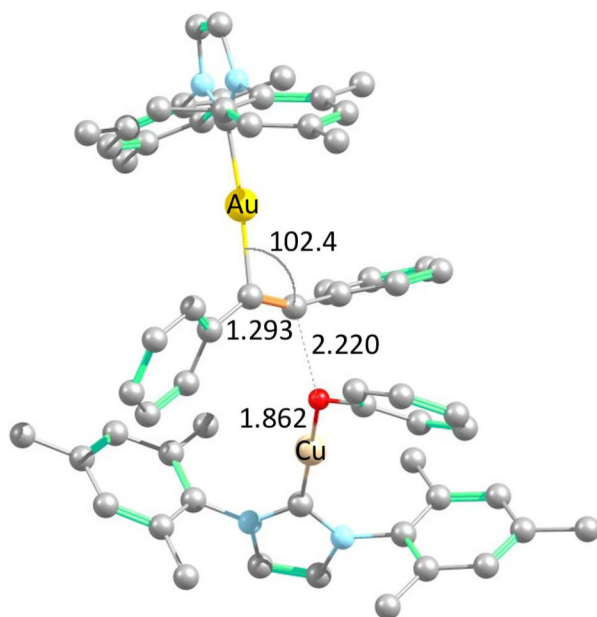
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6	3.319116000	-1.981877000	-0.638503000
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Supporting Information

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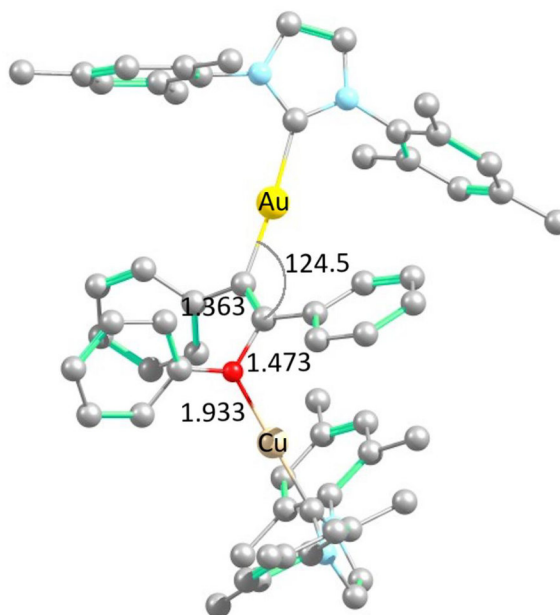
Supporting Information

**37+38-39 TS**

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**39 [Cu(IMes)(PhO)(PhCCPh)(IMes)(Au)]⁺ min**

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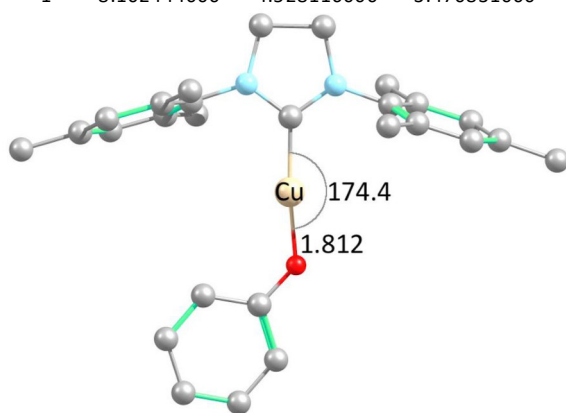
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Supporting Information

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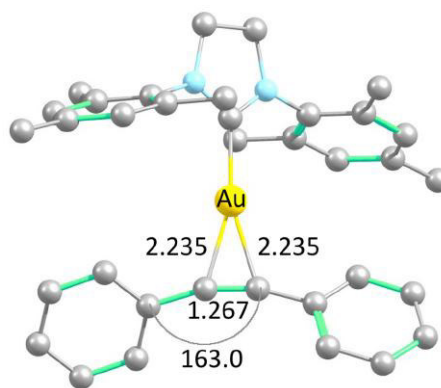
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1	-1.857363000	5.868347000	4.482207000
1	-7.129877000	-5.407194000	-2.255977000
1	-6.364398000	-4.803864000	-3.765192000
1	-8.102444000	-4.528116000	-3.470831000

**40** [Cu(SiMes)(OPh)]

E(sc f) = -1428.89682398 a.u.

29	-0.088414000	0.739742000	-0.021598000
8	0.217231000	2.524807000	-0.067777000
6	-0.576546000	-1.046331000	0.015190000
7	0.262930000	-2.114941000	0.071547000
6	-0.451801000	-3.411776000	0.001078000
6	-1.929870000	-2.987545000	0.133448000
7	-1.853162000	-1.514352000	-0.002714000
6	1.698165000	-2.046821000	0.001865000
6	2.330958000	-1.819972000	-1.248849000
6	3.737746000	-1.806147000	-1.287560000
1	4.236687000	-1.625318000	-2.254528000
6	4.522430000	-2.012137000	-0.134030000
6	6.032192000	-1.976941000	-0.214133000
6	3.859205000	-2.229263000	1.088980000
1	4.453637000	-2.378475000	2.005876000

1	4.180580000	4.109645000	2.203645000
1	3.795293000	2.847704000	-4.484434000
1	3.670444000	1.400339000	-3.432388000
1	5.247648000	2.200908000	-3.661441000
1	1.385803000	6.584235000	-2.432761000
1	2.877078000	7.440389000	-1.958187000
1	1.670074000	7.015645000	-0.711666000
1	4.859659000	-6.558695000	0.164968000
1	5.318760000	-6.179081000	1.859755000
1	6.579918000	-6.406268000	0.614058000
1	-5.411525000	1.702442000	-3.909239000
1	-4.289478000	1.526055000	-2.526881000
1	-5.839143000	2.386643000	-2.309548000
1	-7.676110000	-2.696027000	0.773424000
1	-7.754407000	-0.961819000	1.213504000
1	-6.193528000	-1.821009000	1.268115000
1	-6.534840000	-3.502821000	-4.564071000
1	-7.787187000	-2.369715000	-5.141742000
1	-8.194158000	-3.610581000	-3.908738000
1	-4.837270000	-0.076020000	3.525496000
1	-5.783414000	1.291842000	4.166647000
1	-4.562310000	0.495281000	5.202900000
1	-2.048399000	4.533020000	0.325802000
1	-3.756772000	4.022023000	0.135174000
1	-2.435820000	2.891904000	-0.268368000
6	-0.560367000	3.529300000	5.030930000
1	-0.916356000	3.627948000	6.076269000
1	0.253558000	2.771528000	5.034181000
1	-0.111667000	4.495030000	4.724604000

**41** [Au(SiMes)(PhCCPh)]⁺

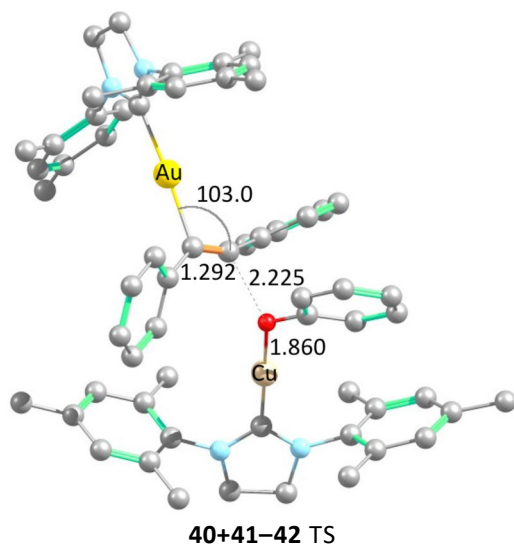
E(sc f) = -1599.54385538 a.u.

6	0.000034000	-1.738208000	0.000146000
7	-1.081216000	-2.507065000	-0.231917000
7	1.081535000	-2.506806000	0.231942000
6	-0.756550000	-3.956691000	-0.159339000
6	0.757315000	-3.956499000	0.158908000
6	-2.401135000	-2.037357000	-0.573836000
6	2.401334000	-2.036870000	0.573982000
6	-2.676977000	-1.674122000	-1.919451000
6	-3.985452000	-1.264941000	-2.236265000
6	-5.013663000	-1.219482000	-1.270223000
6	-4.696756000	-1.584793000	0.053150000
6	-3.402468000	-2.000087000	0.429205000
6	-1.602785000	-1.704907000	-2.982967000
1	-4.211617000	-0.981202000	-3.277531000
6	-6.416296000	-0.813271000	-1.658653000
1	-5.484344000	-1.552002000	0.824168000
6	-3.113630000	-2.397430000	1.859151000

Supporting Information

6	2.453262000	-2.249214000	1.184083000	6	2.677017000	-1.673543000	1.919617000
6	1.526197000	-1.560763000	-2.501352000	6	3.985384000	-1.264103000	2.236504000
6	1.774169000	-2.450407000	2.519564000	6	5.013694000	-1.218572000	1.270555000
6	-3.034614000	-0.693369000	0.016380000	6	4.696980000	-1.584058000	-0.052804000
6	-3.495708000	-0.153817000	1.244719000	6	3.402778000	-1.999592000	-0.428942000
6	-4.681149000	0.606199000	1.232220000	6	1.602785000	-1.704589000	2.983082000
6	-4.917025000	0.292079000	-1.152852000	1	4.211411000	-0.980194000	3.277753000
6	-3.735508000	-0.473100000	-1.195986000	6	6.416247000	-0.812206000	1.659099000
6	-2.722280000	-0.352492000	2.527861000	1	5.484618000	-1.551179000	-0.823768000
6	-3.213788000	-1.014589000	-2.507422000	6	3.114302000	-2.397237000	-1.858885000
6	1.347613000	3.227865000	-0.012336000	79	-0.000182000	0.292912000	0.000143000
6	1.286329000	4.648528000	-0.117730000	6	-0.573749000	2.436773000	0.268311000
6	2.635482000	2.639287000	0.151176000	6	0.573444000	2.436754000	-0.268769000
6	2.449836000	5.428951000	-0.062976000	6	-1.755636000	2.829395000	0.994098000
1	0.295041000	5.112315000	-0.244378000	6	-1.700392000	4.001885000	1.796210000
6	3.793134000	3.430537000	0.204923000	6	-2.968322000	2.097910000	0.906494000
1	2.700501000	1.540196000	0.235229000	6	-2.842386000	4.431093000	2.484857000
6	3.715772000	4.832405000	0.098564000	1	-0.758436000	4.565877000	1.870509000
1	2.367419000	6.525937000	-0.147791000	6	-4.100888000	2.536876000	1.606059000
1	4.774408000	2.942578000	0.333631000	1	-3.014152000	1.190756000	0.283861000
1	4.626769000	5.450017000	0.141843000	6	-4.042667000	3.701540000	2.393130000
1	0.706812000	-2.297196000	-2.636502000	1	-2.794685000	5.342059000	3.101452000
1	2.169802000	-1.593626000	-3.401859000	1	-5.039962000	1.967398000	1.531509000
1	1.048077000	-0.556870000	-2.461101000	1	-4.936451000	4.043679000	2.937781000
1	2.514058000	-2.456591000	3.343436000	6	1.755464000	2.828905000	-0.994572000
1	1.219052000	-3.412842000	2.568904000	6	2.968241000	2.097684000	-0.906146000
1	1.040119000	-1.642965000	2.722864000	6	1.700219000	4.000777000	-1.797605000
1	-3.297844000	0.013749000	3.400062000	6	4.100891000	2.536325000	-1.605787000
1	-1.759334000	0.203495000	2.498473000	1	3.014130000	1.190983000	-0.282859000
1	-2.469957000	-1.418511000	2.708597000	6	2.842296000	4.429670000	-2.486307000
1	6.501294000	-2.284195000	0.741458000	1	0.758191000	4.564563000	-1.872556000
1	6.395740000	-0.954229000	-0.453293000	6	4.042677000	3.700383000	-2.393751000
1	6.411847000	-2.647218000	-1.013895000	1	5.040034000	1.967044000	-1.530581000
1	-3.157556000	-2.124665000	-2.513489000	1	2.794572000	5.340173000	-3.103582000
1	-2.189380000	-0.639387000	-2.715003000	1	4.936540000	4.042240000	-2.938451000
1	-3.865683000	-0.711089000	-3.349501000	1	1.042967000	-2.663207000	2.987784000
6	-5.408522000	0.841057000	0.048068000	1	0.854655000	-0.896275000	2.827690000
1	-5.045645000	1.030814000	2.182751000	1	2.038800000	-1.564520000	3.990694000
1	-5.466263000	0.470624000	-2.092534000	1	3.886698000	-1.997979000	-2.544282000
6	-6.659333000	1.690925000	0.062620000	1	2.127234000	-2.027999000	-2.204318000
1	-7.239148000	1.549926000	0.997565000	1	3.116434000	-3.502474000	-1.985781000
1	-7.322763000	1.459703000	-0.794826000	1	7.051394000	-0.620091000	0.772274000
1	-6.403826000	2.771628000	-0.001099000	1	6.907788000	-1.613038000	2.253011000
1	-2.580097000	-3.426511000	-0.651295000	1	6.416311000	0.099808000	2.290917000
1	-2.368191000	-3.257989000	1.120083000	1	-2.127910000	-2.025212000	2.205283000
1	-0.121614000	-4.093644000	0.811768000	1	-3.112314000	-3.502702000	1.985707000
1	-0.234248000	-3.914479000	-0.967817000	1	-3.887675000	-2.000854000	2.544232000
				1	-2.038838000	-1.564622000	-3.990532000
				1	-1.042926000	-2.663505000	-2.987934000
				1	-0.854687000	-0.896600000	-2.827376000
				1	-6.416599000	0.100008000	-2.288661000
				1	-7.051976000	-0.623251000	-0.771764000
				1	-6.907046000	-1.613193000	-2.254427000
				1	1.001270000	-4.445717000	1.124639000
				1	1.365537000	-4.444929000	-0.629892000
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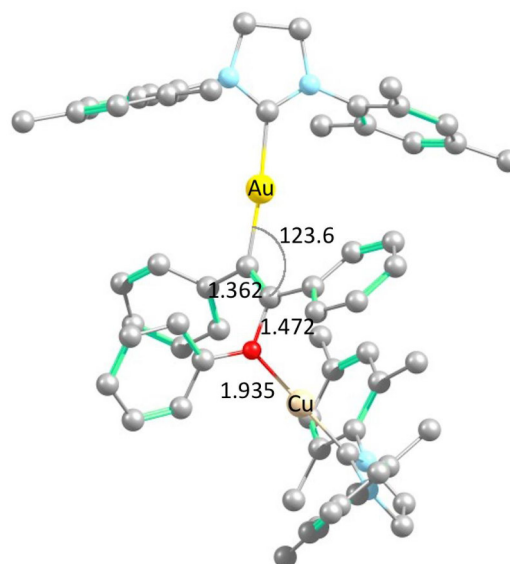
Supporting Information



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$\nu_{\text{min}} = -112.3776 \text{ cm}^{-1}$

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7	5.699023000	-0.609807000	-0.487765000
6	6.581660000	1.229344000	-1.690343000
6	6.962838000	-0.156579000	-1.122771000
6	4.353502000	2.468170000	-1.785377000
6	5.608850000	-1.877770000	0.192007000
6	4.211555000	3.529962000	-0.857077000
6	3.502296000	4.675976000	-1.267765000
6	2.945337000	4.790308000	-2.557267000
6	3.097132000	3.705673000	-3.445851000
6	3.795893000	2.537187000	-3.087311000
6	4.770079000	3.428685000	0.543576000
1	3.387023000	5.509131000	-0.554547000
6	2.232946000	6.051731000	-2.989786000
1	2.659751000	3.769846000	-4.456302000
6	3.919119000	1.381781000	-4.053999000
6	5.209618000	-3.027119000	-0.533349000
6	5.179295000	-4.260959000	0.147842000
6	5.531965000	-4.375819000	1.506488000
6	5.920086000	-3.205840000	2.193987000
6	5.968651000	-1.949087000	1.563159000
6	4.790979000	-2.937761000	-1.983011000
1	4.870903000	-5.162722000	-0.406655000
6	5.492542000	-5.708521000	2.218750000
1	6.197743000	-3.273014000	3.259299000
6	6.368833000	-0.711456000	2.334334000
79	2.782556000	-0.020386000	-0.025525000
6	0.116570000	-0.566143000	-0.109089000
6	0.886587000	-0.291941000	0.891552000
6	-4.882127000	0.941761000	0.211748000
7	-6.029444000	0.565924000	-0.403354000
7	-5.045597000	2.192871000	0.706805000
6	-7.109250000	1.575429000	-0.261704000
6	-6.370148000	2.773614000	0.370915000
6	-6.282881000	-0.723614000	-0.991632000
6	-4.038124000	2.952256000	1.399454000
6	-6.583528000	-1.828976000	-0.154902000
6	-6.877454000	-3.063072000	-0.768455000
6	-6.887176000	-3.221994000	-2.168471000



