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of 3-aryl-1,2,4-oxadiazolones with *ortho-*(trimethylsilyl)phenyl triflates *via* aryne insertion†

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Tuning chemoselectivity in O-/N-arylation

Herein, we first describe finely tunable chemoselectivity in arylation of 3-aryl-1,2,4-oxadiazolones with *ortho*-(trimethylsilyl)phenyl triflates, including *O*-arylation enabled by catalytic amount of silver nitrate and metal-free *N*-arylation. Both the arylation reactions can tolerate a series of functional groups, and afford the corresponding products in moderate to good yields.

Over the past few decades, aryne chemistry has been an ideal strategy for decorating arenes, building heterocycles and assembling natural product scaffold.<sup>1</sup> This is mainly due to the fact that arynes generated in situ possess an inherent electrophilic nature.<sup>2</sup> Several representative routes for obtaining active arynes have been developed in recent years,<sup>3</sup> but most of them generally necessitate the assistance of strong bases, low temperatures, or stoichiometric amounts of toxic metal salts, which extremely hamper the practical application of aryne chemistry. Fortunately, the use of ortho-(trimethylsilyl)phenyl triflates for efficient aryne generation was reported by Kobayashi et al. in 1983, which successfully gained much attention due to the mild conditions and convenient handling processes.<sup>4</sup> Following this, a large number of organic reactions involving arynes, including cyclization reactions,<sup>5</sup> multicomponent reactions,<sup>1d,6</sup> and aryne insertion reactions,<sup>7</sup> and some others8 were successively reported. Particularly, aryne insertion has achieved significant progress in recent years.<sup>7-9</sup> The classic aryne insertion is achieved by addition of a nucleophile to benzyne, which leads to the formation of a carbanion that can be trapped by an electrophile (Scheme 1a). As a typical example, Larock et al. developed a metal-free approach for the synthesis of biraryl ethers (O-arylation) by aryne insertion.<sup>7a,b</sup> Moreover, it was found that amides were also amenable to arvne insertion





(*N*-arylation), yielding aryl amines (Scheme 1b). Further, Biju *et al.* established a rare temperature-dependent reaction of arynes with aliphatic alcohols, affording a series of alkylaryl ethers *via* aryne insertion and multicomponent coupling.<sup>6d</sup> Despite a variety of elegant studies on aryne chemistry, tuning chemoselectivity remains a challenging task and the expansion of the selective aryne insertion for preparing potentially valuable chemicals is still worth exploring.

Moreover, 3-aryl-1,2,4-oxadiazolones serving as coupling partners have received less attention in past years.<sup>10</sup> Interestingly, Zhu et al. recently reported the useful application of oxadiazolone for building up primary aza-aromatic amines under cobalt catalysis.<sup>10b</sup> Wan et al. disclosed the formal [3+2] cycloaddition of 3-aryl-1,2,4oxadiazolones with ynamides, which provided efficient access to aminoimidazoles.<sup>10c</sup> However, 3-aryl-1,2,4-oxadiazolones acting as valuable coupling reagents are still far from being fully explored in organic synthesis.<sup>10</sup> Moreover, we note that oxadiazolone itself contains an active N-H bond, which shows similar activity to the N-H bonds existing in common amides. In addition, isomerization from N-H to O-H (coming from C=O) within oxadiazolone is permissible even though this process is unfavourable under normal conditions (Scheme 1c).<sup>11</sup> Based on these understandings, we conceived that oxadiazolones might act as an N-containing nucleophiles that trap transient benzynes



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(*N*-arylation). In some cases, the isomerization was favoured under definite conditions, generating the nucleophilic oxygen anion species, which could lead to a totally different result (*O*-arylation). Herein, we will first report our investigation into the *O*-arylation and *N*-arylation of 3-aryl-1,2,4-oxadiazolones by finely tuneable aryne insertion.

