

Synthesis Of polyaromatic heterocycles pyrrolo [1,2-a] indoles by Gold(I)-Catalyzed tandem Cyclization/C-H Activaton/Cyclization.

Narendra Sukalal Mali ¹ and Dr. César Rogelio Solorio Alvarado *

¹ Departamento de Química, Universidad de Guanajuato, Noria Alta S/N, Col. Noria Alta, C.P. 36050, Guanajuato, Gto., México; ns.mali@ugto.mx

* Correspondence: csolorio@ugto.mx (C.R.S.A.); Tel.: +52-473-73-20006 ext. 1418 (C.R.S.-A.); cesarrogelio@hotmail.com

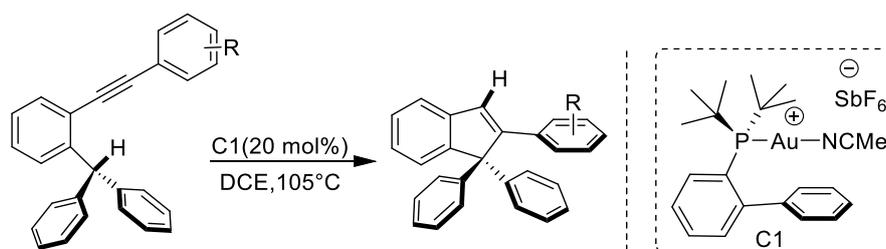
† Presented at the 24th International Electronic Conference on Synthetic Organic Chemistry.

Abstract: The initial results on a novel procedure for the synthesis of pyrrolo[1,2-*a*]indoles via gold(I)-catalyzed tandem cyclization/C-H activation/cyclization is described. The procedure allowed the access to a highly functionalized pyrrolo[1,2-*a*]indoles in a one-pot process starting from anilindiynes. The mechanism of this reaction by using gold(I) catalysis, interestingly proceeded via 5-*endo*-dig cyclization at only one of the alkyne of the diyne fragment, leading to the formation of 2-alkynyndole derivative. We are purposing a Csp³-H bond activation and generating gold(I)-carbene species with [1,5]-H migration and cyclization following by [1,2]-H shift. The result we achieved 1-benzhydryl-2-(phenylethynyl)-1-H-indole moiety first cyclization was confirmed by using ¹H, ¹³C NMR spectroscopy and X-ray. Interestingly we have developed intramolecular cyclization of indole moiety with high yield, short reaction time and room temperature.

Keywords: C-H activation; Cyclization; gold(I) catalysed

1. Introduction

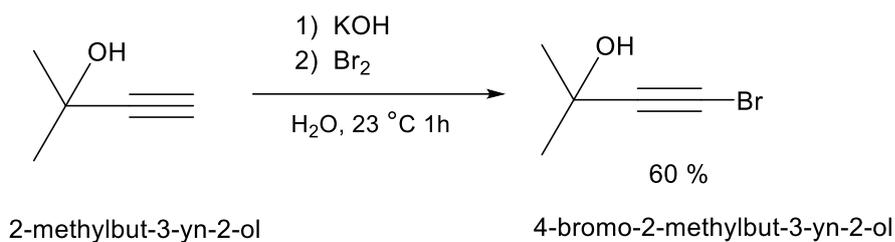
The carbon-hydrogen bond is unfunctional group its unique position in organic chemistry is well illustrated by the standard representation of organic molecule. In 2018, our group synthesized of indenes by direct Csp³-H bond activation by using gold(I) high yielding procedure and new activation modes for the direct gold(I)-catalyzed Csp³-H bond activation alkynyl triphenylmethanes to get 1,1,2-triphenyl indenes derivatives (Scheme 1).



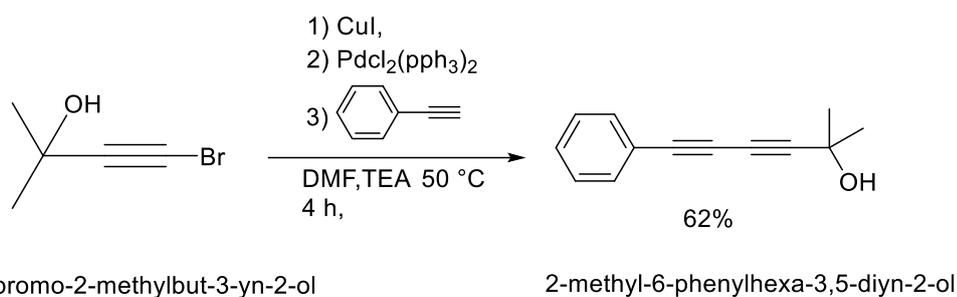
Scheme 1. gold(I)-catalyzed synthesis of indenes by direct Csp³-H bond activation.

