

# Palladium/Copper-Catalyzed Oxidative Coupling of Arylboronic Acids with Isocyanides: Selective Routes to Amides and Diaryl Ketones

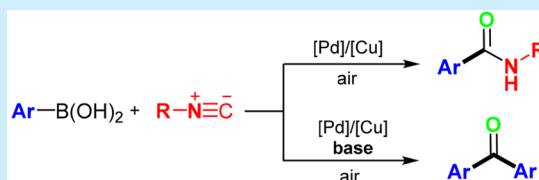
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## S Supporting Information

**ABSTRACT:** An efficient and alternative oxidative cross-coupling strategy starting from arylboronic acids and isocyanides for the selective synthesis of amides and diaryl ketones with palladium/copper catalysis is developed. Various substituted benzamides and benzophenones could be obtained in good yields. The reaction represents an efficient and alternative strategy for the synthesis of carbonyl compounds.



In the past decades, palladium-catalyzed oxidative carbonylation reactions have been extensively used for the construction of numerous important compounds.<sup>1</sup> Compared to the classic transition-metal-catalyzed carbonylation of organic halides (RX) with CO, which was pioneered by Heck and co-workers, these approaches avoid the use of high CO pressure, excess base, aryl halides as electrophiles, and complicated ligands,<sup>2</sup> thus dramatically promoting the development of carbonylation reactions. A typical example is the well-established synthesis of esters using various organometallic compounds (R–M) or hydrocarbons (R–H) as nucleophiles with alcohols.<sup>3</sup> However, few examples have been reported for the synthesis of amides utilizing these approaches, which could be possibly attributed to the strong coordination capability and frangibility to oxidation of amines.<sup>4</sup> Amides are prevalent functional groups widely existing in not only proteins but also pharmaceuticals, functional materials, and other versatile fine synthetic chemicals. Hence, seeking a simple, practical oxidative amidation strategy for the synthesis of amides from readily available starting materials is still highly attractive.

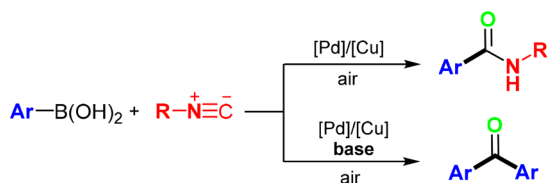
Isocyanides are highly versatile reagents which have been widely used in organic synthesis.<sup>5</sup> As valuable C1 building blocks, isocyanides are isoelectronic with CO, which showed similar reactivity and underwent the same fundamental transformations. Furthermore, as carbonyl sources, compared to the toxic CO gas which was typically used under high pressure in excess amount, isocyanides have incomparable advantages, since they are easily handled liquids or solids and can therefore be used in stoichiometric quantities.<sup>6</sup> Consequently, utilizing isocyanides as CO surrogates offers tremendous opportunities for the synthesis of fine chemicals containing a nitrogen functionality. Recently, direct amidation of aryl halides with isocyanides under transition-metal catalysis has emerged as an effective tool for the formation of amides;<sup>7</sup>

however, these approaches usually need equivalent base and extra ligands. There have been few examples for the direct oxidative synthesis of amides utilizing isocyanides as a source of both a carboxy and amino group.<sup>8</sup> Very recently, Wu<sup>8a</sup> reported a palladium-catalyzed oxidative three component coupling reaction of aryl boronic acids, isocyanides, and amines for the synthesis of amidines. Based on our continuous interest in oxidative cross-couplings and isocyanides chemistry, we envisioned that the direct oxidative cross-coupling of arylboronic acids with isocyanides would be of great opportunity for the direct synthesis of amides, considering that arylboronic acids are commercially available and also air-/moisture-stable. Meanwhile, utilizing arylboronic acids and isocyanides as alternatives for the synthesis of amides would simplify the original strategies and also provide a new route to nitrogen functionality. To the best of our knowledge, there have been no reports in the literature concerning oxidative coupling using organometallics and isocyanides with palladium catalyst. Herein, we demonstrate the first palladium/copper-catalyzed oxidative cross-coupling of arylboronic acids and isocyanides to construct amides and diaryl ketones, respectively (Scheme 1).