At the outset, O-arylation of 3-phenyl-1,2,4-oxadiazol-5(4H)-one (1a) with 2-(trimethylsilyl)phenyl trifluoromethanesulfonate (2a) was chosen as a model reaction to optimize the reaction conditions, as listed in Table 1. According to the previous study, we know that the fluoride source, temperature and reaction medium have a profound effect on the generation of aryne species from ortho-(trimethylsilyl)phenyl triflates.<sup>1b</sup> Therefore, the combination of CH<sub>3</sub>CN/CsF was preferentially adopted for the potential arylation of 1a with 2a in the presence of Ag<sub>2</sub>O (CH<sub>3</sub>CN was simply distilled prior to use). Fortunately, the reaction proceeded at 80  $^\circ\mathrm{C}$ under air ambient for 6 h and generated 3a in 15% yield (entry 1). Furthermore, the structure of 3a was confirmed by single-crystal X-ray diffraction analysis.<sup>12</sup> Then, it was found that Ag<sub>2</sub>CO<sub>3</sub>, silver trifluoromethanesulfonate (AgOTf) or AgSbF<sub>6</sub> did not improve the O-arylation process of 1a (entries 2-4). The use of silver acetate (AgOAc) afforded the arylated product 3a in slightly high isolated yield (entry 5). We observed that the addition of AgNO<sub>3</sub> provided the highest yield of 3a among all the tested silver sources (entry 6). No desired 3a was detected in the absence of CsF, illustrating that the fluoride anion is key to the cleavage of C-Si bond of 2a (entry 7). Several representative F-containing reagents such as KF and tetrabutylammonium fluoride (TBAF), also serving as weak base, were sequentially evaluated in the model reaction. However, both afforded 3a in decreased yields (entries 8 and 9). Additionally, we found that the amounts of CsF and AgNO<sub>3</sub> have a large effect on

Table 1         Optimization of the reaction conditions <sup>a</sup>				
N-C Ph N H 1a	$F_{0} + TMS$	[Ag] (5 mol%) uoride source (0.50 mmol) CH <sub>3</sub> CN, 80 °C, air, 6 h Ph∕∕	$\frac{N-0}{N} + Ph + Ph + N$ $3a^{b} + 4a^{b}$	Ph
		Eluorido	Yield <sup><math>b</math></sup> (%)	
Entry	[Ag]	source	3a	4a
1	$Ag_2O$	CsF	15	_
2	$Ag_2CO_3$	CsF	27	
3	AgOTf	CsF	34	
4	AgSbF <sub>6</sub>	CsF	41	
5	AgOAc	CsF	56	
6	AgNO <sub>3</sub>	CsF	89	
7	AgNO <sub>3</sub>	_	n.r.	
8	AgNO <sub>3</sub>	KF	28	
9	AgNO <sub>3</sub>	TBAF	43	
10	AgNO <sub>3</sub>	CsF	73 <sup>c</sup>	_
11	AgNO <sub>3</sub>	CsF	$90^d$	_
12	AgNO3	CsF	$63^e$	
13	AgNO <sub>3</sub>	CsF	$88^{f}$	
14	AgNO <sub>3</sub>	CsF	89 <sup>g</sup>	_
15	_	CsF	_	67

<sup>*a*</sup> Reaction conditions: **1a** (0.20 mmol), **2a** (0.4 mmol), [Ag] (5 mol%) and fluoride source (0.50 mmol) were added to CH<sub>3</sub>CN (2 mL) at 80 °C in ambient air for 6 h. <sup>*b*</sup> Isolated yield. <sup>*c*</sup> CsF (0.40 mmol). <sup>*d*</sup> CsF (0.60 mmol). <sup>*e*</sup> AgNO<sub>3</sub> (3 mol%). <sup>*f*</sup> AgNO<sub>3</sub> (10 mol%). <sup>*g*</sup> N<sub>2</sub> atmosphere. n.r. = no reaction.

the *O*-arylation of **1a** with **2a**, respectively, under similar reaction conditions, (entries 10–13). Furthermore, performing *O*-arylation under nitrogenatmosphere gave almost the same result when compared with that observed result in ambient air (entry 14). The effect of temperature on this arylation process was analysed, which indicated that no reaction occurred at room temperature, and a reasonable isolated yield of **3a** was obtained at a temperature of 80 °C (Table S1 in ESI†). Solvent screening demonstrated that CH<sub>3</sub>CN is the ideal medium for *O*-arylation of **1a** with **2a** (Table S1 in ESI†). Finally, formation of **3a** was not observed in the absence of silver nitrate, but the *N*-arylated product **4a** was isolated in 67% yield (entry 15).