$E(\text{scf}) = -3028.46995621 \text{ a.u.}$

$E(\text{scf}) = -3028.46995621 \text{ a.u.}$

6	4.478672000	0.478245000	-0.597168000
7	4.926534000	1.687564000	-1.007372000
7	5.522605000	-0.379093000	-0.541370000
6	6.400049000	1.716254000	-1.195742000
6	6.798210000	0.239702000	-0.981163000
6	4.141952000	2.887578000	-1.137003000
6	5.450591000	-1.774904000	-0.190114000
6	3.871176000	3.673081000	0.011373000
6	3.162070000	4.878848000	-0.162921000
6	2.729096000	5.317843000	-1.429836000
6	3.006656000	4.501350000	-2.546092000
6	3.709453000	3.286816000	-2.427850000
6	4.304064000	3.225634000	1.388189000
1	2.952545000	5.500245000	0.723841000
6	2.019074000	6.642215000	-1.597864000
1	2.670402000	4.822381000	-3.546449000
6	3.972364000	2.423788000	-3.640873000
6	5.160153000	-2.730823000	-1.195919000
6	5.147664000	-4.091386000	-0.831816000
6	5.416166000	-4.517432000	0.485051000
6	5.685558000	-3.534350000	1.459254000
6	5.709771000	-2.160567000	1.149235000
6	4.829200000	-2.306504000	-2.608414000
1	4.921998000	-4.843162000	-1.606611000
6	5.444389000	-5.987791000	0.836037000
1	5.885056000	-3.844899000	2.498473000
6	5.961985000	-1.129274000	2.225048000
79	2.552818000	-0.022304000	-0.103794000
6	-0.395550000	-0.729710000	-0.341613000
6	0.675665000	-0.647994000	0.496068000
6	-4.673762000	0.849585000	0.440918000
7	-5.828956000	0.745234000	-0.251294000
7	-4.762982000	1.885882000	1.305445000
6	-6.837768000	1.749659000	0.173796000
6	-6.051051000	2.615687000	1.183812000
6	-6.115076000	-0.238236000	-1.264754000
6	-3.708276000	2.330361000	2.179088000
6	-6.762762000	-1.447328000	-0.899308000
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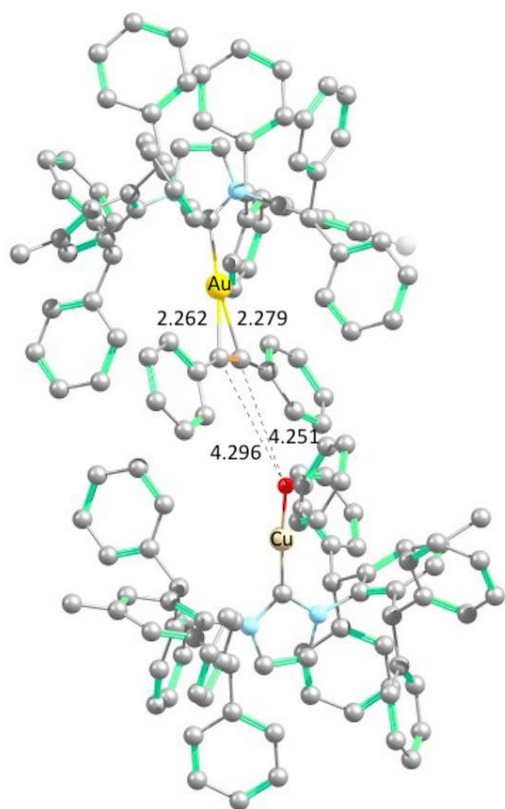
Supporting Information

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6	-6.271006000	-0.846200000	-2.405666000	6	-6.113654000	-0.906727000	-3.593463000
6	-6.559705000	-1.711754000	1.352023000	6	-5.782241000	0.049296000	-2.612512000
1	-7.109491000	-3.928459000	-0.125832000	6	-7.120114000	-1.748556000	0.539002000
6	-7.252595000	-4.545770000	-2.800537000	1	-7.560075000	-3.315941000	-1.645428000
1	-6.560645000	-2.207920000	-4.063506000	6	-7.134121000	-3.112246000	-4.347346000
6	-5.929313000	0.330451000	-3.291676000	1	-5.861515000	-0.693048000	-4.645475000
6	-3.127004000	3.742502000	0.655098000	6	-5.063032000	1.322969000	-2.994058000
6	-2.180842000	4.510117000	1.363637000	6	-2.648800000	3.110675000	1.646909000
6	-2.124890000	4.516688000	2.771292000	6	-1.643311000	3.550058000	2.530150000
6	-3.051004000	3.719429000	3.476549000	6	-1.666812000	3.246936000	3.906395000
6	-4.012544000	2.929316000	2.818248000	6	-2.742922000	2.480480000	4.398188000
6	-3.159084000	3.758633000	-0.856408000	6	-3.773337000	2.010645000	3.560560000
1	-1.467361000	5.127930000	0.793341000	6	-2.577418000	3.455586000	0.176302000
6	-1.090489000	5.333812000	3.510956000	1	-0.815707000	4.156295000	2.126392000
1	-3.028961000	3.714933000	4.579327000	6	-0.554969000	3.702107000	4.822925000
6	-4.976344000	2.068955000	3.603347000	1	-2.784043000	2.236644000	5.472959000
29	-3.358729000	-0.117871000	0.388617000	6	-4.911909000	1.197182000	4.133735000
6	-1.951414000	-2.536464000	0.718035000	29	-3.188979000	-0.265830000	0.266643000
6	-1.125527000	-3.274425000	1.607255000	6	-1.638563000	-2.782757000	0.353039000
6	-2.836762000	-3.249208000	-0.133752000	6	-0.718044000	-3.634991000	-0.275646000
6	-1.197710000	-4.674452000	1.645386000	6	-2.640000000	-3.285211000	1.199132000
1	-0.443049000	-2.723824000	2.272111000	6	-0.819845000	-5.019563000	-0.052882000
6	-2.906710000	-4.651941000	-0.078699000	1	0.069206000	-3.219751000	-0.921704000
1	-3.477836000	-2.682578000	-0.829823000	6	-2.730576000	-4.671494000	1.406941000
6	-2.087142000	-5.374684000	0.805853000	1	-3.332066000	-2.587260000	1.699017000
1	-0.555748000	-5.228859000	2.349265000	6	-1.822065000	-5.543821000	0.782015000
1	-3.608551000	-5.183635000	-0.741304000	1	-0.102559000	-5.694746000	-0.545258000
1	-2.141470000	-6.473694000	0.844893000	1	-3.512469000	-5.068348000	2.073073000
8	-1.865591000	-1.185502000	0.690876000	1	-1.891896000	-6.629281000	0.950043000
6	0.778634000	-0.142810000	2.350762000	8	-1.622933000	-1.393367000	0.127932000
6	1.764946000	-0.697197000	3.204063000	6	0.579453000	-1.098535000	1.913149000
6	-0.302642000	0.567692000	2.928408000	6	-0.378617000	-0.542494000	2.799535000
6	1.659830000	-0.566126000	4.597811000	6	1.483657000	-2.059560000	2.433333000
1	2.609253000	-1.247757000	2.759412000	6	-0.435375000	-0.941148000	4.145387000
6	-0.391460000	0.708794000	4.321765000	1	-1.066875000	0.237638000	2.434190000
6	0.583669000	0.141151000	5.162344000	6	1.410743000	-2.472304000	3.773058000
1	2.426831000	-1.016474000	5.247539000	1	2.249136000	-2.486734000	1.765653000
1	-1.237193000	1.266375000	4.754108000	6	0.452378000	-1.914387000	4.638145000
1	0.505386000	0.250840000	6.255452000	1	-1.180026000	-0.481728000	4.815233000
6	-0.259966000	-0.741950000	-1.481079000	1	2.115741000	-3.231819000	4.147193000
6	-0.627382000	0.382618000	-2.272111000	1	0.403566000	-2.229596000	5.692408000
6	-0.271871000	-2.037550000	-2.068842000	6	-0.576638000	-0.236966000	-1.724308000
6	-0.986988000	0.212608000	-3.614889000	6	-1.435191000	-0.909008000	-2.635274000
1	-0.608109000	1.384433000	-1.816938000	6	0.086909000	0.933773000	-2.176978000
6	-0.636348000	-2.193904000	-3.413906000	6	-1.592439000	-0.448915000	-3.953232000
1	0.012211000	-2.906939000	-1.458906000	1	-1.964918000	-1.820444000	-2.318110000
6	-0.993287000	-1.074824000	-4.188375000	6	-0.075771000	1.390068000	-3.493429000
1	-1.258574000	1.089006000	-4.224270000	1	0.731238000	1.488868000	-1.476806000
1	-0.640830000	-3.199409000	-3.862783000	6	-0.911794000	0.700481000	-4.391584000
1	-1.274113000	-1.204633000	-5.245574000	1	-2.248845000	-1.001140000	-4.644175000
1	-7.049955000	-2.583859000	1.825821000	1	0.448507000	2.303607000	-3.815844000
1	-7.068562000	-0.794300000	1.712911000	1	-1.036782000	1.061010000	-5.424797000
1	-5.514729000	-1.670351000	1.732526000	1	4.737857000	-3.184370000	-3.276802000
1	-5.787694000	0.007696000	-4.341284000	1	5.600434000	-1.634647000	-3.040398000
1	-4.999547000	0.835540000	-2.957159000	1	3.865912000	-1.751895000	-2.640304000
1	-6.733844000	1.098366000	-3.294142000	1	6.805705000	-0.452816000	1.972093000
1	-4.111904000	4.174666000	-1.249259000	1	6.200647000	-1.613117000	3.191659000
1	-3.060087000	2.734672000	-1.275542000	1	5.067699000	-0.487228000	2.377120000
1	-2.337251000	4.378685000	-1.263896000	1	5.379921000	2.954147000	1.422970000
1	-4.827694000	2.197770000	4.692748000	1	3.736377000	2.324930000	1.708631000
1	-4.842204000	0.991864000	3.366554000	1	4.133217000	4.021802000	2.138193000
1	-6.036224000	2.316142000	3.380989000	1	3.523730000	2.869009000	-4.549884000
1	5.836483000	3.120653000	0.550922000	1	3.547882000	1.405871000	-3.510964000
1	4.213714000	2.672524000	1.139567000	1	5.058499000	2.298015000	-3.839408000
1	4.695643000	4.397615000	1.073717000	1	1.230490000	6.589171000	-2.376016000

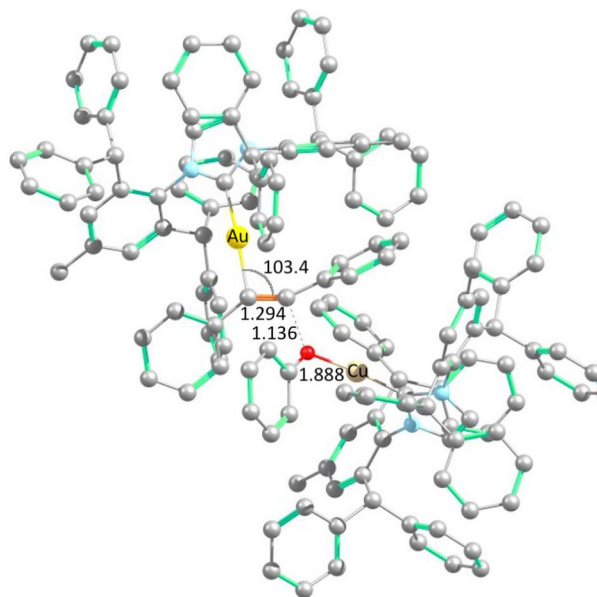
Supporting Information

1	3.454765000	0.460938000	-3.641743000
1	4.978096000	1.135548000	-4.282810000
1	3.419984000	1.613157000	-5.014564000
1	4.654572000	-3.945670000	-2.419965000
1	5.533471000	-2.397680000	-2.607081000
1	3.828197000	-2.391075000	-2.084585000
1	6.606955000	-0.959862000	3.386494000
1	5.554522000	0.044052000	2.338730000
1	7.264765000	-0.216597000	1.901732000
1	-1.070430000	1.009424000	2.276664000
1	1.385664000	5.831925000	-3.670762000
1	2.923664000	6.726236000	-3.542057000
1	1.843785000	6.622472000	-2.123116000
1	4.734831000	-5.705767000	3.031415000
1	6.469270000	-5.941690000	2.692584000
1	5.242268000	-6.536833000	1.527459000
1	-1.535972000	5.868978000	4.374742000
1	-0.611597000	6.084136000	2.851399000
1	-0.286288000	4.681020000	3.915084000
1	-7.043725000	-5.397067000	-2.122385000
1	-6.702646000	-4.713407000	-3.748684000
1	-8.337260000	-4.580797000	-3.044438000
1	7.106991000	2.066405000	-1.182442000
1	6.777308000	1.323367000	-2.778183000
1	7.779489000	-0.111833000	-0.373350000
1	7.270477000	-0.878472000	-1.909244000
1	-7.916479000	1.172619000	0.388481000
1	-7.559881000	1.812775000	-1.246471000
1	-6.869847000	3.163630000	1.280966000
1	-6.246087000	3.624519000	-0.334018000

1	2.731368000	7.435429000	-1.914862000
1	1.552034000	6.982395000	-0.652121000
1	4.756453000	-6.576335000	0.196212000
1	5.168205000	-6.162551000	1.895276000
1	6.463646000	-6.408976000	0.691240000
1	-5.123911000	1.500485000	-4.085117000
1	-3.984531000	1.269793000	-2.727900000
1	-5.478553000	2.214079000	-2.480329000
1	-7.419771000	-2.807581000	0.658674000
1	-7.973236000	-1.128858000	0.892938000
1	-6.270508000	-1.553791000	1.226241000
1	-6.548938000	-2.956945000	-5.275219000
1	-8.209222000	-3.016051000	-4.614955000
1	-6.978573000	-4.157124000	-4.009689000
1	-5.201348000	0.360168000	3.466259000
1	-5.821239000	1.817939000	4.294401000
1	-4.638702000	0.771534000	5.118808000
1	-1.851619000	4.272373000	-0.001468000
1	-3.558632000	3.776297000	-0.229900000
1	-2.247564000	2.585271000	-0.432924000
1	6.658153000	2.094943000	-2.205842000
1	6.862599000	2.402087000	-0.453355000
1	7.582639000	0.107142000	-0.207842000
1	7.159346000	-0.251690000	-1.910439000
1	-7.712146000	1.239403000	0.630847000
1	-7.204331000	2.322956000	-0.702235000
1	-6.550531000	2.694056000	2.170522000
1	-5.865776000	3.648696000	0.818114000
1	-0.072443000	4.628576000	4.452569000
1	0.236100000	2.923597000	4.893729000
1	-0.921755000	3.889337000	5.852075000



43 [Cu(IPr*)(OPh)] + [Au(IPr*)(PhCCPh)]⁺



43-44 TS

$E(\text{scf}) = -1630.34021153891 \text{ a.u.}$

$V_{\text{min}} = -131.1043 \text{ cm}^{-1}$

6	-4.794633000	0.197737000	0.041932000
7	-5.944141000	-0.087615000	-0.641104000
7	-5.087829000	1.382996000	0.657570000
6	-6.919272000	0.885660000	-0.466268000
6	-6.373832000	1.824133000	0.375734000

Supporting Information

E(scf)= -1630.35461917739 a.u.

