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To be cited as: Adv. Synth. Catal. 10.1002/adsc.201900605

Link to VoR: http://dx.doi.org/10.1002/adsc.201900605

DOI: 10.1002/adsc.201((will be filled in by the editorial staff))

# **Gold(I)-Catalyzed Synthesis of Six-Membered P,O-Heterocycles** *via* Hydration/Intramolecular Cyclization Cascade Reaction

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Received: ((will be filled in by the editorial staff))

Supporting information for this article is available on the WWW under http://dx.doi.org/10.1002/adsc.201#######.((Please delete if not appropriate))

**Abstract.** Herein, we report the synthesis of sixmembered P,O-heterocycles from dialkynylphosphine oxides. By using gold(I) complexes, the chemoselectivity of the reaction was switched from literature-reported double hydration to a hydration/intramolecular cyclization cascade. Control experiments indicated that the first alkyne hydration product is an intermediate of the reaction. In addition, a density functional theory (DFT) calculation allowed to rationalize the observed chemoselectivity.

**Keywords:** Gold-catalysis; P,O-Heterocycles; Chemoselectivity switch; Cyclization; DFT calculation

Homogeneous gold catalysis has become one of the most important tools in organic synthetic toolbox. Owing to their advantages in activation of carboncarbon  $\pi$  bonds, gold catalysts have shown their power the transformation of alkyne-containing in substrates.<sup>[1]</sup> For example, fruitful achievements have been made in the gold-catalyzed rearrangement of propargyl esters,<sup>[2]</sup> cycloisomerizations of enynes,<sup>[3]</sup> cyclizations of diynes,<sup>[4]</sup> oxidation of alkynes by Noxides<sup>[5]</sup> and transformations of propargyl alcohols and propargyl amines.<sup>[6]</sup> Gold complexes have also been used to promote the synthesis of heterocyclic phosphorus compounds, which are useful in organic synthesis, medicinal chemistry, and material science. In 2013, Lee reported the gold(I)-catalyzed sequential alkyne activation for the preparation of 4,6disubstituted phosphorus 2- pyrones.<sup>[7]</sup> At the same year, the author reported the synthesis of phosphacoumarins gold(I)-catalyzed via a hydroarylation of aryl alkynylphosphonates.<sup>[8]</sup> Very recently, Virieux and Pirat developed a cascade reaction to bridgehead methanophos-phocines by gold(I)-catalyzed intramolecular double hydroarylation.<sup>[9]</sup> In 2018, Zi reported a novel chiral gold(I)-catalyzed desymmetrization of prochiral phenols with P- stereogenic centers, affording P-

chiral cyclic phosphine oxides in good yields with high enantioselectivities.<sup>[10]</sup>

In contrast to other transition-metal catalysts, gold complexes show specific catalytic activities. For example, in our recent research on the [4 + 1]cycloaddition of propargyl alcohols and  $\alpha$ -diazoesters, it was found that gold(I) catalyst promoted the reaction *via* an alternative pathway to Pd(II) complexes.<sup>[11]</sup> In 2013, Gao and Xu reported the Pd(II)-catalyzed hydration alkynylphosphonates of to ketophosphonates. When dialkynylphosphine oxides were subjected to the standard conditions, double hydration products 2 were obtained (Scheme 1a).<sup>[17]</sup> Interestingly, in our recent investigation, we found that when gold(I) complexes were added instead of Pd(II) the chemoselectivity of the reaction was switched from double hydration to a hydration/intramolecular cyclization cascade. To continuously explore the specific catalytic activity of gold complexes, herein we want to report gold(I)-catalyzed а hydration/cyclization cascade reaction for the synthesis of six-membered P,O-heterocycles 3 (Scheme 1b).



Scheme 1. Literature reports and our exploration.

In our initial study, dialkynylphosphine oxide 1a was treated with AuCl<sub>3</sub> in the presence of 1 equivalent of water in DCE (1,2-dichloroethane) at 80 °C for 36 h. To our delight, a six-membered P-O heterocycle 3a