Next, the generality of O-arylation was studied by employing optimized reaction conditions, and the result is summarized in Table 2. First, a range of 3-aryl-1,2,4-oxadiazolones were prepared and then utilized for O-arylation. The result indicated that the 3-aryl-1,2,4-oxadiazolones bearing an electron-rich group at 4-position on the phenyl ring, such as Me, t-Bu, and MeO, afforded arylated products 3b-d in good to excellent yields. This O-arylation is slightly sensitive to the electronic effect that resulted from the substituents. Both F and Cl incorporated into the phenyl ring led to decreased yields of 3e and 3f, respectively. Replacing the halogens with strong electron-withdrawing groups such as CF<sub>3</sub>, NO<sub>2</sub>, and COOMe only produced the arylated products in acceptable yields (3g-i). Introduction of meta substituents into the phenyl ring has a weak effect on O-arylation (3j-l). However, steric hindrance clearly hampered this process as indicated by the yield obtained through the O-arylation of 3-aryl-1,2,4-oxadiazolones containing an ortho-methoxyl group on the phenyl ring (3d vs. 3m). Furthermore, the commonly

 Table 2
 Scope of 3-aryl-1,2,4-oxadiazolones and ortho-(trimethylsilyl)-phenyl triflates<sup>a</sup>



 $^a$  Reaction conditions: 1 (0.20 mmol), 2 (0.40 mmol), AgNO<sub>3</sub> (5 mol%), and CsF (0.50 mmol) at 80 °C under air ambient for 6 h.  $^b$  Isolated yield.  $^c$  X-ray structure of 3a.

used conjugated groups including 1,1'-biphenyl and naphthyl groups were found to be less active than the former groups, but they still led to the formation of the desired products in good yields (**3n-p**). At last, we obtained satisfactory results from *O*-arylation of furanyl- or thiophenyl-substituted oxadiazolone with **2a** under optimal reaction conditions (**3q** and **3r**).

We next focused on expanding the scope of *ortho*-(trimethylsilyl)phenyl triflates. Some typical aryne precursors 2 were prepared and used for *O*-arylation of **1a** under optimal conditions (Table 2). Notably, the substituted groups or atoms on the phenyl ring did not affect the insertion process. Most of the symmetric substituted aryne precursors are well compatible with the *O*-arylation protocol, leading to the synthesis of target products in good yields (**3s-w**). It was also observed that *O*-arylation of an asymmetric aryne precursor with **1a** smoothly proceeded under the above condition, but gave poor selectivity (**3x-z**, **3x'-z'**), which indicated that the bulkiness and electron effect of the methyl group did not affect the aryne insertion. However, the reaction of indolyne with **1a** afforded the product with enhanced selectivity (**3ab**: **3ab**' = **3**: **1**).

Inspired by the findings reported by Larock et al.,<sup>7a,b</sup> we considered that the 3-aryl-1,2,4-oxadiazolones containing an active N-H bond could also serve as nucleophiles and attack the fleeting aryne intermediates to complete the N-arylation process (Table 3). Unfortunately, this metal-free N-arylation did not proceed at room temperature, demonstrating that 3-aryl-1,2,4-oxadiazolones were not active enough for the N-arylation reaction. Therefore, we next explored the model N-arylation process of 1a with 2a (Table S2 in ESI<sup>+</sup>), and the optimized conditions were as follows: 1a (0.20 mmol), 2a (0.40 mmol), and CsF (2.5 equiv.), in CH<sub>3</sub>CN at 80 °C for 10 h. It was found that a number of 3-aryl-1,2,4oxadiazolones could react with symmetric arynes 2 under the optimal conditions, affording the N-arylated products in good to excellent yields (4a-l, Table 3). For the asymmetric arynes, poor selectivity was observed in the *N*-arylations (4m-n, 4m'-n'). In fact, the obtained N-arylated products 4 can also be harnessed for the synthesis of amidines.13

Furthermore, we were still curious about the role of AgNO<sub>3</sub> in the unique *O*-arylation of 3-aryl-1,2,4-oxadiazolones with *ortho*-(trimethylsilyl)phenyl triflates because there was no

 Table 3
 Investigation into the N-arylation reaction of 3-aryl-1,2,4-oxadiazolones<sup>a</sup>



 $^a$  Reaction conditions: 1 (0.20 mmol), 2a (0.40 mmol), and CsF (0.50 mmol) at 80  $^\circ \rm C$  under air ambient for 10 h.  $^b$  Isolated yield.