6	-5.679313000	0.092049000	0.034197000	6	-6.086625000	-1.261782000	-1.486631000
7	-6.690767000	-0.394935000	-0.741043000	6	-4.138795000	2.061579000	1.525410000
7	-6.311051000	0.958364000	0.877244000	6	-6.989028000	-2.284403000	-1.115169000
6	-7.919890000	0.152144000	-0.398898000	6	-7.136779000	-3.385907000	-1.965780000
6	-7.677236000	1.014903000	0.643519000	6	-6.417905000	-3.476157000	-3.164863000
6	-6.471165000	-1.362784000	-1.803216000	6	-5.529282000	-2.445981000	-3.518615000
6	-5.591901000	1.698955000	1.900629000	6	-5.344923000	-1.337604000	-2.691196000
6	-7.000223000	-2.668202000	-1.675091000	6	-7.794505000	-2.196409000	0.170724000
6	-6.813762000	-3.570250000	-2.728553000	1	-7.822584000	-4.190958000	-1.686359000
6	-6.129881000	-3.194601000	-3.892141000	6	-6.584181000	-4.650763000	-4.066528000
6	-5.611821000	-1.892291000	-3.998934000	1	-4.970046000	-2.524012000	-4.455120000
6	-5.765669000	-0.966633000	-2.965838000	6	-4.369410000	-0.236245000	-3.080490000
6	-7.760995000	-3.094700000	-0.430450000	6	-3.605197000	3.311174000	1.133768000
1	-7.210901000	-4.586196000	-2.640490000	6	-2.725430000	3.963140000	2.005335000
6	-5.952626000	-4.156477000	-5.015680000	6	-2.388054000	3.402914000	3.244389000
1	-5.078238000	-1.605567000	-4.909887000	6	-2.928600000	2.160397000	3.614575000
6	-5.184485000	0.434329000	-3.097351000	6	-3.802322000	1.473215000	2.769967000
6	-5.482277000	3.104797000	1.797357000	6	-3.988253000	3.948641000	-0.191481000
6	-4.819420000	3.799604000	2.814862000	1	-2.298746000	4.926498000	1.717041000
6	-4.281560000	3.125969000	3.919811000	6	-1.472757000	4.118096000	4.179711000
6	-4.402591000	1.728090000	4.003793000	1	-2.658309000	1.729329000	4.582193000
6	-5.048050000	0.997271000	3.005593000	6	-4.390928000	0.133782000	3.187506000
6	-6.071224000	3.857100000	0.615274000	79	-3.037168000	-0.852732000	0.126301000
1	-4.720836000	4.886591000	2.746718000	6	-0.326946000	-1.237280000	0.590784000
6	-3.582048000	3.873489000	5.001863000	6	-1.218140000	-2.043142000	0.109053000
1	-3.977787000	1.208618000	4.868331000	6	4.656750000	-0.084995000	-0.103992000
6	-5.165164000	-0.516638000	3.110651000	7	5.503810000	0.579978000	0.759048000
79	-3.677450000	-0.317742000	-0.030979000	7	5.379717000	-0.074739000	-1.276856000
6	-1.416894000	-0.069757000	0.122749000	6	6.692186000	0.970226000	0.154266000
6	-1.630599000	-1.245019000	-0.287519000	6	6.611276000	0.554635000	-1.149391000
6	5.672895000	-0.002278000	-0.087360000	6	5.134894000	0.986562000	2.109656000
7	6.523464000	0.737429000	0.708044000	6	4.935710000	-0.652306000	-2.539267000
7	6.426919000	-0.171624000	-1.228235000	1	7.483055000	1.503978000	0.693594000
6	7.739502000	1.010083000	0.093167000	1	7.320427000	0.639240000	-1.979783000
6	7.677980000	0.427476000	-1.146777000	6	5.217791000	0.064701000	3.181865000
6	6.142665000	1.298073000	1.998697000	6	4.721469000	0.455131000	4.429898000
6	5.977624000	-0.907048000	-2.403439000	6	4.201527000	1.740227000	4.637145000
1	8.531267000	1.591152000	0.579341000	6	4.243666000	2.677602000	3.595580000
1	8.410808000	0.380265000	-1.959692000	6	4.743493000	2.330629000	2.336678000
6	6.259221000	0.523795000	3.178836000	6	5.879089000	-1.291028000	3.000754000
6	5.801796000	1.073028000	4.380655000	1	4.744218000	-0.248335000	5.267593000
6	5.263046000	2.366729000	4.433161000	1	3.897965000	3.696032000	3.779188000
6	5.235987000	3.149685000	3.270992000	6	4.963455000	3.395781000	1.274710000
6	5.699787000	2.642149000	2.053482000	6	4.086557000	0.089601000	-3.393548000
6	6.903503000	-0.851900000	3.158348000	6	3.696356000	-0.479527000	-4.610720000
1	5.862147000	0.486407000	5.302171000	6	4.134392000	-1.756180000	-4.988862000
1	4.859569000	4.172986000	3.321996000	6	5.005384000	-2.462239000	-4.146710000
6	5.804846000	3.546007000	0.836144000	6	5.428379000	-1.921315000	-2.929214000
6	5.235134000	-0.241465000	-3.407750000	6	3.622320000	1.492558000	-3.033469000
6	4.790123000	-0.978283000	-4.510162000	1	3.041976000	0.081245000	-5.283190000
6	5.085810000	-2.342856000	-4.637203000	1	5.362721000	-3.450130000	-4.451302000
6	5.874883000	-2.971470000	-3.663254000	6	6.440343000	-2.668990000	-2.075989000
6	6.342132000	-2.266867000	-2.550134000	1	5.478711000	-1.740732000	2.046503000
6	4.965437000	1.251599000	-3.325864000	1	4.791046000	2.924464000	0.263683000
1	4.206444000	-0.484852000	-5.290096000	1	3.446423000	1.527013000	-1.919915000
1	6.129678000	-4.028375000	-3.779261000	1	6.190967000	-2.483936000	-0.990996000
6	7.273430000	-2.937507000	-1.553503000	29	3.071827000	-1.000549000	0.281353000
1	6.540838000	-1.386192000	2.232466000	6	1.812324000	-3.337264000	1.282384000
1	5.606612000	2.922201000	-0.082859000	6	0.974791000	-3.836186000	2.313743000
1	4.843608000	1.525257000	-2.237924000	6	2.879658000	-4.161969000	0.833061000
1	7.017909000	-2.554498000	-0.522970000	6	1.208837000	-5.098332000	2.878197000
29	4.031482000	-0.762954000	0.364273000	1	0.125201000	-3.217385000	2.659026000
6	2.493676000	-2.712772000	1.665357000	6	3.115037000	-5.416525000	1.415823000
				1	3.523735000	-3.799913000	0.005729000
				6	2.283591000	-5.895771000	2.443942000
				1	0.539679000	-5.464159000	3.673125000

Supporting Information

6	1.488858000	-2.960405000	2.646054000	1	3.957352000	-6.029050000	1.054904000
6	3.481721000	-3.725508000	1.481799000	1	2.462705000	-6.884889000	2.890748000
6	1.485590000	-4.141313000	3.402441000	8	1.617204000	-2.106980000	0.756372000
1	0.708087000	-2.190818000	2.803395000	6	-1.286922000	-3.388648000	-0.473062000
6	3.472830000	-4.902049000	2.246808000	6	-2.456798000	-4.177806000	-0.340698000
1	4.257758000	-3.570111000	0.703138000	6	-0.194124000	-3.913680000	-1.209644000
6	2.479684000	-5.121061000	3.219656000	6	-2.526681000	-5.457992000	-0.910657000
1	0.692517000	-4.298398000	4.152278000	1	-3.314251000	-3.774346000	0.222051000
1	4.257178000	-5.659325000	2.080354000	6	-0.275302000	-5.188005000	-1.788155000
1	2.473080000	-6.046196000	3.815451000	1	0.715950000	-3.305959000	-1.315877000
8	2.469641000	-1.581377000	0.949059000	6	-1.437566000	-5.966633000	-1.639281000
6	-1.438163000	-2.581597000	-0.783681000	1	-3.441518000	-6.058540000	-0.789813000
6	-2.492881000	-3.375268000	-1.301357000	1	0.581434000	-5.580924000	-2.356688000
6	-0.116430000	-3.105572000	-0.737199000	1	-1.493938000	-6.967944000	-2.092084000
6	-2.230586000	-4.669549000	-1.769804000	6	0.085109000	0.058541000	1.075262000
1	-3.517772000	-2.969462000	-1.337712000	6	-0.161653000	1.219564000	0.293062000
6	0.125849000	-4.403241000	-1.206192000	6	0.718214000	0.203036000	2.339569000
1	0.704732000	-2.493482000	-0.329497000	6	0.186842000	2.487775000	0.779641000
6	-0.923183000	-5.186308000	-1.722591000	1	-0.642855000	1.110046000	-0.690830000
1	-3.054524000	-5.279579000	-2.170290000	6	1.068043000	1.474188000	2.813709000
1	1.148161000	-4.806178000	-1.156069000	1	0.922444000	-0.693229000	2.940603000
1	-0.722159000	-6.205476000	-2.084835000	6	0.802528000	2.618731000	2.038145000
6	-0.850320000	1.140260000	0.650910000	1	-0.028175000	3.382482000	0.172027000
6	-1.545424000	2.377318000	0.646972000	1	1.562949000	1.572396000	3.792532000
6	0.464576000	1.069648000	1.192848000	1	1.086131000	3.616647000	2.409228000
6	-0.946734000	3.522255000	1.189469000	1	-4.513909000	-0.506530000	2.258610000
1	-2.560408000	2.431952000	0.218352000	1	-3.881094000	0.153808000	-2.133164000
6	1.048777000	2.228796000	1.721783000	1	-7.174220000	-1.644453000	0.937077000
1	1.019674000	0.113712000	1.189927000	1	-6.896002000	-4.347132000	-5.077709000
6	0.349939000	3.450780000	1.730134000	1	-7.331309000	-5.371586000	-3.705330000
1	-1.499570000	4.475053000	1.187811000	1	-5.638038000	-5.204657000	-4.179285000
1	2.068024000	2.172879000	2.138270000	1	-2.007627000	4.442863000	5.086806000
1	0.822099000	4.350679000	2.154656000	1	-1.021380000	5.017496000	3.739018000
1	-5.093087000	-0.955246000	2.067160000	1	-0.647051000	3.470762000	4.512294000
1	-4.841028000	0.778623000	-2.072715000	1	-4.225129000	3.120558000	-0.923891000
1	-7.334268000	-2.536182000	0.454295000	6	-5.772307000	0.276277000	3.804614000
1	-6.528798000	-3.846284000	-5.902415000	6	-6.613175000	-0.849896000	3.820281000
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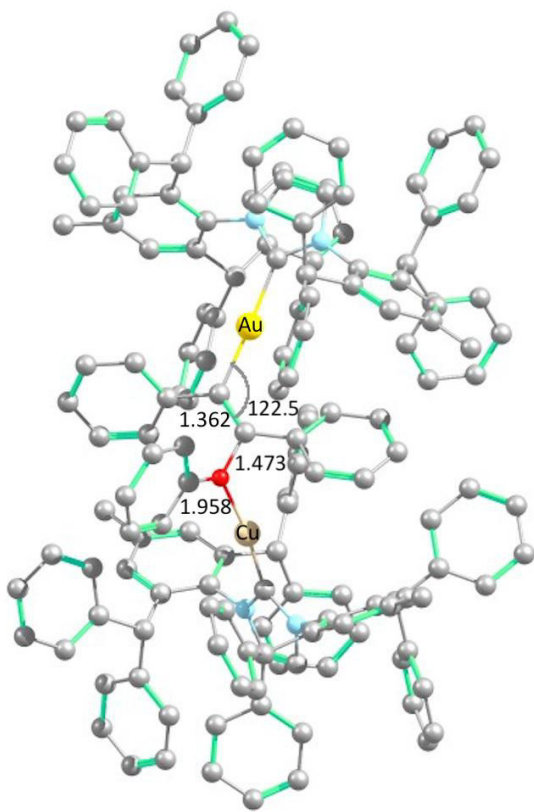
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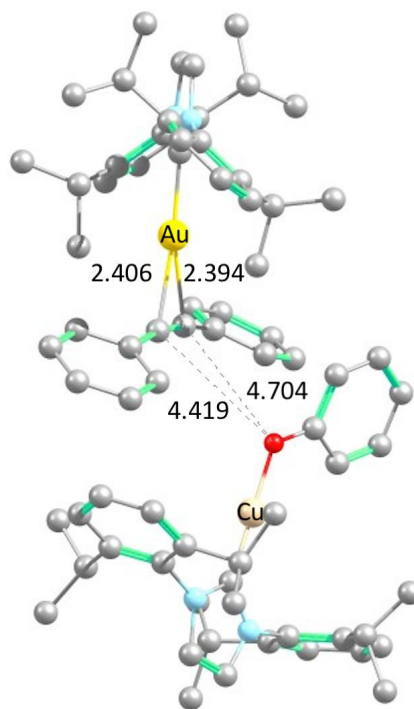
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1	4.714979000	-2.469417000	3.352686000
6	6.839755000	-2.518688000	6.607159000
6	4.923675000	-3.273044000	5.337924000
1	7.433975000	-2.536793000	7.519602000
1	4.020002000	-3.879256000	5.249197000
6	5.681041000	-3.296399000	6.512807000
1	5.372647000	-3.919995000	7.349552000
6	4.756049000	2.906342000	5.727976000
1	4.302721000	3.901797000	5.633335000
1	3.993125000	2.244824000	6.167240000
1	5.565579000	2.991151000	6.469939000
6	4.594912000	-3.121629000	-5.810820000
1	4.093694000	-4.050847000	-5.499430000
1	3.878254000	-2.563358000	-6.428236000
1	5.426758000	-3.414386000	-6.470414000
1	-8.849944000	-0.117996000	-0.908637000
1	-8.350688000	1.656267000	1.220296000



44 [Cu(IPr*)(PhO)(PhCCPh)(IPr*)Au]⁺ min

6	10.177199000	-1.088500000	2.520925000
1	11.258646000	-1.054492000	2.401953000
6	5.552397000	-2.260831000	4.126742000
6	6.322142000	-2.295402000	5.300010000
6	4.472636000	-3.142941000	3.981640000
1	7.169980000	-1.620454000	5.417400000
1	3.863809000	-3.136272000	3.075119000
6	6.012486000	-3.204800000	6.314238000
6	4.168340000	-4.052762000	4.998469000
1	6.616629000	-3.231916000	7.220245000
1	3.332598000	-4.741964000	4.867750000
6	4.935499000	-4.085292000	6.166415000
1	4.700477000	-4.797151000	6.955623000
6	3.654534000	2.114197000	5.973661000
1	3.082448000	3.050852000	5.959948000
1	2.994742000	1.334169000	6.382056000
1	4.467600000	2.249660000	6.706255000
6	3.705329000	-2.354575000	-6.285553000
1	3.354935000	-3.390566000	-6.161390000
1	2.891814000	-1.796336000	-6.768705000
1	4.540537000	-2.386804000	-7.003320000
1	-7.905158000	0.828019000	-0.938768000
1	-6.785169000	2.753311000	0.783058000



45 [Cu(IPr)(PhO)] + [Au(IPr)(PhCCPh)]⁺

E(scf) = -1631.160515853887 a.u.

6	-5.273434000	0.499252000	-0.325494000
7	-6.433792000	-0.168682000	-0.062492000
7	-5.656545000	1.500510000	-1.169512000
6	-7.522736000	0.396793000	-0.720438000
6	-7.024362000	1.456904000	-1.435084000
6	-6.470066000	-1.322053000	0.825364000
6	-4.728660000	2.465264000	-1.744086000
1	-8.538392000	-0.001929000	-0.631599000
1	-7.517986000	2.179910000	-2.093376000
6	-5.946940000	-1.193252000	2.133720000

Supporting Information

E(scf)= -1630.35909316135 a.u.

6	4.693239000	0.151818000	-0.077890000	6	-6.024434000	-2.299896000	2.991365000
7	5.747404000	-0.254167000	0.697764000	6	-6.610799000	-3.494645000	2.570264000
7	5.212957000	1.228084000	-0.747708000	6	-7.108304000	-3.609846000	1.273054000
6	6.875328000	0.538016000	0.528349000	6	-7.033960000	-2.537320000	0.371336000
6	6.535610000	1.484241000	-0.406562000	6	-5.322661000	0.087842000	2.669413000
6	5.661529000	-1.383805000	1.610536000	1	-5.635375000	-2.222150000	4.008471000
6	4.457519000	2.013508000	-1.711484000	1	-6.682020000	-4.339156000	3.258955000
6	6.424418000	-2.545207000	1.356097000	1	-7.564073000	-4.550124000	0.951997000
6	6.328862000	-3.619438000	2.249797000	6	-7.564679000	-2.722509000	-1.041680000
6	5.513534000	-3.543787000	3.385168000	6	-3.598039000	1.993603000	-2.450665000
6	4.780074000	-2.370864000	3.634148000	6	-2.747217000	2.935203000	-3.047312000
6	4.836303000	-1.285439000	2.759055000	6	-3.013252000	4.301704000	-2.956029000
6	7.351647000	-2.641279000	0.155511000	6	-4.122199000	4.751653000	-2.239571000
1	6.897888000	-4.531697000	2.051959000	6	-4.989088000	3.849223000	-1.606644000
6	5.417250000	-4.690754000	4.332969000	6	-3.245579000	0.519224000	-2.580662000
1	4.150982000	-2.319091000	4.526576000	1	-1.866111000	2.592879000	-3.595233000
6	4.037020000	-0.021225000	3.037617000	1	-2.350378000	5.019617000	-3.443371000
6	4.141167000	3.358017000	-1.415614000	1	-4.318004000	5.824147000	-2.169310000
6	3.460190000	4.116336000	-2.376422000	6	-6.165103000	4.393598000	-0.810805000
6	3.118680000	3.567278000	-3.618018000	1	-5.342826000	0.910671000	1.901622000
6	3.442260000	2.228897000	-3.895093000	6	-3.851624000	-0.165764000	3.045319000
6	4.094609000	1.432508000	-2.951943000	6	-6.133147000	0.606672000	3.863257000
6	4.527609000	3.993366000	-0.090025000	1	-7.137595000	-1.934085000	-1.714658000
1	3.199020000	5.153121000	-2.153201000	6	-7.139725000	-4.073262000	-1.629259000
6	2.414067000	4.385186000	-4.647168000	6	-9.091625000	-2.579224000	-1.031959000
1	3.168337000	1.807720000	-4.866485000	1	-4.059690000	-0.134460000	-2.160696000
6	4.393597000	-0.029807000	-3.249250000	6	-3.104680000	0.123165000	-4.054903000
79	2.796509000	-0.647622000	-0.168109000	6	-1.958100000	0.234664000	-1.792201000
6	-0.139396000	-0.991546000	-0.919881000	1	-6.554461000	3.603673000	-0.117793000
6	0.901429000	-1.533590000	-0.227606000	6	-5.746696000	5.577897000	0.069151000
6	-4.605735000	-0.007324000	0.082655000	6	-7.289983000	4.792651000	-1.774227000
7	-5.543798000	0.710357000	-0.622709000	1	-3.198926000	0.701815000	2.820737000
7	-5.206637000	-0.152456000	1.311375000	1	-3.742428000	-0.301128000	4.136896000
6	-6.673870000	0.995570000	0.130421000	1	-3.450845000	-1.113915000	2.634582000
6	-6.457191000	0.445295000	1.369375000	1	-5.732077000	1.556743000	4.236905000
6	-5.341635000	1.205147000	-1.979238000	1	-7.181609000	0.781079000	3.587165000
6	-4.597322000	-0.843247000	2.440854000	1	-6.140519000	-0.095113000	4.706184000
1	-7.520217000	1.565542000	-0.268857000	1	-7.396418000	-4.133737000	-2.694857000
1	-7.075313000	0.434102000	2.273176000	1	-6.058092000	-4.230346000	-1.545259000
6	-5.614300000	0.368053000	-3.088545000	1	-7.635669000	-4.919650000	-1.139385000
6	-5.329701000	0.848813000	-4.369613000	1	-9.507898000	-2.719336000	-2.037868000
6	-4.816715000	2.139843000	-4.565791000	1	-9.569383000	-3.325561000	-0.384749000
6	-4.642718000	2.986484000	-3.462362000	1	-9.407226000	-1.589811000	-0.677705000
6	-4.928283000	2.547766000	-2.166061000	1	-2.900994000	-0.950356000	-4.159175000
6	-6.240905000	-1.003968000	-2.900999000	1	-4.019947000	0.341827000	-4.618638000
1	-5.516029000	0.215361000	-5.242085000	1	-2.283906000	0.650551000	-4.557086000
1	-4.290345000	4.008842000	-3.621088000	1	-1.906383000	-0.808913000	-1.430980000
6	-4.876012000	3.516926000	-0.996733000	1	-1.056045000	0.289736000	-2.452732000
6	-3.818222000	-0.106620000	3.369895000	1	-1.726512000	0.994313000	-1.021622000
6	-3.200094000	-0.794574000	4.415906000	1	-6.558912000	5.867043000	0.747872000
6	-3.368416000	-2.179465000	4.577166000	1	-4.873020000	5.336394000	0.684698000
6	-4.202299000	-2.875844000	3.693994000	1	-5.497706000	6.469102000	-0.519675000
6	-4.837329000	-2.223416000	2.630180000	1	-8.151506000	5.200223000	-1.230628000
6	-3.691539000	1.404784000	3.270390000	1	-6.966691000	5.565621000	-2.483007000
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1	-4.365617000	-3.947338000	3.838112000	79	-3.395973000	-0.011937000	0.405290000
6	-5.814999000	-2.991848000	1.754941000	6	-1.488111000	-1.302242000	1.057474000
1	-5.683841000	-1.521179000	-2.068594000	6	-1.148597000	-0.113604000	1.259532000
1	-4.480188000	2.958948000	-0.100421000	6	5.796361000	0.241118000	0.196985000
1	-3.689395000	1.688002000	2.179225000	7	6.855817000	-0.636297000	0.292748000
1	-5.869761000	-2.504463000	0.740501000	7	6.338165000	1.394281000	0.726228000
29	-2.993386000	-0.737021000	-0.502777000	6	7.990775000	-0.061540000	0.849214000
				6	7.659632000	1.240317000	1.127580000
				6	6.816378000	-2.034113000	-0.124929000
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Supporting Information