Initial efforts were focused on the reaction of phenylboronic acid **1a** with *tert*-butyl isocyanide **2a** (Note: isocyanides are quite toxic reagents and stink; please handle them with caution) utilizing Pd(OAc)<sub>2</sub> and Cu(OAc)<sub>2</sub> as the catalysts in water and toluene at 100 °C for 16 h under air atmosphere. To our delight, the desired product *N*-*tert*-butyl benzamide **3a** was produced in 18% yield (Table 1, entry 1). Solvent screening revealed that toluene appeared to be the best solvent (Table 1, entries 2–4). In comparison with Pd(OAc)<sub>2</sub>, PdCl<sub>2</sub> can help

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Scheme 1. Oxidative Cross-Coupling of Arylboronic Acids and Isocyanides To Construct Amides and Diaryl Ketones

Table 1. Condition Optimization of Palladium/Copper-Catalyzed Oxidative Cross-Coupling between 1a and 2a<sup>a</sup>

		$\text{Ph-B(OH)}_2 + \text{C}\equiv\text{N}^+-\text{tBu} \xrightarrow[\text{16 h, air}]{[\text{Pd}]/[\text{Cu}], \text{toluene, 100 }^\circ\text{C}}$			
		1a	2a	3a	4a
entry	[Pd]	[Cu]	yield <sup>b</sup> (%)		
1	Pd(OAc) <sub>2</sub>	Cu(OAc) <sub>2</sub>	18	trace	
2 <sup>c</sup>	Pd(OAc) <sub>2</sub>	Cu(OAc) <sub>2</sub>	n.d.	n.d.	
3 <sup>d</sup>	Pd(OAc) <sub>2</sub>	Cu(OAc) <sub>2</sub>	trace	trace	
4 <sup>e</sup>	Pd(OAc) <sub>2</sub>	Cu(OAc) <sub>2</sub>	trace	trace	
5	Pd(PPh <sub>3</sub> ) <sub>2</sub> Cl <sub>2</sub>	Cu(OAc) <sub>2</sub>	33	trace	
6	PdCl <sub>2</sub>	Cu(OAc) <sub>2</sub>	39	7	
7	PdCl <sub>2</sub>	CuI	trace	trace	
8	PdCl <sub>2</sub>	Cu(OH) <sub>2</sub>	67	18	
9 <sup>f</sup>	PdCl <sub>2</sub>	Cu(OH) <sub>2</sub>	75	trace	
10 <sup>g</sup>	PdCl <sub>2</sub>	Cu(OH) <sub>2</sub>	72	trace	
11		Cu(OH) <sub>2</sub>	n.d.	n.d.	
12	PdCl <sub>2</sub>		n.d.	n.d.	
13 <sup>h,i</sup>	PdCl <sub>2</sub>	Cu(OH) <sub>2</sub>	25	51	
14 <sup>h,j</sup>	PdCl <sub>2</sub>	Cu(OH) <sub>2</sub>	trace	70	
15 <sup>h,j,k</sup>	PdCl <sub>2</sub>	Cu(OH) <sub>2</sub>	trace	85	
16 <sup>h,j,l</sup>	PdCl <sub>2</sub>	Cu(OH) <sub>2</sub>	trace	75	
17 <sup>h,j,m</sup>	PdCl <sub>2</sub>	Cu(OH) <sub>2</sub>	trace	70	
18 <sup>h,j,n</sup>	PdCl <sub>2</sub>	Cu(OH) <sub>2</sub>	trace	72	
19 <sup>o</sup>	PdCl <sub>2</sub>	Cu(OH) <sub>2</sub>	trace	trace	