precedent to the tuneable reaction. Subsequently, several experiments were conducted to gain insight into the effect of Ag(1) on the two different arylations. As illustrated in Table S2 (ESI†), complete *N*-arylation was observed in the absence of Ag(1). Clearly, the use of 1 mol% AgNO<sub>3</sub> would make the reaction of **1a** with **2a** to absolutely proceed toward *O*-arylation, and completely suppress the *N*-arylation. Then, **4a** was specially treated under the above conditions, and no **3a** was detected, indicating that phenyl group transfer would not happen (Scheme 2, eqn (1)). Again, the result indicated that only **1a**, containing a N–H unit, could react with benzyne in the presence or absence of AgNO<sub>3</sub> to produce the corresponding arylated products. Moreover, we found that the gram-scale synthesis of **3a** is very successful through the *O*-aylation of **1a** with **2a**, which provides an efficient approach to synthesize 1,2,4-oxadiazole (Scheme 2, eqn (2)).

For better understanding the O-arylation process, the density functional theory (DFT) calculation was carried out to investigate the role of Ag(i), as shown in Fig. 1,<sup>14</sup> which also helped us to shed light on the mechanism proposed in Scheme 3. Initially, the use of excess CsF led to the formation of benzyne intermediates. We then envisioned that a possible isomerization of 1a into 1a-OH assisted by Ag(I) was the key step for O-arylation (Scheme 3, path A). However, the results from the DFT calculations (Fig. 1a) indicated that at least 59.53 kcal  $mol^{-1}$  of free energy barrier is necessary for the proton transfer from N to O within 1a. Adversely, the addition of Ag(I) into the system would require much higher free energy barrier (up to 87.42 kcal mol<sup>-1</sup>) for the same isomerization, presumably because Ag(1) decreases the electron density of the carbonyl group in 1a. This result demonstrated that the proposal for the isomerization of 1a assisted by Ag(I) is extremely unreasonable. Subsequently, a stepwise mechanism for the O-arylation process was proposed (Scheme 3, path B). We assumed that the interaction of 1a with Ag(1) by weak coordination generated unstable complexes,<sup>15</sup>



**Fig. 1** (a) Free energy profile of **1a** isomerization with and without Ag(ı). (b) Free energy profile of the *O*-arylation pathway with Ag(ı).



Scheme 3 Proposed reaction mechanism of the O-/N-arylation process.

followed by attacking benzyne to afford intermediate I-Ag, which is less stable (3.35 kcal mol<sup>-1</sup>) than 1a-Ag (Fig. 1b). In addition, it was also found that the presence of Ag(1) leads to the reduction in distance (1.473 Å) between the O atom of the carbonyl group and the alkynyl carbon atom of benzyne when compared with that (3.902 Å) in the absence of Ag(1). Further, an intramolecular proton transformation (from N to C) of I-Ag gives 3a, where a relatively lower energy barrier (19.24 kcal mol<sup>-1</sup>) for the transition state  $TS_{1a-Ag \rightarrow 3a-Ag}$ . was observed. Remarkably, the above results indicated that Ag(1) can drastically lower the energy barrier in forging the C(aryl)–O bonds of aryl ether. For the *N*-arylation process, 1a was deprotonated by a base to give the electronically negative species I, which then directly attacked benzyne to form the *N*-arylated product 4a.

In summary, we first reported the highly chemoselective arylation of 3-aryl-1,2,4-oxadiazolones with *ortho*-(trimethyl-silyl)phenyl triflates under air ambient. In the arylation-oriented systems, the catalytic activity of silver nitrate plays an important role in *O*-arylation of oxadiazolone with aryne, which yields a series of disubstituted 1,2,4-oxadiazole in moderate to good yields. In contrast, only *N*-arylated oxadiazolone was observed in the absence of silver nitrate. Further efforts to achieve a valuable transformation of the arylated 3-aryl-1,2,4-oxadiazolones and mechanistic investigation are underway in our laboratory.

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## Conflicts of interest

There are no conflicts to declare.

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- 14 For the DFT calculation, see details in ESI<sup>†</sup>.
- 15 The addition of AgNO<sub>3</sub> can efficiently assist the *O*-arylation of **1a** with **2a**, which can be observed by the according <sup>1</sup>H NMR experiment, see details in ESI<sup>†</sup>.