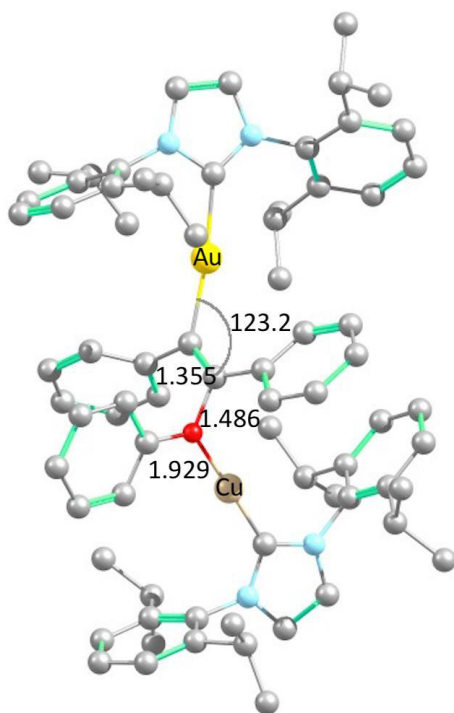
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1	0.499516000	-2.776845000	-2.691075000	6	6.486557000	-4.364831000	0.416633000
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1	-3.466929000	-3.327741000	-1.008763000	6	7.575088000	-1.323340000	-2.477888000
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1	0.208507000	-4.860314000	-4.047355000	1	6.818732000	-5.759661000	-1.195879000
1	-3.755542000	-5.421779000	-2.355563000	1	6.232681000	-5.147291000	1.132967000
1	-1.913188000	-6.197491000	-3.889444000	6	6.145748000	-2.686929000	2.270033000
8	-1.402565000	-1.738407000	-1.052277000	6	4.962912000	2.935359000	2.090705000
6	0.762124000	-2.823583000	0.499808000	6	4.330178000	4.178058000	2.232738000
6	1.749170000	-3.835790000	0.374779000	6	4.351611000	5.114531000	1.197870000
6	-0.317152000	-3.068777000	1.390636000	6	5.013273000	4.827788000	0.004222000
6	1.645861000	-5.046002000	1.077607000	6	5.668781000	3.600747000	-0.178865000
1	2.610132000	-3.655977000	-0.289441000	6	4.949642000	1.949990000	3.248082000
6	-0.408918000	-4.269650000	2.110550000	1	3.826809000	4.419036000	3.169703000
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1	2.423156000	-5.815831000	0.951514000	6	6.421120000	3.344551000	-1.474651000
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1	1.076473000	1.359119000	-0.235132000	1	5.254477000	0.934296000	2.885277000
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1	4.158968000	-0.625073000	-2.309430000	1	7.019324000	-2.411898000	-4.305265000
1	3.617527000	0.345794000	2.048324000	1	5.691934000	-1.503175000	-3.577930000
1	6.928465000	-2.002813000	-0.676977000	1	9.412956000	-0.663147000	-3.452775000
1	5.705727000	-4.398320000	5.354000000	1	9.660497000	-1.283271000	-1.814629000
1	6.056410000	-5.538772000	4.050440000	1	9.365416000	-2.399069000	-3.150891000
1	4.386096000	-5.074233000	4.389939000	1	4.541363000	-3.032044000	3.707257000
1	3.006123000	4.460933000	-5.572818000	1	4.024313000	-3.153804000	2.019024000
1	2.208025000	5.411909000	-4.316629000	1	4.948731000	-4.462352000	2.762943000
1	1.448858000	3.933063000	-4.923475000	1	7.121698000	-2.833125000	4.218044000
1	4.610745000	3.177632000	0.689119000	1	7.521490000	-4.163148000	3.131179000
6	5.856071000	-0.267292000	-3.580703000	1	8.245053000	-2.573531000	2.876741000
6	6.393198000	-1.547812000	-3.366517000	1	5.989946000	1.703946000	5.151892000
6	6.670033000	0.744139000	-4.107610000	1	6.979306000	2.453300000	3.893139000
1	5.765329000	-2.349338000	-2.978613000	1	5.725306000	3.390953000	4.709425000
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6	7.730075000	-1.808747000	-3.674059000	1	3.220976000	2.716392000	4.367723000
6	8.009744000	0.478782000	-4.409466000	1	2.799112000	1.586112000	3.074617000
1	8.138258000	-2.807570000	-3.512500000	1	6.031171000	3.311407000	-3.619918000
1	8.637931000	1.269006000	-4.819644000	1	4.598162000	3.002147000	-2.633327000
6	8.542661000	-0.794997000	-4.193742000	1	5.233887000	4.645277000	-2.790606000
1	9.584019000	-1.001048000	-4.436314000	1	8.261622000	4.031939000	-2.424914000
6	3.473121000	-0.572771000	-4.330303000	1	7.433337000	5.292383000	-1.512275000
6	3.892922000	-0.736504000	-5.656193000	1	8.331033000	4.034024000	-0.658228000
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1	4.916628000	-0.493317000	-5.944358000	6	2.013343000	-1.331412000	-1.978239000
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6	2.999175000	-1.219558000	-6.617570000	6	2.612448000	-2.625173000	-1.892983000
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6	1.683555000	-1.529201000	-6.262896000	1	3.487826000	-2.749193000	-1.228361000
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Supporting Information

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1	-4.157581000	4.058995000	3.249098000	6	-1.418510000	-3.194022000	3.170382000
1	-5.839154000	0.364553000	4.737353000	6	-2.159174000	-4.048758000	2.354932000
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1	-7.745044000	1.619302000	5.677946000	1	-0.563530000	-3.578575000	3.728457000
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1	-7.879983000	4.090932000	5.415552000	6	-4.018349000	-4.540117000	0.724395000
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1	-1.276967000	1.557349000	2.024551000	6	-7.453578000	1.488472000	-0.738605000
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Supporting Information

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1	-5.688362000	-4.162320000	-7.266584000
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46 [Cu(IPr)(PhO)(PhCCPh)(IPr)Au]⁺ min

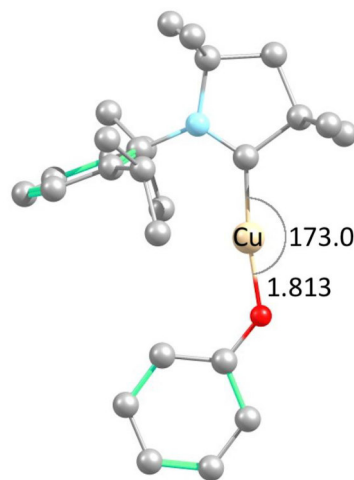
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6	8.428733000	0.407180000	-2.284650000
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Supporting Information

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47 [Cu(L¹)(OPh)]

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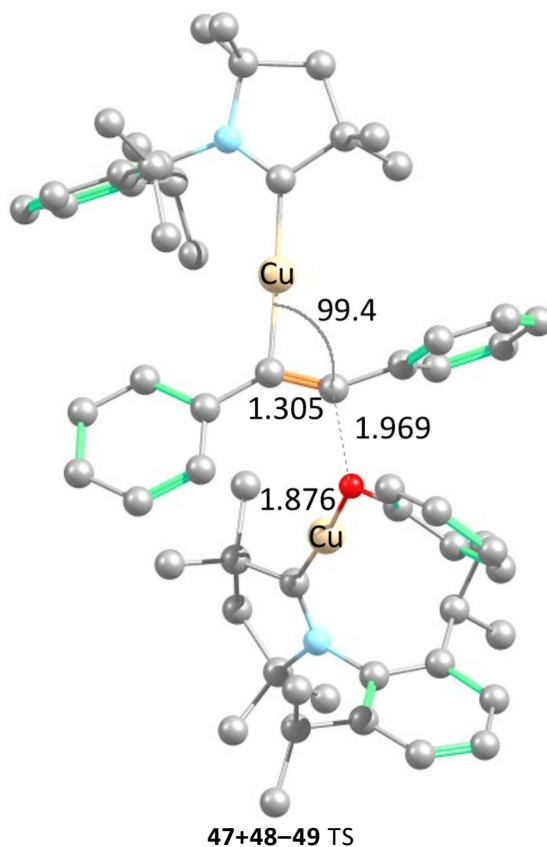
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Supporting Information

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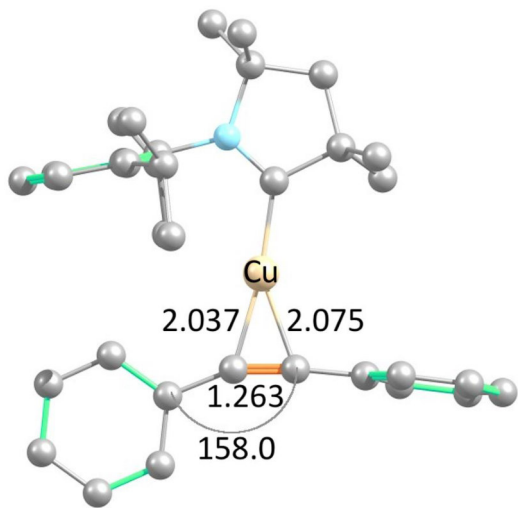
Supporting Information

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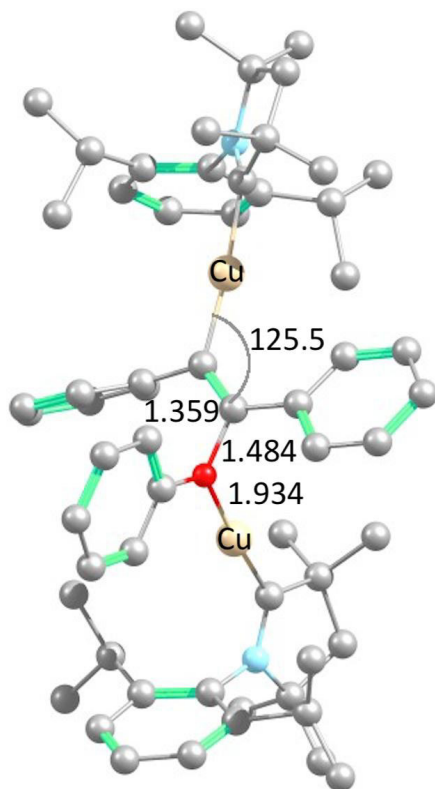
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Supporting Information

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Supporting Information

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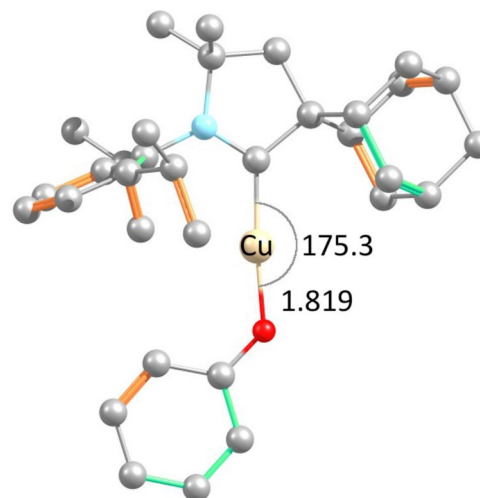
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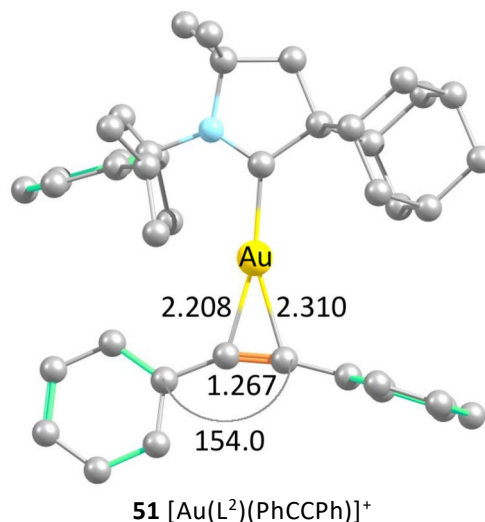
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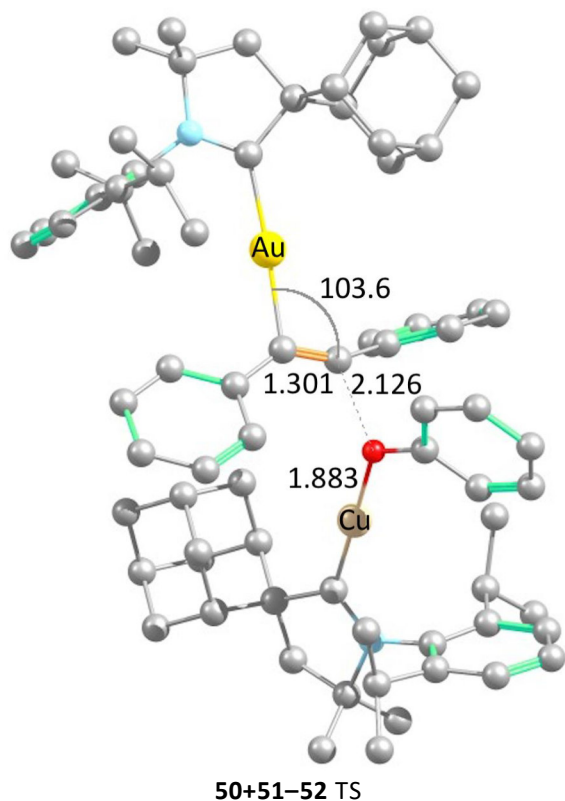
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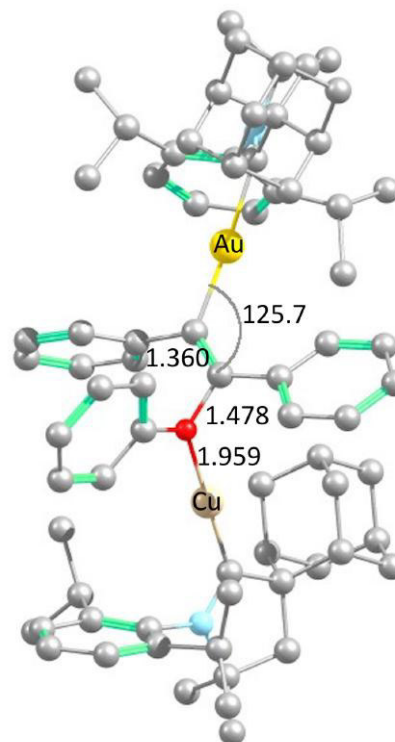
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1	1.731139000	-4.119469000	1.763920000