2. Experimental Section (Preparation of starting material)

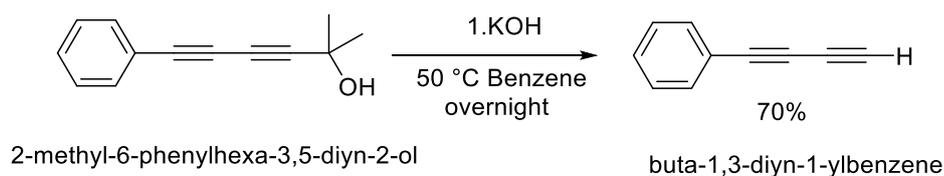
The synthesis of starting material alkynes was developed. Initially we started with addition of Br₂ to 2 methylbut-3-yn-2-ol leading to the formation of the corresponding 4-bromo-2-methylbut-3-2-ol.



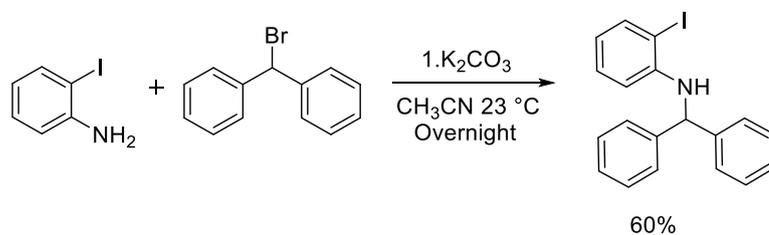
In the next step we were used 4-bromo-2-methylbut-3-2-ol with phenylacetylene gave rise to 2-ethyl-6-phenylhexa-3,5-diyn-2-ol.



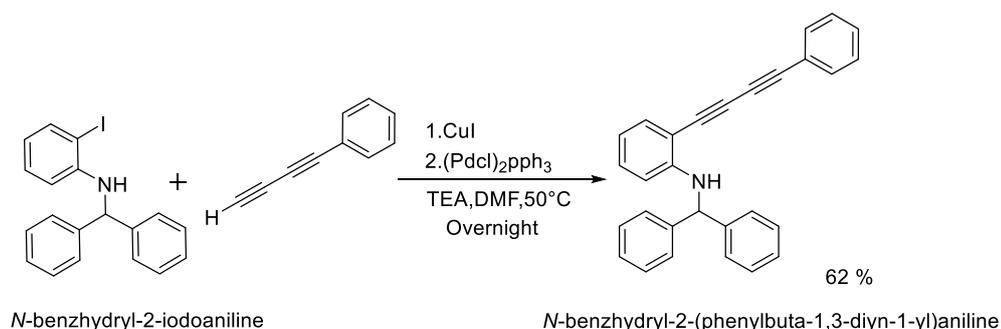
Among we used 2-methyl- 6-phenylhexa-3,5-diyn-2-ol reacted with KOH foe evolving acetone and we obtained buta-1-3-diyn-1-ylbenzeze.



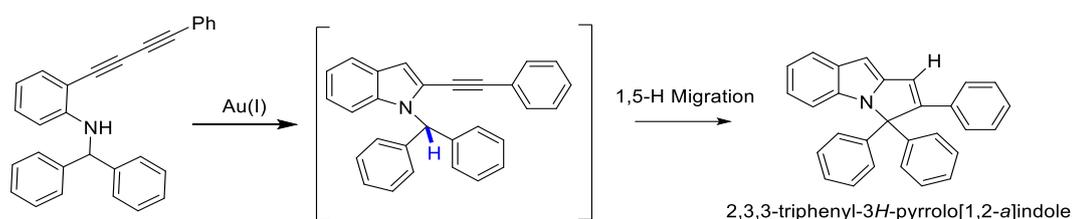
Further we treated 2-iodoaniline with benzhydryl bromide we get *N*-benzhydryl 2-iodoanilne.