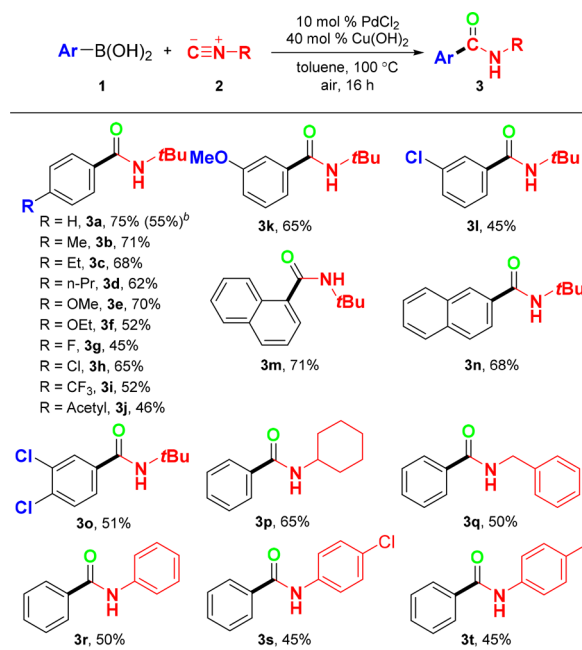
<sup>a</sup>Unless otherwise noted, the reactions were carried out with 0.3 mmol of 1a, 0.3 mmol of 2a, 10 mol % of [Pd], 40 mol % of [Cu] in 1 mL of toluene at 100 °C for 16 h under air atmosphere. <sup>b</sup>Yields presented are of isolated products. <sup>c</sup>DMSO as the solvent. <sup>d</sup>DCE as the solvent. <sup>e</sup>1,4-Dioxane as the solvent. <sup>f</sup>0.36 mmol of 2a was used. <sup>g</sup>0.45 mmol of 2a was used. <sup>h</sup>3 mL of toluene was used. <sup>i</sup>0.9 mmol of 1a was used. <sup>j</sup>1.5 mmol of 1a was used. <sup>k</sup>2 equiv of NH<sub>4</sub>Cl was added. <sup>l</sup>2 equiv of NH<sub>3</sub>·H<sub>2</sub>O was added. <sup>m</sup>2 equiv of KI was added. <sup>n</sup>2 equiv of KOAc was added. <sup>o</sup>The reactions were carried out under a nitrogen atmosphere. n.d. = not detected.

increase the yield to 39% (Table 1, entries 5 and 6). Meanwhile, the copper source was also examined. Cu(OH)<sub>2</sub> was revealed to be the best copper salt in this reaction, which greatly enhanced the reaction yield to 67%, while CuI was almost ineffective (Table 1, entries 7 and 8). Moreover, by slightly changing the ratio of 1a/2a to 1:1.2, the desired product was isolated in 75% yield (Table 1, entry 9). Further increasing the amount of 2a made no difference at all (Table 1, entry 10). Control experiments showed that both PdCl<sub>2</sub> and Cu(OH)<sub>2</sub> are essential to this reaction (Table 1, entries 11 and 12).

Notably, during the condition optimization process, some benzophenone 4a was detected as byproduct in entries 6 and 8, which could be possibly originated from the reaction of excess amount of arylboronic acids with isocyanides. Indeed, by increasing the amount of 1a to 3 and 5 equiv, the yield of 4a

could be increased to 51% and 70%, respectively (Table 1, entries 13 and 14). Meanwhile, introducing a weak acidic additive such as NH<sub>4</sub>Cl (2 equiv) to accelerate the hydrolysis process could further increase the yield of 4a to 85% (Table 1, entry 15). As expected, other basic additives such as NH<sub>3</sub>·H<sub>2</sub>O or KOAc and neutral salts such as KI made no difference (Table 1, entries 16–18). Notably, when the reaction was carried out under N<sub>2</sub> atmosphere, only a trace amount of product was detected, demonstrating the essential role of air in this reaction (Table 1, entry 19).