Supporting Information

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1	6.607344000	2.662885000	-4.164671000
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1	7.961938000	2.335413000	-3.033753000
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6	1.058848000	2.509360000	2.679557000
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6	0.772133000	-2.191499000	3.595866000
1	1.132177000	-0.213151000	2.775327000
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6	0.291359000	4.117943000	-1.651118000
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52 [Cu(L²)(PhO)(PhCCPh)(L²)Au]⁺

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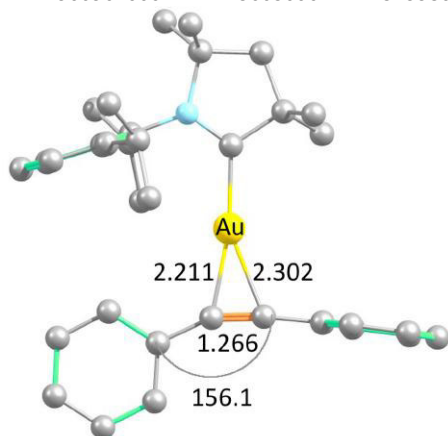
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Supporting Information

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6	7.840869000	-2.068897000	-0.007288000	6	-1.794798000	-2.764337000	0.531256000
1	8.578143000	-2.748329000	-0.480971000	6	-0.831700000	-3.757758000	0.287112000
1	8.404237000	-1.362768000	0.634033000	6	-2.960760000	-3.049466000	1.259151000
1	7.180943000	-2.682838000	0.635550000	6	-1.049651000	-5.053654000	0.787993000
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7	-5.544950000	-0.721050000	-0.220731000	6	-3.162288000	-4.349284000	1.752237000
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Supporting Information

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53 [Au(L¹)(PhCCPh)]⁺

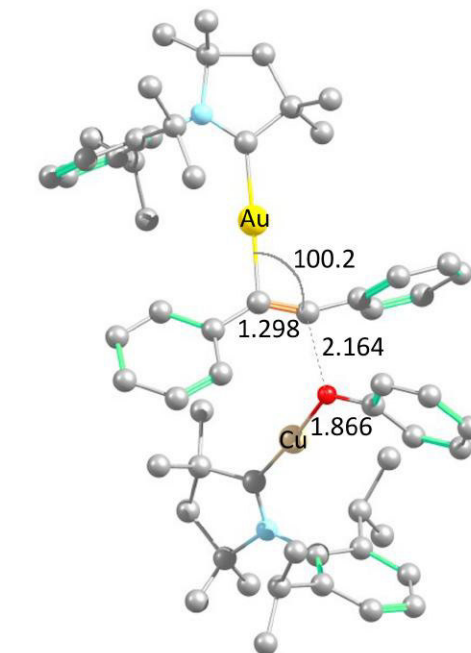
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Supporting Information

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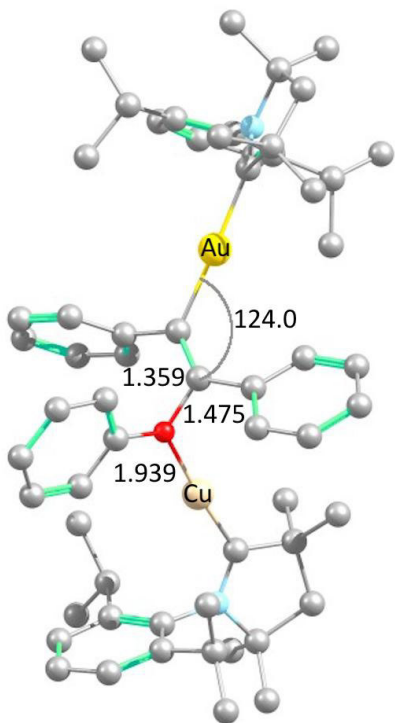
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Supporting Information

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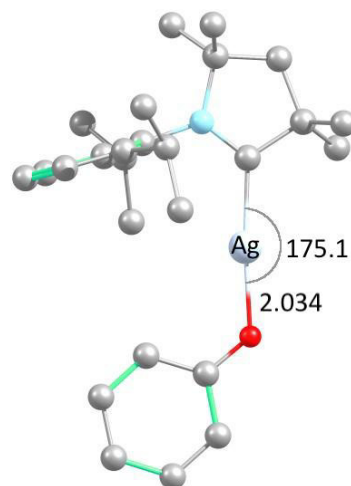
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Supporting Information

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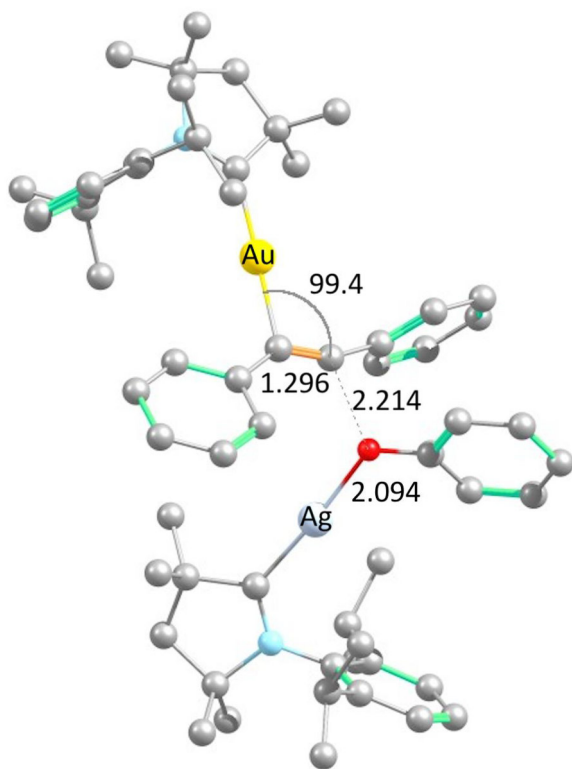
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1	2.847909000	3.290922000	2.418755000
1	2.633491000	1.616904000	1.782896000
1	2.786948000	1.898118000	3.549173000
1	5.150029000	4.033121000	3.319966000
1	5.080738000	2.714888000	4.519615000
1	6.499962000	2.856755000	3.440175000
6	5.236032000	1.361284000	-2.011957000
1	6.595828000	2.910527000	-1.268834000
1	7.406018000	1.743661000	-2.346215000
1	8.638141000	2.215298000	0.454294000
6	7.653642000	1.847934000	0.809044000
1	7.039581000	2.732737000	1.062817000
1	7.828124000	1.256654000	1.730359000
1	7.595841000	-0.797432000	-1.463653000
6	7.966155000	-0.168793000	-0.631157000
1	8.948267000	0.247277000	-0.934189000
1	8.136162000	-0.813702000	0.253017000
6	4.346056000	2.544205000	-2.448045000
1	4.808932000	3.063664000	-3.313362000
1	3.336577000	2.197366000	-2.748278000
1	4.222926000	3.283970000	-1.630456000
6	5.301666000	0.324292000	-3.164768000
1	5.950514000	-0.540287000	-2.918372000
1	4.290603000	-0.067418000	-3.398400000
1	5.707670000	0.809074000	-4.077040000
1	-2.803341000	4.303448000	1.899112000
1	-1.926453000	1.372863000	2.772757000
1	-2.562111000	2.660044000	3.850853000
1	-3.615522000	3.786778000	0.384173000

55 [Ag(L¹)(OPh)]

E(scf)= -1288.67666381 a.u.

6	1.234016000	-1.229832000	-0.085062000
7	1.912945000	-0.092255000	-0.028014000
6	3.446598000	-0.234662000	-0.019254000
6	3.589770000	-1.727074000	-0.410457000
6	1.266502000	1.212721000	0.052495000
6	0.919272000	1.750609000	1.326279000
6	0.367000000	3.048816000	1.359773000
6	0.139944000	3.778839000	0.187185000
6	0.421004000	3.199712000	-1.056552000
6	0.976250000	1.907555000	-1.158672000
6	1.001791000	0.957833000	2.634114000
1	0.091006000	3.488027000	2.331087000
1	-0.288117000	4.792253000	0.240902000
1	0.186191000	3.756600000	-1.976925000
6	1.125213000	1.279269000	-2.547697000
1	1.558229000	0.021862000	2.431622000
6	-0.414771000	0.545547000	3.097909000
6	1.742666000	1.714255000	3.755947000
1	1.709450000	0.343022000	-2.438188000
6	-0.262517000	0.879757000	-3.100589000
6	1.873438000	2.184726000	-3.547546000
1	-0.357101000	-0.086612000	4.008894000
1	-1.035598000	1.433638000	3.338748000
1	-0.947658000	-0.032095000	2.312425000
1	1.851224000	1.066444000	4.650801000
1	2.756611000	2.041378000	3.445995000
1	1.185075000	2.618960000	4.076940000
1	-0.159270000	0.366448000	-4.079736000
1	-0.794311000	0.194622000	-2.406555000
1	-0.907843000	1.770748000	-3.248835000
1	2.026121000	1.651742000	-4.509255000
1	1.298489000	3.106107000	-3.777598000
1	2.867264000	2.498163000	-3.167304000
47	-0.790397000	-1.402525000	-0.075690000
6	-3.761498000	-0.830469000	-0.052453000
6	-5.123463000	-1.258794000	-0.055244000
6	-3.521859000	0.575258000	-0.009278000
6	-6.173460000	-0.331113000	-0.016810000
1	-5.321604000	-2.341906000	-0.088768000
6	-4.581211000	1.494732000	0.029118000
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Supporting Information



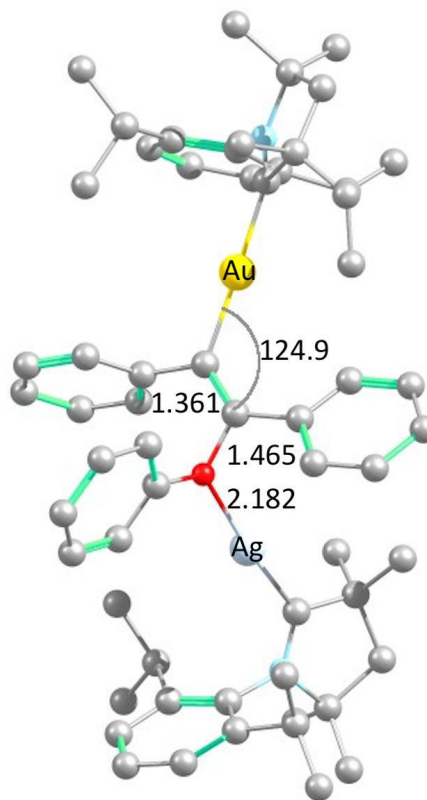
53+55-56 TS

$E(\text{scf}) = -2798.41094427 \text{ a.u.}$

$\nu_{\text{min}} = -113.2462 \text{ cm}^{-1}$

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6	-0.337531000	1.316113000	0.374743000
6	-0.937640000	0.253937000	0.812789000
6	3.939169000	-1.645455000	-0.546517000
7	5.238708000	-1.691736000	-0.768123000
6	5.770211000	-3.057052000	-1.266753000
6	4.436049000	-3.749875000	-1.638413000
6	6.135436000	-0.562804000	-0.536867000
6	6.712395000	-0.369939000	0.751830000
6	7.639140000	0.684404000	0.899213000
6	7.966459000	1.528012000	-0.168343000
6	7.333424000	1.359874000	-1.406464000
6	6.400453000	0.324915000	-1.621797000
6	6.306370000	-1.162752000	1.997870000
1	8.104155000	0.854884000	1.882556000
1	8.699792000	2.337516000	-0.028217000
1	7.562090000	2.056638000	-2.227683000
6	5.652912000	0.272975000	-2.958053000
1	5.656624000	-2.000376000	1.675308000
6	5.462291000	-0.274446000	2.940690000
6	7.510412000	-1.761265000	2.754841000
1	5.113767000	-0.694583000	-3.012763000
6	4.579971000	1.384977000	-3.012009000
6	6.586428000	0.355982000	-4.182951000
1	5.111513000	-0.859424000	3.816443000
1	6.051896000	0.585372000	3.320947000
1	4.570295000	0.137833000	2.422095000
1	7.160882000	-2.391268000	3.598888000
1	8.149213000	-2.390235000	2.101939000
1	8.156592000	-0.969407000	3.186955000

1	-7.214662000	-0.696133000	-0.020235000
1	-4.357695000	2.574749000	0.061762000
1	-6.748050000	1.777926000	0.055658000
8	-2.795394000	-1.744300000	-0.090361000
6	2.210404000	-2.402782000	-0.146453000
6	2.158151000	-3.152411000	1.210257000
6	1.819593000	-3.378173000	-1.277611000
1	2.444685000	-2.501175000	2.060732000
1	0.817019000	-3.816630000	-1.094517000
1	3.836377000	-1.802283000	-1.490000000
1	4.415002000	-2.215455000	0.145881000
6	4.112724000	0.708575000	-1.031611000
1	3.788525000	0.503843000	-2.069587000
1	3.906013000	1.772591000	-0.797931000
1	5.211178000	0.560449000	-0.987776000
6	4.007879000	0.071854000	1.382342000
1	5.110394000	-0.047513000	1.362293000
1	3.789585000	1.115311000	1.684531000
1	3.608250000	-0.609849000	2.157666000
1	2.556210000	-4.207303000	-1.338946000
1	1.135899000	-3.534696000	1.408384000
1	2.855682000	-4.016099000	1.188714000
1	1.791276000	-2.868722000	-2.262959000

56 [Ag(L¹)(PhO)(PhCCPh)(L¹)Au]⁺ min

$E(\text{scf}) = -2798.43149257 \text{ a.u.}$

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6	0.082085000	0.428638000	-1.139883000
6	-0.968634000	0.836979000	-0.376746000
6	4.291478000	-1.575025000	0.562730000
7	5.561783000	-1.353910000	0.825378000
6	6.338215000	-2.580772000	1.369876000