	O,	Me H <sub>2</sub> O		ζ, Me .P.	o ™e ∵P	
	Ph	P conditions Ph	Ph Ph Ph Ph	• +	Ph O Ph	
		1a	2a	3a	4a	
Entry	Catalyst	Solvent/ Time(h)	Conversion (1a %) <sup>[b]</sup>	<b>3a:2a</b> <sup>[c]</sup>	Yield ( <b>3a</b> %) <sup>[d]</sup>	Yield (4a %) <sup>[d]</sup>
1	AuCl <sub>3</sub>	DCE/36h	37	7:1	21	-
2	Ph <sub>3</sub> PAuCl	DCE/36h	-	-	-	-
3	AgNTf <sub>2</sub>	DCE/36h	15	-	Trace	10
4	$AuCl_3/3AgNTf_2$	DCE/36h	59	6:1	45	-
5	Ph <sub>3</sub> PAuNTf <sub>2</sub>	DCE / 36h	75	>20:1	65	-
6	$JohnPhosAuNTf_2\\$	DCE / 36h	92	4:1	73	-
7	SphosAuNTf <sub>2</sub>	DCE / 36h	91	>20:1	88(87)	-
8	IPrAuNTf <sub>2</sub>	DCE / 12h	100	>20:1	96(94)	-
9	BinapAu <sub>2</sub> (NTf <sub>2</sub> ) <sub>2</sub>	DCE / 36h	38	8:1	25	_ (
10	IPrAuSbF <sub>6</sub>	DCE / 18h	100	13:1	90(84)	-
11	IPrAuPF <sub>6</sub>	DCE / 18h	100	>20:1	97(96)	-
12	IPrAuOTf	DCE / 30h	100	>20:1	96(94)	-
13 <sup>[e]</sup>	IPrAuPF <sub>6</sub>	DCE / 36h	73	>20:1	69	-
$14^{[f]}$	IPrAuPF <sub>6</sub>	DCE / 36h	100	>20:1	97(96)	-
15 <sup>[g]</sup>	IPrAuPF <sub>6</sub>	DCE / 16h	100	>20:1	97(96)	-
16 <sup>[h]</sup>	IPrAuPF <sub>6</sub>	DCE / 13h	100	>20:1	95(95)	-
17 <sup>[g]</sup>	IPrAuPF <sub>6</sub>	CH <sub>3</sub> CN/ 24h	100	>20:1	96(94)	-
18 <sup>[g]</sup>	IPrAuPF <sub>6</sub>	THF/ 36h	88	11:1	79	-
19 <sup>[g]</sup>	IPrAuPF <sub>6</sub>	Dioxane/ 36h	78	9:1	69	-
20 <sup>[g]</sup>	PdCl <sub>2</sub>	DCE / 36h	70	1:4	10	20
21 <sup>[g]</sup>	PdCl <sub>2</sub>	Dioxane / 36h	88	1:10	5	15
22	<i>p</i> -TSOH	DCE / 12h	0	-	-	_
23	p-TSOH	MeOH / 12h	0	-	-	-

#### Table 1. Optimization of the Reaction Conditions.<sup>[a]</sup>

<sup>a)</sup> General reaction conditions: The reaction was conducted in a sealed tube under an argon atmosphere at 80 °C with 0.3 mmol of **1a**, 0.3 mmol of H<sub>2</sub>O and 0.015 mmol of catalyst in 3 mL of solvent. <sup>b)</sup> The conversion of **1a** was determined by <sup>1</sup>H NMR analysis. <sup>c)</sup> The ratio of **3a:2a** was determined by <sup>1</sup>H NMR analysis. <sup>d)</sup> Yield determined by <sup>1</sup>H NMR analysis; the number in parentheses represents the yields of isolated products. <sup>e)</sup> 0.009 mmol of IPrAuPF<sub>6</sub> was added. <sup>f)</sup> The reaction was conducted at 60 °C. <sup>g)</sup> 0.6 mmol of H<sub>2</sub>O was added. <sup>h)</sup> 1.5 mmol of H<sub>2</sub>O was added.