Then move to final step for formation of starting material by taking buta-1-3 -diyn-1-ylbenzeze with *N*-benzhydryl 2-iodoanilne and we get *N*-benzhydryl-2-(phenylbuta-1,3-diyn-1-yl).



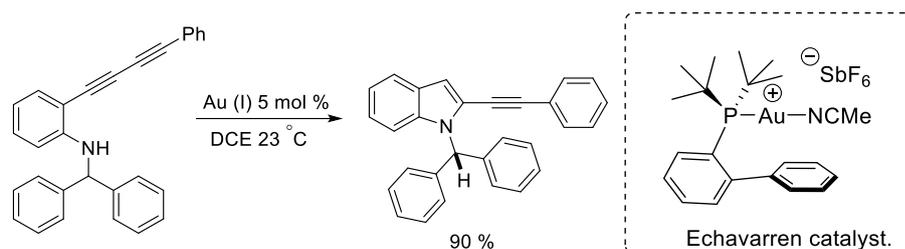
As assuming we have been trying to be developing of polyaromatic heterocyclic pyrrolo[1,2-a] indoles by using Au(I)- catalyst.



Scheme 2. Synthesis Of polyaromatic heterocycles pyrrolo [1,2-*a*] indoles by Au(I)-Catalyzed tandem Cyclization/C-H Activator/Cyclization.

3. Results and Discussion

In the synthesis of heterocyclic compound Initial tandem gold(I)-catalyzed screening was carried out by using highly reactive cationic gold(I)-complex (Echavarren catalyst). Initially we use between 5-20 mol% then we decided to 5 mol% gold(I) catalyst in DCM at room temperature and we have achieved 90 % yield.



Scheme 3. Synthesis of polyaromatic heterocycles pyrrolo[1,2-*a*] indoles by Au(I)-catalyzed Tandem cyclization/C-H activation/cyclization.

Crystallographic data: The cyclization of indole moiety we have confirmed by with the help of X- ray crystallographic technique in (figure 2).

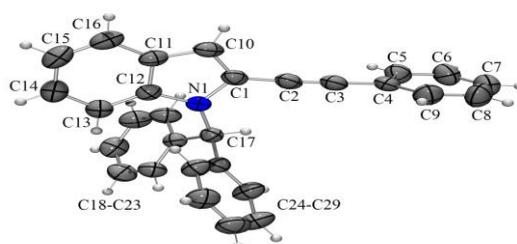


Figure 2. crystallographic data of *N*-benzhydryl-2-(phenylbuta-1,3-diyne-1-yl)aniline .

4. Conclusions

The synthesis of polyaromatic heterocycles pyrrole [1,2- a] indoles by Au(I)-catalysed tandem cyclization/C-H activation/cyclization. Further had been developed 5-endo-diagonal cyclisation by using gold(I) catalyst. In future we trying to change for one more cyclization by changing intermediate conditions.

Author Contributions: All authors contributed equally to this work.

Acknowledgments: Thanks to CONACyT for financial support (PhD fellowship). We acknowledge the facilities of the DCNyE, the Chemistry Department,

Conflicts of Interest: The authors declare no conflict of interest. The funders had no role in the design of the study; in the collection, analyses, or interpretation of data; in the writing of the manuscript, or in the decision to publish the results.

References

1. P.D.Nahide, C.R.S.Alvarado, *org.biomol.chem* ,2018,00,1-3.
2. Fetisov, Evgenii O.; Gloriov, Igor P.; Nechaev, Mikhail S.; Kahlal, Samia; Saillard, Jean-Yves; Oprunenko, Yuri F. From *Journal of Organometallic Chemistry* (2017), 830, 212-218.
3. Minaeva, Valentina A.; Baryshnikov, Gleb V.; Minaev, Boris F.; Karaush, Natalia N.; Xiong, Xiao-Dong; Li, Ming-De; Phillips, David Lee; Wong, Henry N. C. From *Spectrochimica Acta, Part A: Molecular and Biomolecular Spectroscopy* (2015), 151, 247-261
4. Nayak, Maloy; Singh, Dileep Kumar; Kim, Ikyon. From *Tetrahedron* (2017), 73(14), 1831-1840.

Publisher's Note: MDPI stays neutral with regard to jurisdictional claims in published maps and institutional affiliations.



© 2020 by the authors. Submitted for possible open access publication under the terms and conditions of the Creative Commons Attribution (CC BY) license (<http://creativecommons.org/licenses/by/4.0/>).