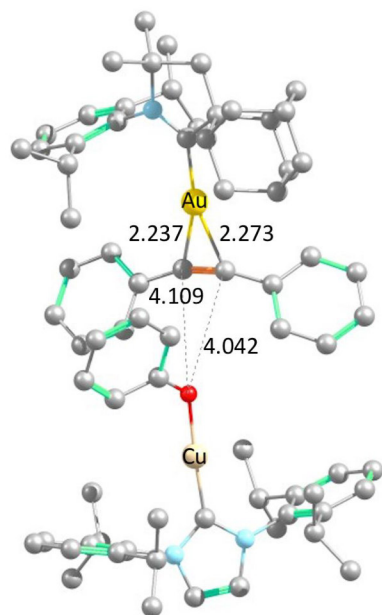
Supporting Information

1	4.006737000	1.327960000	-3.961383000	6	5.309651000	-3.705838000	1.090065000
1	3.861043000	1.297292000	-2.169392000	6	6.208821000	-0.056432000	0.644079000
1	5.043210000	2.392373000	-2.955364000	6	6.195289000	0.889064000	1.710314000
1	6.006699000	0.216452000	-5.118966000	6	6.897904000	2.097778000	1.516621000
1	7.084264000	1.345092000	-4.256233000	6	7.566902000	2.372786000	0.317928000
1	7.381487000	-0.416238000	-4.153923000	6	7.508703000	1.454141000	-0.737618000
47	2.904164000	-0.061003000	0.234592000	6	6.824944000	0.227216000	-0.610444000
6	2.197540000	2.600352000	1.569380000	6	5.379696000	0.714588000	2.994900000
6	1.593738000	3.252135000	2.679733000	1	6.910822000	2.844213000	2.325756000
6	3.287932000	3.242524000	0.925497000	1	8.118402000	3.318269000	0.197154000
6	2.082725000	4.485832000	3.136600000	1	7.998739000	1.697589000	-1.692730000
1	0.747047000	2.760269000	3.184557000	6	6.687341000	-0.670486000	-1.844445000
6	3.772139000	4.474104000	1.393248000	1	5.020075000	-0.331806000	3.036316000
1	3.757959000	2.746667000	0.059459000	6	4.123346000	1.613382000	2.953234000
6	3.174269000	5.105498000	2.500007000	6	6.199045000	0.978328000	4.274983000
1	1.608112000	4.967250000	4.007128000	1	6.280808000	-1.648977000	-1.516811000
1	4.627293000	4.947681000	0.884304000	6	5.656530000	-0.066331000	-2.825573000
1	3.556516000	6.071729000	2.863707000	6	8.028777000	-0.938691000	-2.556976000
8	1.729282000	1.402048000	1.164594000	1	3.505740000	1.465478000	3.863185000
6	-0.686221000	-0.882776000	1.713555000	1	4.392675000	2.688625000	2.897453000
6	-1.462269000	-2.064671000	1.607916000	1	3.487555000	1.378564000	2.071918000
6	0.313666000	-0.818259000	2.719847000	1	5.591175000	0.750650000	5.174917000
6	-1.236329000	-3.153452000	2.464713000	1	7.118590000	0.359693000	4.318991000
1	-2.251816000	-2.121577000	0.842096000	1	6.509099000	2.040949000	4.354086000
6	0.523245000	-1.904554000	3.583442000	1	5.506429000	-0.737213000	-3.696887000
1	0.918290000	0.095643000	2.802600000	1	4.670292000	0.082659000	-2.334195000
6	-0.244394000	-3.077705000	3.458382000	1	5.991802000	0.920373000	-3.207473000
1	-1.848993000	-4.062687000	2.361118000	1	7.885261000	-1.663328000	-3.384944000
1	1.294923000	-1.831706000	4.366471000	1	8.449178000	-0.015233000	-3.006195000
1	-0.075628000	-3.926572000	4.139817000	1	8.792586000	-1.352571000	-1.867924000
6	-0.195401000	2.524132000	-0.386653000	47	2.945612000	-0.197796000	-0.158515000
6	-0.545079000	3.780101000	0.179919000	6	1.605717000	2.357164000	-1.515150000
6	0.325059000	2.483431000	-1.709927000	6	0.755997000	2.897742000	-2.494290000
6	-0.391697000	4.957890000	-0.567215000	6	2.747919000	3.051331000	-1.082946000
1	-0.945029000	3.814809000	1.203257000	6	1.067890000	4.153949000	-3.044106000
6	0.469951000	3.664813000	-2.447216000	1	-0.137559000	2.344062000	-2.817684000
1	0.604432000	1.511533000	-2.144505000	6	3.045243000	4.304688000	-1.642689000
6	0.113063000	4.904073000	-1.878022000	1	3.392831000	2.612032000	-0.303767000
1	-0.664421000	5.926059000	-0.119528000	6	2.207271000	4.862088000	-2.624967000
1	0.864611000	3.623789000	-3.474490000	1	0.406245000	4.579490000	-3.814957000
1	0.232771000	5.831189000	-2.460391000	1	3.938330000	4.850020000	-1.299900000
6	3.302315000	-2.989445000	-0.887455000	1	2.441091000	5.845270000	-3.060786000
6	2.880730000	-3.682041000	0.435220000	8	1.375727000	1.091020000	-0.954926000
6	2.052907000	-2.792995000	-1.773344000	6	-0.752790000	1.868097000	0.683463000
1	3.741779000	-3.857858000	1.110612000	6	-0.195503000	1.496473000	1.932380000
1	1.262248000	-2.237098000	-1.228040000	6	-1.134632000	3.218840000	0.500125000
1	4.272981000	-3.667763000	-2.733127000	6	-0.021733000	2.443101000	2.956514000
1	4.456898000	-4.830295000	-1.392667000	1	0.082111000	0.443412000	2.103628000
6	6.712526000	-2.900897000	-2.467955000	6	-0.945911000	4.166927000	1.519644000
1	6.211141000	-2.435874000	-3.337620000	1	-1.581261000	3.525256000	-0.458681000
1	7.612023000	-2.305577000	-2.211948000	6	-0.390290000	3.785047000	2.753708000
1	7.055148000	-3.908434000	-2.779966000	1	0.400278000	2.127243000	3.924380000
6	6.526466000	-3.776191000	-0.134835000	1	-1.241527000	5.214446000	1.348699000
1	6.879847000	-4.757487000	-0.511144000	1	-0.253509000	4.527306000	3.555772000
1	7.417997000	-3.201522000	0.184143000	6	0.191969000	-0.659087000	-2.139630000
1	5.890334000	-3.963946000	0.751273000	6	1.138962000	-0.587776000	-3.196543000
6	-4.721987000	0.765127000	-0.845896000	6	-0.619765000	-1.820326000	-2.056778000
7	-5.723968000	-0.078463000	-0.676530000	6	1.244572000	-1.618124000	-4.145437000
6	-6.584178000	1.559408000	-2.166630000	1	1.782150000	0.299786000	-3.296583000
6	-7.069201000	0.387518000	-1.277029000	6	-0.511705000	-2.846689000	-3.007012000
6	-5.589556000	-1.352391000	0.024227000	1	-1.334764000	-1.909842000	-1.224037000
6	-5.798063000	-1.413044000	1.432532000	6	0.418793000	-2.752077000	-4.058846000
6	-5.728168000	-2.682514000	2.045490000	1	1.974371000	-1.527262000	-4.965541000
6	-5.444761000	-3.838873000	1.309500000	1	-1.152480000	-3.738480000	-2.917803000
6	-5.182216000	-3.742870000	-0.063272000	1	0.502000000	-3.559909000	-4.802746000
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Supporting Information

6	-5.991821000	-0.182933000	2.324358000	6	3.020981000	-3.049443000	2.118346000
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6	-4.834043000	-2.454329000	-2.215688000	1	5.605412000	-4.258600000	0.174675000
1	-6.136400000	0.697258000	1.667871000	1	5.282461000	-4.442084000	1.917574000
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6	-7.227691000	-0.292069000	3.241473000	1	7.509992000	-2.966104000	-0.458927000
1	-5.115141000	-1.458350000	-2.614069000	1	8.347756000	-1.925337000	0.750692000
6	-3.299173000	-2.572016000	-2.356091000	1	8.165578000	-3.681357000	1.041406000
6	-5.546139000	-3.517957000	-3.076566000	6	6.633894000	-2.400697000	2.869445000
1	-4.839943000	1.006106000	3.765935000	1	7.177726000	-3.296445000	3.231656000
1	-4.499604000	-0.752994000	3.850016000	1	7.281532000	-1.521144000	3.053939000
1	-3.829151000	0.222163000	2.502759000	1	5.713344000	-2.298951000	3.475919000
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1	-7.108283000	-1.094064000	3.999496000	6	-6.841294000	-1.181252000	-2.090043000
1	-2.997989000	-2.495563000	-3.422102000	6	-7.184038000	-0.999499000	-0.590134000
1	-2.781327000	-1.766098000	-1.792624000	6	-5.550295000	-0.556385000	1.408480000
1	-2.934873000	-3.547102000	-1.969368000	6	-5.765293000	0.669889000	2.101974000
1	-5.300672000	-3.372092000	-4.148915000	6	-5.603340000	0.664990000	3.503719000
1	-5.226145000	-4.546557000	-2.809366000	6	-5.224079000	-0.491906000	4.194191000
1	-6.648814000	-3.473391000	-2.968275000	6	-4.954375000	-1.667422000	3.482421000
6	-5.176812000	1.981029000	-1.647717000	6	-5.099194000	-1.729718000	2.081145000
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6	-4.197001000	2.269173000	-2.806105000	6	-5.288000000	-4.287341000	1.942684000
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1	-5.913689000	3.060634000	0.152389000	1	-8.177095000	2.138764000	2.014567000
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1	1.639286000	-3.780955000	-2.065818000	1	-2.667885000	-2.197720000	0.883861000
1	2.136227000	-3.071500000	0.986363000	1	-2.717865000	-3.197322000	2.374500000
1	2.418900000	-4.664996000	0.206346000	1	-5.008414000	-5.169483000	1.329741000
1	2.292021000	-2.233499000	-2.701372000	1	-4.929379000	-4.483366000	2.974608000
				1	-6.394878000	-4.233934000	1.979700000
				6	-5.478868000	-0.471751000	-2.338006000
				1	-6.739593000	-2.262931000	-2.315804000
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				1	-8.702507000	-2.525125000	-0.397790000
				6	-7.716335000	-2.288948000	0.051236000
				1	-7.050709000	-3.153538000	-0.132885000
				1	-7.863356000	-2.175564000	1.144130000
				1	-7.907720000	1.081791000	-0.826748000
				6	-8.199367000	0.130634000	-0.341246000
				1	-9.179093000	-0.174672000	-0.761376000
				1	-8.343911000	0.313838000	0.741618000
				6	-4.565030000	-1.291975000	-3.272761000
				1	-5.040673000	-1.395503000	-4.270709000
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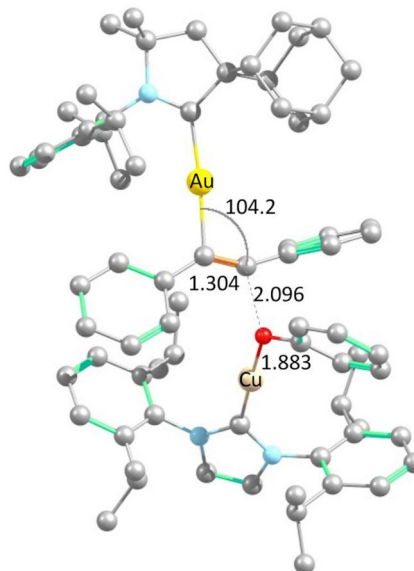
Supporting Information

57 [Cu(IPr)(OPh)] + [Au(L²)(PhCCPh)]⁺

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7	6.761795000	-0.837512000	0.245026000
7	6.462094000	1.035553000	-0.810147000
6	8.015995000	-0.424994000	-0.200440000
6	7.826714000	0.757681000	-0.868374000
6	6.530920000	-2.053731000	0.998194000
6	5.860315000	2.223361000	-1.379850000
1	8.922079000	-1.006124000	-0.002749000
1	8.533470000	1.422305000	-1.374748000
6	6.342436000	-3.266991000	0.283291000
6	6.134457000	-4.438727000	1.039655000
6	6.121220000	-4.404891000	2.441426000
6	6.316963000	-3.193571000	3.118627000
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6	6.329508000	-3.329103000	-1.244981000
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1	5.959544000	-5.333265000	3.011717000
1	6.306424000	-3.180190000	4.219727000
6	6.757395000	-0.687582000	3.187612000
6	5.817835000	3.404874000	-0.592302000
6	5.266769000	4.559225000	-1.186995000
6	4.783955000	4.538288000	-2.503313000
6	4.836343000	3.356022000	-3.254612000
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6	6.337552000	3.461429000	0.845039000
1	5.223750000	5.495313000	-0.607761000
1	4.366237000	5.454324000	-2.950294000
1	4.453050000	3.352709000	-4.287175000
6	5.428906000	0.898917000	-3.561144000
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6	4.900813000	-3.587776000	-1.770912000
6	7.332637000	-4.362457000	-1.798177000
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1	2.953290000	-4.718831000	-0.118010000
1	2.087388000	-2.475237000	1.946707000
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57-58 TS

E(scf)= -3444.48543868 a.u.

vmin= -141.0648 cm⁻¹

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7	5.969180000	0.016542000	0.910998000
7	4.952506000	1.919684000	1.150558000
6	6.845898000	0.853148000	1.595746000
6	6.203031000	2.054780000	1.748833000
6	6.290980000	-1.343658000	0.527497000
6	3.992786000	3.001517000	1.063113000
1	7.841380000	0.521491000	1.906468000
1	6.521851000	2.989018000	2.221168000
6	6.842109000	-1.572407000	-0.762033000
6	7.166153000	-2.903567000	-1.097650000
6	6.957977000	-3.953148000	-0.192124000
6	6.419800000	-3.694147000	1.076595000
6	6.075341000	-2.384375000	1.470383000
6	7.108661000	-0.447530000	-1.762927000
1	7.594091000	-3.119921000	-2.088961000
1	7.223913000	-4.983827000	-0.475425000
1	6.267541000	-4.527415000	1.780381000
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6	3.014304000	3.131351000	2.084193000
6	2.121551000	4.218401000	1.987720000
6	2.201714000	5.132326000	0.927517000
6	3.182683000	4.980778000	-0.061350000
6	4.105011000	3.914841000	-0.018529000
6	2.940454000	2.174505000	3.274807000
1	1.350747000	4.355320000	2.761940000
1	1.493745000	5.974140000	0.873382000
1	3.235452000	5.707605000	-0.886911000
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Supporting Information

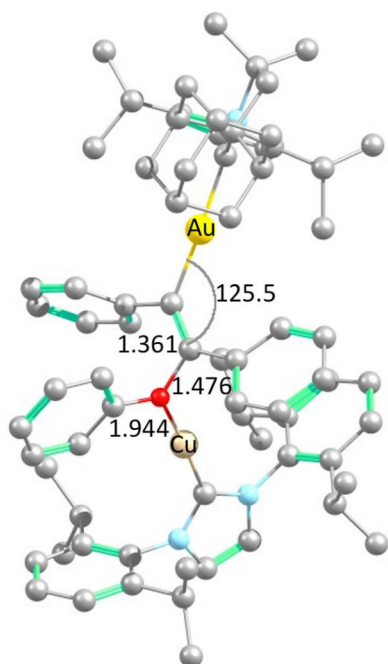
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6	5.196997000	3.749590000	1.845092000	6	6.604506000	-2.368578000	3.949243000
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6	6.344711000	1.075142000	-4.791792000	6	1.506906000	1.670132000	3.533600000
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1	4.522183000	-4.577400000	-1.437336000	6	4.581193000	3.679549000	-2.509511000
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1	4.610809000	-0.309131000	3.538721000	1	9.185530000	-0.099133000	-1.089971000
1	5.440345000	-1.101339000	4.913340000	1	9.052338000	-1.186021000	-2.506798000
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Supporting Information

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6	-5.714264000	-1.831982000	-0.590284000	7	-5.449178000	0.656681000	0.445971000
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1	-7.501019000	-1.664035000	-4.485706000	1	-2.235623000	1.584891000	1.878386000
1	-8.559434000	-1.307745000	-3.088718000	1	-2.148558000	3.256122000	2.530896000
6	-5.146552000	1.485646000	2.630918000	1	-4.541328000	2.858110000	4.624833000
6	-3.655056000	1.902639000	2.640958000	1	-4.289650000	4.310070000	3.620465000
1	-5.242596000	0.461078000	3.050783000	1	-5.848720000	3.437273000	3.540578000
6	-5.928470000	2.485483000	3.519888000	6	-5.751831000	-2.489737000	-0.588340000
6	-5.520296000	2.963127000	0.615105000	6	-4.473996000	-3.069088000	-1.242119000
6	-4.036796000	3.386572000	0.649689000	1	-6.260059000	-1.816623000	-1.312518000
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6	-3.496759000	3.338670000	2.094002000	6	-3.387549000	-3.265240000	1.014270000
1	-3.279041000	1.846716000	3.685533000	1	-4.363042000	-2.120711000	2.601174000
1	-3.036760000	1.192291000	2.048655000	6	-5.602529000	-3.837245000	2.037000000
1	-2.421834000	3.619811000	2.098137000	6	-3.770098000	-4.037186000	-0.265326000
6	-4.301756000	4.324140000	2.970293000	1	-4.760517000	-3.603508000	-2.174370000
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1	-6.210370000	4.976621000	1.081444000	6	-4.721812000	-5.197454000	0.099337000
1	-7.410385000	3.729992000	1.475910000	1	-2.883621000	-3.941123000	1.738639000
6	-5.791911000	3.916885000	2.953644000	1	-2.654272000	-2.464333000	0.773977000
1	-4.181142000	5.361855000	2.588996000	1	-5.084267000	-4.511905000	2.752598000
1	-3.914544000	4.319473000	4.012806000	1	-6.510543000	-3.471761000	2.562406000
1	-6.997601000	2.201077000	3.614334000	6	-5.993274000	-4.622313000	0.762172000
1	-5.510498000	2.441558000	4.549123000	1	-4.214499000	-5.905808000	0.790763000
1	-6.382024000	4.620142000	3.579993000	1	-4.993522000	-5.777011000	-0.810503000
1	-9.475338000	-0.499323000	0.391969000	1	-7.660096000	-3.315510000	0.173824000
1	-8.510590000	-0.099357000	-1.056411000	1	-6.937551000	-4.215343000	-1.172787000
1	-8.531532000	-1.784969000	-0.417488000	1	-6.685720000	-5.448560000	1.032907000
1	-6.720565000	-1.009430000	2.833746000	1	-8.349306000	1.008075000	2.356012000
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Supporting Information

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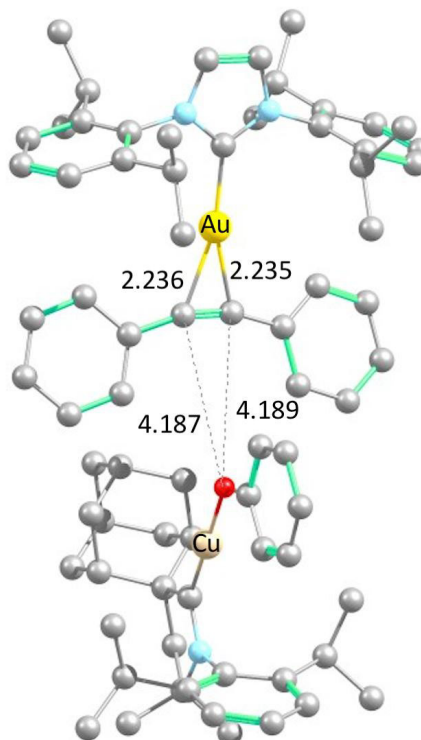


58 [Cu(IPr)(PhO)(PhCCPh)(L²)Au]⁺ min

E(scf)= -3444.50564665 a.u.