was obtained as a main product over double hydration product **2a** (Table 1, entry 1). Encouraged by this result, we further optimized the reaction conditions for the formation of **3a**. Unfortunately, when Ph<sub>3</sub>PAuCl was used as a catalyst, no conversion of **1a** was observed (Table 1, entry 2). AgNTf<sub>2</sub> (NTf<sub>2</sub> = bis(trifluoromethanesulfonyl)imide) was also used to promote the reaction, which resulted in the formation of a hydration product **4a** in low yield (entry 3). Addition of AgNTf<sub>2</sub> in combination with AuCl<sub>3</sub> provided an increase in reaction efficiency, affording **3a** in 45% yield (entry 4). Fortunately, when treating **1a** and water with  $Ph_3PAuNTf_2$  for 36 h, 75% conversion of **1a** was achieved, affording **3a** in 65% yield with the ratio of **3a** to **2a** over 20:1 (entry 5). In further optimization on gold catalysts (entries 6-7), it was found that when IPrAuNTf<sub>2</sub> was employed, 100% conversion of **1a** was achieved. In addition, the reaction delivered **3a** in 94% isolated yield with **3a:2a** over 20:1 ratio (entry 8). The counter anion of the cationic gold(I) complexes was also investigated (entries 10-12), among which -PF<sub>6</sub> and -OTf (OTf = trifluoromethanesulfonate) gave comparative result (96% vs 94%). Reducing the catalyst loading to 3 mol % resulted in incomplete conversion of 1a (entry 13). A longer time was needed when the reaction temperature was decreased to 60 °C (entry 14). It was notable that, when 2 equivalents and 5 equivalents of water were added respectively, the yields of **3a** were not affected (entry 15-16). Polar solvents, such as MeCN (acetonitrile), THF (tetrahydrofuran) and dioxane (entries 17-19) were screened, among which THF and dioxane was proved not to be suitable for the formation of **3a**. The formation of double hydration product 2a could be promoted by the water-miscible solvents, which admit more equivalents of water as well as facilitate the proton transfer of hydration.<sup>[13]</sup> PdCl<sub>2</sub> was also examined in both DCE and dioxane. As a result, the double hydration product 2a was obtained as main product in both DCE and dioxane (entries 20-21), which is in accordance with the literature reports.<sup>[12]</sup> *p*-TSOH (*p*-toluenesulfonic acid) was reported as an efficient catalyst for promoting the hydration/cyclization cascade of 1,4-diyn-3-ones.<sup>[14]</sup> However, no conversion of 1a was observed when p-TSOH was added (entries 22-23).



**Scheme 2**. Substrate Scope. General reaction conditions: The reaction was conducted in a sealed tube under an argon atmosphere at 80 °C with 0.3 mmol of **1**, 0.6 mmol of H<sub>2</sub>O and 0.015 mmol of IPrAuPF<sub>6</sub> in 3 mL of DCE for 16 h.

After establishing the optimized conditions (Table 1, entry 15; 2 equivalent of water and 5 mol % of IPrAuPF<sub>6</sub> in DCE at 80 °C), we turned our attention to the substrate scope (Scheme 2). Starting materials bearing substituted phenyl groups were examined first, which delivered the corresponding products 3a-3i in good to excellent yields (81%-98%). 1-Naphthyl group substituted product **3j** was also obtained in 79% yield. Both thiophene-2-yl-substituted product 3k and thiophene-3-yl-substituted product **3** were obtained in 91% yield. Aliphatic starting material also worked well, delivering the corresponding products 3m and 3n in 92% and 88% yield, respectively. R<sup>3</sup> group was also evaluated. When R<sup>3</sup> were phenyl group and *tert*-butyl group, 30 and 3p were obtained in 89% and 92% yields, respectively. When R<sup>3</sup> was an ethoxy group, the reaction afforded 3q in 93% yield. A product with different  $R^1$  and  $R^2$  group (3r) was obtained in 75% vield. Starting materials bearing two dialkynylphosphine oxide units were also evaluated. delivering 3s and 3t in 88% and 92% yield, respectively. Interestingly, when **1u** was subjected to the standard condition, a six-membered P,Oheterocycle 3u was obtained, in which a ketone unit was formed via the hydration of alkyne.

Besides water, amines and sodium sulfide were also used as nucleophiles to react with dialkynylphosphine oxide 1, giving six-membered P,N- and P,Sheterocycles (Scheme 3). It is worth noting that, owing to the stronger nucleophilicity of amine, the reaction of amines with 1 could be catalyzed by silver salts. For example, the reaction of **1a** with aniline in the presence of 10 mol % of AgNO<sub>3</sub> afforded 5a in 88% yield. p-Phenylenediamine was also added to react with 1a. A a result, 90% of 5b was obtained in the presence of IPrAuPF<sub>6</sub> and 30% of **5b** was isolated in the presence of AgNO<sub>3</sub>, respectively. The reaction of sodium sulfide with 1a afforded a six-membered P.Sheterocycle **6a**. In analogy to amine, the strong nucleophilicity of sodium sulfide made this reaction occurring in the absence of a catalyst, although the yield is relatively lower (See SI for details).