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6	-0.341207000	-1.121416000	-0.449577000
6	0.558959000	-0.692103000	0.477130000
6	-4.653163000	0.816053000	-0.303859000
7	-5.924669000	0.493932000	0.110896000
7	-4.789288000	2.050584000	-0.894187000
6	-6.830105000	1.497678000	-0.219053000
6	-6.113550000	2.478991000	-0.854538000
6	-6.298174000	-0.732971000	0.788377000
6	-3.727740000	2.816790000	-1.519925000
1	-7.894663000	1.422017000	0.022905000
1	-6.425705000	3.435124000	-1.285257000
6	-6.361911000	-0.731616000	2.208052000
6	-6.752905000	-1.933032000	2.836257000
6	-7.071395000	-3.074981000	2.087438000
6	-7.006667000	-3.041340000	0.687457000
6	-6.624609000	-1.869914000	0.001051000
6	-6.059293000	0.506824000	3.053367000
1	-6.814816000	-1.970786000	3.935102000
1	-7.380768000	-3.999311000	2.600430000
1	-7.264627000	-3.943936000	0.111843000
6	-6.580034000	-1.863421000	-1.527472000
6	-3.435715000	2.571451000	-2.888033000
6	-2.432010000	3.362679000	-3.484259000
6	-1.761244000	4.354275000	-2.756030000
6	-2.080144000	4.579871000	-1.409280000
6	-3.072208000	3.820475000	-0.755868000
6	-4.198545000	1.543983000	-3.725422000
1	-2.177734000	3.201859000	-4.543235000
1	-0.985571000	4.964097000	-3.245264000
1	-1.551291000	5.368711000	-0.852736000
6	-3.452063000	4.128721000	0.694060000
1	-5.687445000	1.301153000	2.372223000
6	-4.948912000	0.241115000	4.090843000

1 -7.384286000 2.353286000 1.677412000
 1 -7.660790000 -0.272894000 -1.058728000
 1 -8.893563000 0.181211000 0.154526000
 1 -7.939008000 1.458015000 -0.651209000



59 [Cu(L²)(OPh)] + [Au(IPr)(PhCCPh)]⁺

E(scf)= -3444.50294818 a.u.

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7	6.236697000	1.169599000	0.050846000
7	6.289063000	-0.960921000	-0.394384000
6	7.568966000	0.840521000	-0.186510000
6	7.602195000	-0.501708000	-0.466913000
6	5.782068000	2.503714000	0.398677000
6	5.900608000	-2.341780000	-0.618484000
1	8.365731000	1.588981000	-0.136402000
1	8.434165000	-1.168897000	-0.712501000
6	5.804075000	2.886960000	1.766779000
6	5.398843000	4.203580000	2.070563000
6	4.995192000	5.090396000	1.061873000
6	4.982491000	4.678430000	-0.277989000
6	5.379050000	3.376254000	-0.647138000
6	6.264927000	1.951912000	2.886651000
1	5.409068000	4.541908000	3.118533000
1	4.691649000	6.116611000	1.322210000
1	4.663490000	5.385449000	-1.059515000
6	5.384207000	2.968280000	-2.120871000
6	5.550161000	-2.741272000	-1.935782000
6	5.215542000	-4.098250000	-2.125761000
6	5.237675000	-5.009043000	-1.060425000
6	5.588675000	-4.581621000	0.228282000
6	5.930927000	-3.237268000	0.484509000
6	5.541518000	-1.780304000	-3.125174000
1	4.938098000	-4.448623000	-3.131975000
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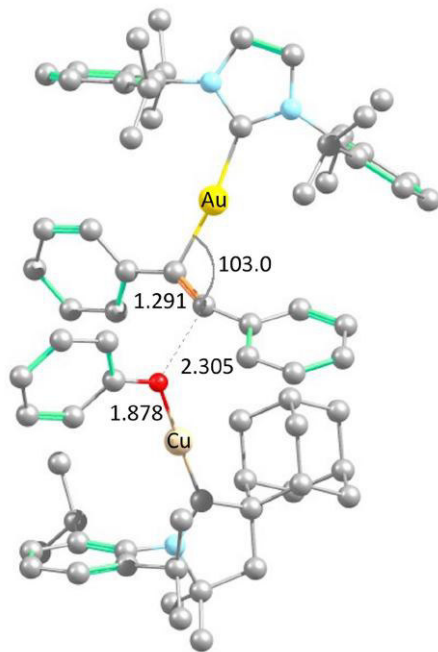
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1	-6.304324000	-0.839029000	-1.855184000	1	6.467599000	0.956506000	2.438128000
6	-5.489820000	-2.817888000	-2.059351000	6	5.171226000	1.749847000	3.956726000
6	-7.960395000	-2.181983000	-2.141032000	6	7.583799000	2.448760000	3.519929000
1	-4.803625000	0.924020000	-3.030700000	1	5.666391000	1.895524000	-2.176296000
6	-5.178420000	2.248188000	-4.691551000	6	3.984821000	3.100890000	-2.757805000
6	-3.257652000	0.586071000	-4.481795000	6	6.444504000	3.763435000	-2.914804000
1	-4.024712000	3.259299000	1.082587000	1	5.811982000	-0.770211000	-2.751115000
6	-2.226247000	4.312496000	1.610121000	6	6.602708000	-2.176687000	-4.175336000
6	-4.375594000	5.367100000	0.766246000	6	4.137104000	-1.668923000	-3.756562000
1	-4.718219000	1.169857000	4.653001000	1	6.490697000	-1.707877000	1.885792000
1	-5.254789000	-0.523686000	4.834850000	6	5.243640000	-3.108307000	2.935368000
1	-4.011739000	-0.108027000	3.610923000	6	7.688794000	-3.450109000	2.298672000
1	-7.126455000	1.972159000	4.293936000	1	5.514509000	1.029679000	4.728026000
1	-8.134308000	1.271509000	2.985158000	1	4.925127000	2.698100000	4.478577000
1	-7.761655000	0.304485000	4.443913000	1	4.234420000	1.353584000	3.513370000
1	-5.438359000	-2.772478000	-3.167012000	1	7.936562000	1.737119000	4.295057000
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1	-7.917523000	-2.109031000	-3.247576000	1	4.003435000	2.741573000	-3.807391000
1	-8.294725000	-3.210370000	-1.890372000	1	3.227861000	2.507190000	-2.205145000
1	-8.740516000	-1.479433000	-1.782476000	1	3.637606000	4.155035000	-2.776363000
1	-5.760947000	1.501491000	-5.270639000	1	6.475018000	3.423458000	-3.970778000
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1	-4.634436000	2.888063000	-5.417945000	1	7.459956000	3.637492000	-2.485751000
1	-3.847065000	-0.191550000	-5.010331000	1	6.620584000	-1.440366000	-5.005432000
1	-2.656841000	1.116129000	-5.250070000	1	7.620605000	-2.220760000	-3.735967000
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1	-2.549974000	4.423293000	2.665661000	1	4.140400000	-0.922495000	-4.577575000
1	-1.534078000	3.448375000	1.552869000	1	3.803033000	-2.635080000	-4.189045000
1	-1.647670000	5.224654000	1.354028000	1	3.378622000	-1.354761000	-3.010099000
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1	-5.295308000	5.236548000	0.160447000	1	5.055363000	-4.197804000	3.034185000
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6	-0.835742000	-3.783031000	0.531600000	1	8.495256000	-3.205521000	1.577011000
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6	-1.043549000	-5.024327000	1.158261000	6	1.271960000	0.524049000	0.401806000
1	0.079506000	-3.589120000	-0.045748000	6	1.293466000	-0.708756000	0.111041000
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6	-0.652403000	0.545574000	2.315469000	6	-2.152752000	1.078451000	-5.205983000
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1	-0.946502000	1.299824000	1.567164000	1	-2.022518000	1.317937000	-6.272697000
6	0.142481000	-1.345622000	4.226963000	8	-2.610429000	0.161215000	-1.128618000
1	1.148838000	-2.357098000	2.584878000	6	0.906904000	-2.063304000	-0.185687000
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1	-1.619340000	1.583905000	3.960669000	6	1.802376000	-3.156263000	-0.057593000
1	0.455713000	-2.095506000	4.970831000	6	-0.848904000	-3.599889000	-0.890560000
1	-0.923246000	-0.116275000	5.678995000	1	-1.133307000	-1.443474000	-0.726036000
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Supporting Information

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6	4.607973000	2.154139000	0.978490000	1	1.837642000	4.804597000	2.177106000
6	6.793396000	-0.026487000	-1.154344000	1	-0.528869000	5.425088000	1.604021000
1	6.693718000	0.368617000	-2.188048000	6	-5.722373000	-0.118122000	0.872716000
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6	7.084942000	2.486655000	-0.804751000	6	-5.837729000	-0.413576000	2.373844000
6	7.605111000	0.941122000	1.083083000	6	-8.101452000	-0.087492000	1.353556000
6	4.614188000	2.079711000	2.402749000	6	-7.164623000	0.349109000	-1.044771000
6	4.051174000	3.272085000	0.290479000	6	-7.319915000	-0.035904000	2.683826000
6	4.120307000	3.190308000	3.119301000	1	-7.349011000	1.000704000	3.082638000
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1	4.118566000	3.157751000	4.219774000	6	-8.835578000	-1.427169000	1.146535000
6	3.572726000	4.348397000	1.065946000	6	-7.311176000	-0.723861000	-1.971932000
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1	5.517057000	0.130800000	2.485486000	6	-7.725336000	0.934949000	-3.731459000
6	3.770268000	0.110895000	3.727449000	1	-7.722179000	-1.206242000	-4.048292000
6	6.018885000	1.125904000	4.330908000	6	-7.512699000	1.973496000	-2.815776000
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1	4.053614000	-0.829003000	4.246155000	1	-6.994003000	-2.267427000	-0.510725000
1	3.218444000	0.745534000	4.451861000	6	-5.686189000	-2.642200000	-2.171069000
1	3.070179000	-0.144974000	2.904700000	6	-8.178913000	-3.136145000	-2.086001000
1	6.351375000	0.178449000	4.803630000	1	-6.851116000	2.505588000	0.501242000
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1	5.431339000	4.808597000	-1.637827000	1	-8.241680000	-3.182453000	-3.193249000
6	5.943303000	-2.162162000	0.119292000	1	-5.167835000	4.217753000	-0.155095000
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Supporting Information

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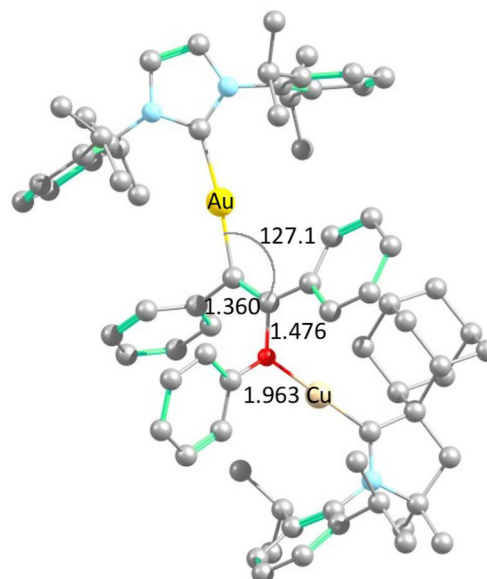
59-60 TS

E(scf)= -3444.48540835 a.u.

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6	-5.650551000	-2.071728000	-0.631734000
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6	-3.975629000	4.808006000	-0.185974000
6	-3.810038000	5.170716000	1.158296000
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6	-5.638095000	-3.006270000	0.437706000
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1	-5.230726000	-5.843669000	-1.471732000
1	-5.258766000	-4.159019000	-3.310916000
6	-5.536300000	-1.441474000	-3.142671000
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1	-9.293555000	-1.487157000	0.139482000

60 [Cu(L²)(PhO)(PhCCPh)(IPr)Au]⁺ min

E(scf)= -3444.50979404 a.u.

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1	-3.435124000	6.150944000	1.377553000
1	-4.351660000	4.619415000	3.122547000
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6	-5.081499000	-2.528341000	-2.113557000
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Supporting Information

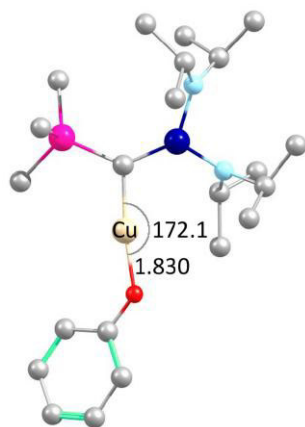
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Supporting Information

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1	6.275544000	0.918994000	2.163710000	6	4.241137000	-2.442180000	-2.447737000
6	4.976490000	-0.217757000	3.438363000	6	6.643595000	-2.523511000	-3.266856000
6	7.474579000	0.110023000	3.763902000	1	6.257590000	0.824400000	2.106239000
1	4.528355000	-2.573105000	-3.423166000	6	5.028718000	-0.345404000	3.416195000
1	4.735959000	-3.733986000	-2.071122000	6	7.555749000	-0.112715000	3.550989000
1	3.981522000	-2.138666000	-1.766282000	1	3.909005000	-2.295242000	-3.496393000
1	7.010038000	-2.521784000	-4.028120000	1	4.184142000	-3.528333000	-2.226287000
1	8.254244000	-2.304327000	-2.753720000	1	3.507092000	-1.928969000	-1.790595000
1	7.279579000	-3.802341000	-2.816094000	1	6.331177000	-2.279410000	-4.303256000
1	4.787749000	0.620958000	4.141188000	1	7.684055000	-2.163844000	-3.130931000
1	4.140803000	-0.248043000	2.705736000	1	6.661738000	-3.630344000	-3.186652000
1	4.945472000	-1.164181000	4.017102000	1	4.918710000	0.457981000	4.174195000
1	7.304632000	1.002508000	4.401342000	1	4.141023000	-0.309456000	2.748606000
1	7.525305000	-0.766852000	4.442216000	1	5.010614000	-1.321516000	3.944100000
1	8.467607000	0.216895000	3.281986000	1	7.469803000	0.744245000	4.250739000
6	4.563049000	2.210210000	-2.456467000	1	7.634127000	-1.029419000	4.171551000
6	3.058430000	1.856127000	-2.543079000	1	8.507809000	-0.005046000	2.992934000
1	5.151496000	1.451425000	-3.017037000	6	4.194213000	2.355380000	-2.362014000
6	4.769071000	3.603550000	-3.099898000	6	2.682246000	2.022212000	-2.380977000
6	4.158809000	3.294105000	-0.214605000	1	4.742401000	1.613018000	-2.982230000
6	2.658818000	2.950731000	-0.314784000	6	4.383472000	3.770490000	-2.961883000
1	4.462069000	3.322391000	0.856129000	6	3.921870000	3.356721000	-0.060179000
6	4.385901000	4.686702000	-0.855324000	6	2.414297000	3.032256000	-0.096465000
6	2.217918000	2.913711000	-1.793202000	1	4.281131000	3.340345000	0.993084000
1	2.756423000	1.810534000	-3.612434000	6	4.132013000	4.770574000	-0.659441000
1	2.869546000	0.845268000	-2.115893000	6	1.895122000	3.058255000	-1.548663000
1	1.141723000	2.640897000	-1.855578000	1	2.325230000	2.019298000	-3.434101000
6	2.445395000	4.304209000	-2.427253000	1	2.500035000	0.996478000	-1.986021000
1	2.070494000	3.707959000	0.246777000	1	0.814272000	2.800756000	-1.561905000
1	2.445814000	1.972766000	0.177643000	6	2.108123000	4.469669000	-2.140534000
1	3.795629000	5.443467000	-0.293678000	1	1.862999000	3.767282000	0.528225000
1	5.448981000	4.998710000	-0.770803000	1	2.209790000	2.039221000	0.369444000
6	3.945047000	4.666002000	-2.338219000	1	3.579829000	5.509461000	-0.038965000
1	1.833655000	5.069781000	-1.900601000	1	5.201313000	5.069806000	-0.616990000
1	2.114568000	4.303512000	-3.489478000	6	3.615060000	4.811061000	-2.116683000
1	5.842716000	3.887445000	-3.121154000	1	1.534734000	5.220149000	-1.553378000

Supporting Information

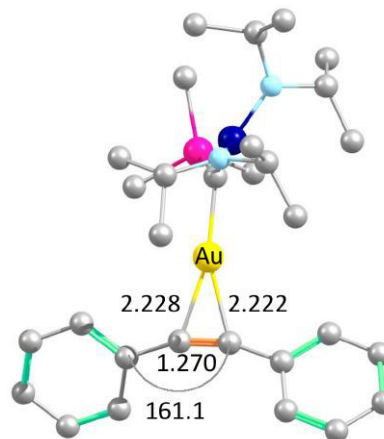
1	4.444003000	3.556856000	-4.162373000
1	4.118968000	5.665759000	-2.791940000
1	9.228176000	1.982592000	0.043233000
1	8.075520000	1.660835000	1.370480000
1	8.912345000	0.294580000	0.548044000
1	7.201618000	0.755525000	-2.821032000
1	8.748238000	1.471794000	-2.278040000
1	8.392928000	-0.239220000	-1.908268000

**61** [Cu(PSC)(OPh)]

E(scf)= -1875.77922671 a.u.

6	-0.206585000	0.939467000	0.129111000
14	-0.260029000	2.810791000	0.413018000
29	1.478312000	0.219323000	-0.188542000
6	4.301288000	-0.387200000	-0.400123000
6	5.312997000	-1.153616000	-1.050823000
6	4.730489000	0.620843000	0.511919000
6	6.672177000	-0.918939000	-0.799459000
1	4.992814000	-1.935106000	-1.758454000
6	6.093815000	0.846733000	0.755958000
1	3.960187000	1.218639000	1.028926000
6	7.079981000	0.081862000	0.104385000
1	7.429709000	-1.528724000	-1.320588000
1	6.390732000	1.634467000	1.469074000
1	8.149101000	0.262390000	0.297812000
8	3.020549000	-0.648536000	-0.656492000
15	-1.403405000	-0.200134000	-0.034330000
6	-0.371370000	3.735819000	-1.245470000
1	0.421014000	3.386925000	-1.940239000
1	-1.350145000	3.605112000	-1.750930000
1	-0.221416000	4.824521000	-1.080315000
6	1.370440000	3.303817000	1.249201000
1	1.524706000	2.742080000	2.194178000
1	2.238666000	3.097188000	0.588956000
1	1.371847000	4.389002000	1.490603000
6	-1.669086000	3.358565000	1.569931000
1	-2.676598000	3.103443000	1.186223000
1	-1.557169000	2.888311000	2.569754000
1	-1.629512000	4.459894000	1.714022000
7	-1.122704000	-1.824935000	0.352654000
7	-3.071348000	0.024450000	-0.287032000
6	-0.445121000	-2.148903000	1.653746000
1	-0.338899000	-1.169764000	2.167690000
6	0.966001000	-2.736017000	1.494494000
1	1.622148000	-2.081375000	0.881816000
1	0.951225000	-3.746721000	1.034472000
1	1.435167000	-2.843463000	2.494245000

1	1.722590000	4.513436000	-3.183004000
1	5.457953000	4.042895000	-3.032153000
1	4.000155000	3.767120000	-4.005656000
1	3.778331000	5.825590000	-2.540133000
1	8.997498000	1.977827000	-0.163210000
1	7.927300000	1.646098000	1.227206000
1	8.680734000	0.284365000	0.318746000
1	6.782331000	0.885483000	-2.928173000
1	8.370159000	1.555255000	-2.451333000
1	8.003972000	-0.161609000	-2.120564000

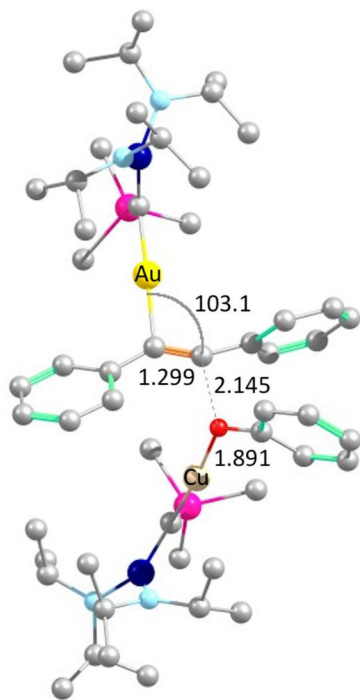
**62** [Au(PSC)(PhCCPh)]⁺

E(scf)= -2046.42745431 a.u.

79	0.934155000	-0.190396000	-0.271111000
6	3.123195000	-0.049616000	0.120567000
6	2.753467000	1.084618000	-0.314919000
6	2.740459000	2.490315000	-0.633266000
6	1.809519000	3.044170000	-1.549836000
6	3.710381000	3.337082000	-0.030040000
6	1.850615000	4.411543000	-1.855430000
1	1.068293000	2.384285000	-2.026550000
6	3.743701000	4.701350000	-0.347776000
1	4.431328000	2.913093000	0.685221000
6	2.815795000	5.242582000	-1.257491000
1	1.130089000	4.832467000	-2.573854000
1	4.500744000	5.349598000	0.120344000
1	2.848199000	6.315325000	-1.503742000
6	3.963175000	-1.160665000	0.490074000
6	3.461264000	-2.290756000	1.185029000
6	5.344533000	-1.106695000	0.155869000
6	4.320896000	-3.340053000	1.537841000
1	2.392520000	-2.331688000	1.445083000
6	6.194077000	-2.159705000	0.518770000
1	5.737714000	-0.236727000	-0.391410000
6	5.687065000	-3.277570000	1.207929000
1	3.923215000	-4.213603000	2.077231000
1	7.262419000	-2.110146000	0.256822000
1	6.359847000	-4.103055000	1.487759000
6	-0.963472000	-0.865691000	-0.621846000
14	-1.059396000	-2.252088000	-1.938357000
15	-2.201301000	-0.222558000	0.282568000
6	-2.692289000	-3.217096000	-1.893269000
1	-2.678009000	-3.990116000	-2.691320000
1	-2.802768000	-3.751012000	-0.925858000
1	-3.592373000	-2.592508000	-2.051318000
6	0.327984000	-3.482817000	-1.536407000
1	0.311539000	-4.317453000	-2.269842000

Supporting Information

6	-1.34325000	-3.05186300	2.51837400	1	1.32960200	-3.00681700	-1.58621800
1	-0.86909900	-3.22915800	3.50608000	1	0.20561700	-3.92139200	-0.52416100
1	-1.50049700	-4.04582700	2.04749400	6	-0.72293600	-1.50445900	-3.64794200
1	-2.33757500	-2.59260600	2.69533400	1	-0.66395900	-2.31408100	-4.40629900
6	-1.19183700	-2.91098700	-0.67412400	1	-1.50540400	-0.79136100	-3.97855900
1	-0.82833400	-3.81378900	-0.13939700	1	0.24857900	-0.96731900	-3.65373400
6	-0.23956700	-2.65762600	-1.85303700	7	-3.74727100	0.05752200	-0.30388200
1	0.79790200	-2.47412800	-1.50922300	7	-2.00665700	0.42297100	1.82035700
1	-0.55578100	-1.76728700	-2.43868200	1	-4.90532000	1.48041000	-1.26844000
1	-0.23317200	-3.52645400	-2.54390400	6	-4.01141500	0.87654000	-1.54437100
6	-2.62378200	-3.21893500	-1.13982900	6	-4.38297200	0.01965100	-2.76215600
1	-2.62066500	-4.09696200	-1.81847700	1	-5.18865700	-0.70764800	-2.53633700
1	-3.06373500	-2.36687400	-1.69649700	1	-3.50463600	-0.53961200	-3.13943000
1	-3.28573400	-3.45243500	-0.28172400	1	-4.75157000	0.66985000	-3.58147400
6	-4.00569100	-0.51583200	0.75529000	6	-2.89511600	1.87080400	-1.87380300
1	-3.50269500	-1.43311900	1.13234800	1	-3.22916000	2.52751200	-2.70233700
6	-5.36497400	-0.95896200	0.19551200	1	-1.96511900	1.36335300	-2.20067900
1	-5.25781900	-1.67686000	-0.64206000	1	-2.65408200	2.52319400	-1.01007200
1	-5.98763200	-0.10705600	-0.14741200	1	-5.64372900	-0.75693200	-0.49934300
1	-5.93107400	-1.47011600	1.00888000	6	-5.00123000	-0.45362900	0.35704000
6	-4.16377900	0.43832900	1.95266400	6	-5.75715800	0.62698400	1.14723300
1	-4.73961400	-0.05505400	2.76387700	1	-5.89953400	1.55818700	0.56235900
1	-4.69818800	1.37030600	1.67638400	1	-5.23439800	0.88298600	2.09030500
1	-3.17492700	0.72432500	2.36509800	1	-6.76686100	0.25520500	1.41614100
6	-3.62281500	0.69589400	-1.50173300	6	-4.76542100	-1.70646600	1.20274400
1	-4.46916600	0.05341500	-1.83133200	1	-5.74055500	-2.12779100	1.51970900
6	-2.62964000	0.72894100	-2.67076400	1	-4.19528500	-1.47537600	2.12497500
1	-2.26561000	-0.28640500	-2.92863700	1	-4.22972000	-2.49136600	0.63224700
1	-1.74643400	1.36374100	-2.45886900	1	-3.30219300	1.98394300	1.35304300
1	-3.13855800	1.14114600	-3.56606600	6	-2.45330500	1.84239300	2.05474900
6	-4.19343300	2.09713800	-1.22013900	6	-1.37358000	2.87182000	1.67014600
1	-4.68073400	2.49960600	-2.13279400	1	-0.95373700	2.66062900	0.66522700
1	-3.39225500	2.80234500	-0.92124200	1	-0.53057600	2.89190300	2.38784100
1	-4.95534000	2.08350500	-0.41593100	1	-1.81776000	3.88856400	1.64741500
				6	-2.99897900	2.07466100	3.46954500
				1	-3.46329700	3.08050100	3.51306700
				1	-2.20523300	2.05151100	4.24336500
				1	-3.77779700	1.33512700	3.74618400
				1	-2.00215400	-0.18974900	3.80375000
				6	-1.31982700	-0.31999000	2.93519400
				6	0.04773200	0.26991200	3.31910600
				1	-0.01806900	1.32384800	3.64906700
				1	0.75784600	0.21639500	2.46588900
				1	0.47568200	-0.31176800	4.16097100
				6	-1.20752700	-1.83173300	2.69677600
				1	-0.88527000	-2.30965700	3.64369700
				1	-0.46241400	-2.08197900	1.91576100
				1	-2.17506200	-2.28824200	2.40803400



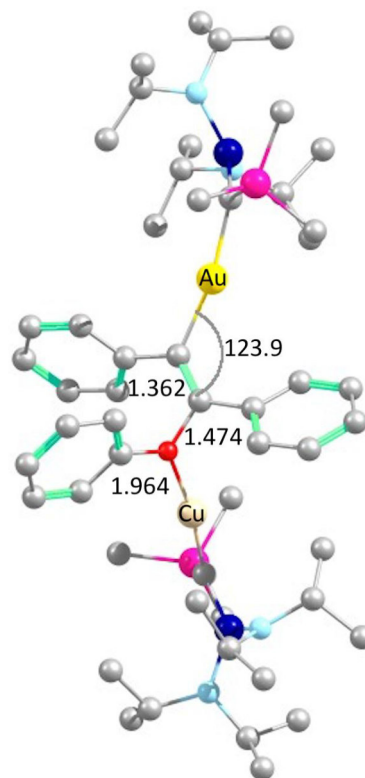
61+62-63 TS

E(scf)= -3922.21037522 a.u.

Supporting Information

 $\nu_{\min} = -135.3696 \text{ cm}^{-1}$

79	-2.351240000	-0.451431000	0.040099000
6	-0.176821000	1.202800000	-0.139408000
6	-0.406993000	0.190613000	0.641825000
29	3.098491000	0.872833000	-0.381640000
6	1.858610000	3.379853000	0.215732000
6	1.299710000	4.176660000	1.250071000
6	2.514260000	4.034252000	-0.859698000
6	1.416933000	5.575029000	1.216404000
1	0.782059000	3.675423000	2.083262000
6	2.628109000	5.433231000	-0.883581000
1	2.934954000	3.418773000	-1.672241000
6	2.082066000	6.213326000	0.152672000
1	0.986517000	6.174924000	2.034769000
1	3.146538000	5.920443000	-1.725308000
1	2.172865000	7.310329000	0.131028000
8	1.757430000	2.031754000	0.278348000
6	0.249975000	-0.483234000	1.774807000
6	1.007919000	0.245802000	2.726304000
6	0.081267000	-1.877094000	1.972432000
6	1.562200000	-0.401104000	3.841953000
1	1.154623000	1.323338000	2.572641000
6	0.658808000	-2.523649000	3.076536000
1	-0.518925000	-2.446565000	1.245165000
6	1.393955000	-1.786782000	4.022682000
1	2.129507000	0.186182000	4.581687000
1	0.518268000	-3.608444000	3.208115000
1	1.826449000	-2.288742000	4.902746000
6	-0.524043000	2.096014000	-1.212738000
6	-1.127968000	3.353135000	-0.942300000
6	-0.251578000	1.740627000	-2.561871000
6	-1.458617000	4.220249000	-1.994639000
1	-1.341534000	3.634408000	0.098552000
6	-0.591918000	2.609889000	-3.606193000
1	0.213164000	0.766017000	-2.772893000
6	-1.193428000	3.852623000	-3.325501000
1	-1.924378000	5.192998000	-1.772633000
1	-0.386069000	2.319268000	-4.648321000
1	-1.454283000	4.536141000	-4.148874000
14	3.869825000	-1.022614000	-2.756898000
6	4.316399000	-0.394255000	-1.021535000
15	5.660036000	-0.772343000	-0.134249000
6	5.275254000	-1.907313000	-3.683099000
6	3.433871000	0.502863000	-3.804176000
6	2.336653000	-2.138390000	-2.629293000
7	6.433984000	-2.270997000	-0.108464000
7	6.362097000	0.257237000	1.005820000
1	4.889599000	-2.308817000	-4.644877000
1	6.086270000	-1.190349000	-3.931574000
1	5.720057000	-2.750594000	-3.121092000
1	3.149546000	0.196671000	-4.834237000
1	2.591503000	1.079687000	-3.369210000
1	4.303954000	1.188139000	-3.885380000
1	1.521039000	-1.622277000	-2.080269000
1	1.961810000	-2.398507000	-3.642291000
1	2.545565000	-3.087617000	-2.093795000
6	5.708716000	-3.531918000	0.277515000
6	7.877760000	-2.483444000	-0.463636000
6	6.626613000	-0.276398000	2.383035000
6	6.579992000	1.720458000	0.741588000
1	6.454442000	-4.095846000	0.882792000
6	5.330439000	-4.404947000	-0.928383000
6	4.496460000	-3.290207000	1.182453000
1	6.190108000	-4.588948000	-1.604274000
1	4.518623000	-3.933360000	-1.516602000

**63** [Cu(PSC)(PhO)(PhCCPh)(PSC)Au]⁺ min

E(scf) = -3922.2237487 a.u.

79	-2.650747000	-0.436343000	-0.064345000
6	0.349666000	-0.671608000	-0.540750000
6	-0.760759000	0.095918000	-0.721686000
29	3.122754000	0.329533000	-0.200763000
6	1.650965000	-0.438308000	-2.648643000
6	0.837559000	-1.353487000	-3.336617000
6	2.585693000	0.358204000	-3.330438000
6	0.980520000	-1.473196000	-4.730072000
1	0.096762000	-1.955319000	-2.790245000
6	2.718440000	0.223681000	-4.722771000
1	3.189598000	1.088624000	-2.766911000
6	1.918634000	-0.692514000	-5.428131000
1	0.346401000	-2.191368000	-5.273277000
1	3.445854000	0.852840000	-5.259264000
1	2.020470000	-0.792034000	-6.519501000
8	1.593629000	-0.318829000	-1.248086000
6	-0.704872000	1.350378000	-1.523752000
6	0.094604000	2.447362000	-1.115140000
6	-1.496767000	1.509554000	-2.689194000
6	0.104014000	3.650621000	-1.841188000
1	0.695588000	2.357698000	-0.195871000
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Supporting Information

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This thesis presents the computational-mechanistic study of the hydrophenoxylation of diphenylacetylene assisted by [Cu(NHC)] and [Au(NHC)] catalysts. In such process, the first reaction step is the generation of the nucleophile-electrophile couple: PhO-[M(NHC)] and PhCCPh-[M(NHC)]. This couple is responsible of the reaction rate, which is defined by the nucleophilic attack in the rate determining step (rds) such as 2016 Poater's proposal. Thus, we performed the study of the metal effect in the rds exchanging copper-, silver- and gold-IPr catalysts in the pre-activated species. Also, the ligand effect in the Cu/Au catalysis was done using NHC ligands such as IMe, IMes, SIMes and IPR*. These studies allowed us to give a clear explanation in the preference for hetero-dual-metal catalysis instead of homo-dual and assessing steric hindrance effects in the rds. Furthermore, in order to improve and expand the dual catalysis field, we introduced CAAC and PSC ligands in our study.

En esta tesis se presenta un estudio mecanístico-computacional de la hidrofenoxilación del difenilacetileno asistida por catalizadores de [Cu(NHC)] y [Au(NHC)]. En tal proceso, la primera etapa de reacción es la generación de la pareja nucleófilo-electrófilo: PhO-[M(NHC)] y PhCCPh-[M(NHC)]. Estas especies son responsables de la velocidad de la reacción, lo cual convierte al ataque nucleofílico en la etapa determinante de la reacción tal como propuso Poater en 2016. Por esto se desarrolló el estudio del efecto del metal en la etapa determinante de la reacción intercambiando los catalizadores de cobre, plata y oro-IPr en las especies pre activadas. También se analizó el efecto del ligando en la catálisis de Cu/Au usando ligandos NHC como IMe, IMes, SIMes y IPR*. Estos estudios nos permitieron dar una explicación clara acerca de la preferencia por la catálisis hetero-dual metálica frente a la homo-dual y el efecto de impedimento estérico de los ligandos en la etapa determinante de la reacción. Además, con el objetivo de mejorar y expandir el campo de la catálisis dual, introducimos los ligandos CAAC y PSC.

En aquesta tesi es presenten els estudis mecanístic-computacionals de l'hidrofenoxilació del difenilacetilè assistida pels catalitzadors de [Cu(NHC)] i [Au(NHC)]. En aquest procés, la primera etapa de reacció és la generació de la parella nucleòfil-electrófil: PhO-[M(NHC)] i PhCCPh-[M(NHC)]. Aquestes espècies són responsables de la velocitat de la reacció, la qual hi torna a l'atac nucleofílic en l'etapa determinant de la reacció tal com va proposar Poater al 2016. Per això, es va desenvolupar l'estudi de l'efecte del metall en l'etapa determinant de la reacció intercanviant els catalitzadors de coure, plata i or-IPr a les espècies pre activades. També es va realitzar l'efecte del lligant a la catàlisi de Cu / Au fent servir lligands NHC com IMe, IMes, SIMes i IPR*. Aquests estudis ens van permetre donar una explicació clara sobre la preferència per la catàlisi hetero-dual metàl·lica de cara a la homo-dual i l'efecte d'impediment estèric dels lligands en l'etapa determinant de la reacció. A més, amb l'objectiu de millorar i expandir el camp de la catàlisi dual, en vam introduir els lligands CAAC i PSC.