**Scheme 3.** Synthesis of six-membered P,N- and P,Sheterocycles. <sup>a)</sup> IPrAuPF<sub>6</sub> (5 mol %) was used as a catalyst. <sup>b)</sup> AgNO<sub>3</sub> (10 mol %) was added as a catalyst. <sup>c)</sup> The reaction was conducted in the absence of a catalyst.

The reduction of phosphine oxides is one of the major methods for the synthesis of phosphines. In our further investigation, by the use of Werner's method,<sup>[15]</sup> **3a** was reduced by PhSiH<sub>3</sub> in the presence of CF<sub>3</sub>SO<sub>3</sub>H and was directly converted to **7a** by subsequent addition of BH<sub>3</sub>·THF to the reaction mixture (eq 1).



To gain some insights into the reaction mechanism of the P,O-heterocycle formation, several control experiments were conducted (Scheme 4). By addition of D<sub>2</sub>O instead of H<sub>2</sub>O, 95% of **3a** was obtained, with P,O-heterocycle deuterated in 80% ratio (Scheme 4a). During the optimization of the reaction conditions, 4a was obtained as a by-product (Table 1, entry 3). We hypothesized that 4a was the plausible intermediate for the formation of 3a. As we expected, when 4a was subjected to the standard condition, **3a** was obtained in 96% yield within 4 min (Scheme 4b). 2a was also a plausible intermediate to deliver **3a** by an intramolecular dehydration reaction. However, when 2a was subjected to the standard condition, no reaction was observed (Scheme 4c).



Scheme 4. Mechanistic investigation.

Based on the control experiments, a plausible reaction mechanism is proposed by taking 1n as an example. First, a gold(I)-catalyzed alkyne hydration occurs, generating 4n as an intermediate.<sup>[13]</sup> In the following, two pathways (path I and path II) result in the formation of two products 2n and 3n. In path I, a gold(I)-catalyzed intramolecular 6-endo-dig cyclization occurs via TS1, generating intermediate Int1, which then undergoes proton shift and protondeauration to give **3n**.<sup>[16]</sup> In path II, the second gold(I)-catalyzed alkyne hydration occurs via TS2 to give Int3, which finally delivers double hydration product 2n. In our study, P,O-heterocycles were obtained in good chemoselectivity over double hydration product. To better understand the chemoselectivity, density functional theory (DFT) calculations were performed.<sup>[17]</sup> To simplify the calculation, a phenyl substituted NHC ligand was employed (see SI for computational details). The DFT calculation result indicates that the transition state for intramolecular cyclization the (**TS1**, +10.78kcal mol<sup>-1</sup>) is lower in free energy than that for the second alkyne hydration (**TS2**,  $\pm 19.25$  kcal mol<sup>-1</sup>) by  $\Delta\Delta G^{*}=$  8.47 kcal mol<sup>-1</sup> (Scheme 5). The DFT that intramolecular calculation indicates the cyclization is favored over the intermolecular alkyne hydration in the presence of a gold(I) catalyst.



Scheme 5. Plausible Mechanism.

In conclusion, we have reported the facile synthesis of six-membered P,O-, P,N- and P,S-heterocycles. By using gold(I) complexes, the chemoselectivity of the reaction was switched from literature-reported double hydration to a hydration/intramolecular cyclization cascade. Control experiments indicate that ketone **4** is the possible intermediate, which undergoes two different pathways, resulting in the formation of product **2** and **3**. The DFT calculation provided rationalization for the observed chemoselectivity. Further investigation into expanding the scope of the reaction to other nucleophiles and the application of P,O-, P,N- and P,S-heterocycles in material science are currently underway in our lab.

#### **Experimental Section**

General procedures for the gold(I)-catalyzed synthesis of six-membered P, O-heterocycles

IPrAuPF<sub>6</sub> (0.015 mmol), phosphine oxide **1** (0.3 mmol), and water (0.6 mmol) are dissolved in 3 mL of DCE in a 10 mL sealed tube. The reaction mixture was stirred under argon at 80 °C for 16 h. Then, the solvent was removed and the crude product was purified *via* column chromatography on silica gel (methanol/dichloromethane, 1:80) to give the corresponding product.

#### Acknowledgements

Financial support by the National Natural Science Foundation of China (21502110), the Natural Science Foundation of Shaanxi Province (2019JQ-323), the young top-notch talent of "Special Support Plan for High-Level Talents in Shaanxi Province", the 111 Project (B14041) and the Fundamental Research Funds for the Central Universities (GK201903039) are greatly appreciated.

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### COMMUNICATION

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Adv. Synth. Catal. Year, Volume, Page – Page

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