With the above optimized reaction conditions in hand, the oxidative cross-coupling of different arylboronic acids with isocyanide derivatives to construct various benzamides were first explored. As depicted in Scheme 2, this reaction has good

Scheme 2. Substrate Scope for Oxidative Cross-Coupling of Different Arylboronic Acids with Isocyanide Derivatives To Construct Various Benzamides<sup>a</sup>

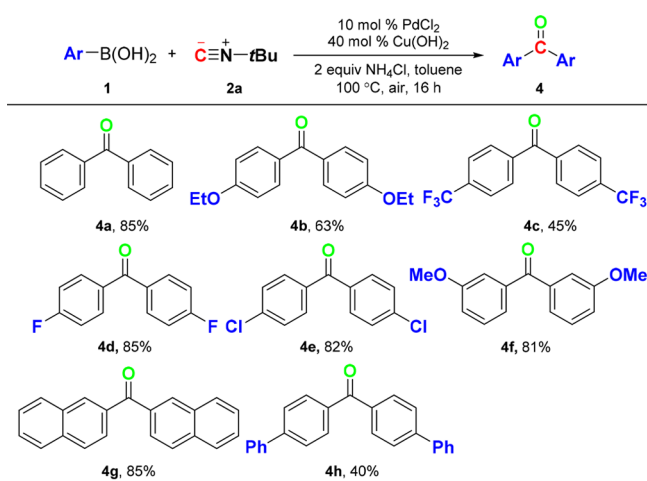
<sup>a</sup>Reactions of 1 and 2. Reaction conditions: 0.3 mmol of 1, 0.36 mmol of 2, 10 mol % of PdCl<sub>2</sub>, 40 mol % of Cu(OH)<sub>2</sub>, 1 mL of toluene, 100 °C, air, 16 h. Yields presented are of isolated products. <sup>b</sup>Yield in parentheses was the reaction with 5 mmol scale.

applicability for both substituted arylboronic acids and isocyanide derivatives. As for arylboronic acids, substrates with electron-neutral groups such as Me (3b), Et (3c), or n-Pr (3d), electron-rich groups such as OMe (3e) or OEt (3f), electron-poor groups such as CF<sub>3</sub> (3i), acetyl (3j), and halogen groups such as F (3g) or Cl (3h) could be facilely converted into the desired products in 45–71% yields. Arylboronic acids with meta substituents on the phenyl ring could also be well tolerated (3k and 3l). Meanwhile, naphthaleneboronic acids were revealed to be good substrates in this reaction (3m and 3n). Additionally, 3,4-dichlorophenylboronic acid could also react with 2a to deliver the corresponding benzamide 3o in 51% yield. We also tried the reaction of alkyl and alkenyl boronic acids; however, these substrates were totally inert under standard conditions. As for isocyanide derivatives, cyclohexyl-, benzyl-, and phenyl-substituted isocyanides all

proved to be compatible, affording the desired products in 45–65% yields (**3p–t**).

Inspired by the good results of benzamides synthesis, we turned our attention to the substrate scope of oxidative carbonylation with arylboronic acids and *tert*-butyl isocyanides to synthesize different benzophenones (Scheme 3). Arylbor-

**Scheme 3. Substrate Scope for Oxidative Carbonylation of Different Arylboronic Acids with *tert*-Butyl Isocyanide To Synthesize Different Benzophenones<sup>a</sup>**

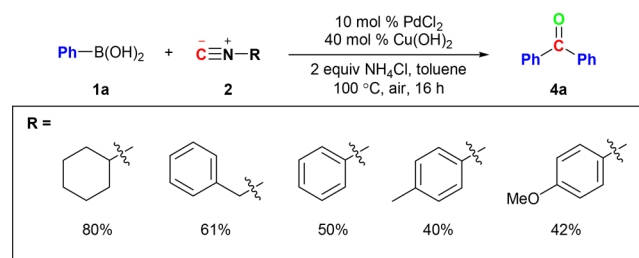


<sup>a</sup>Reaction conditions: 1.5 mmol of **1**, 0.3 mmol of **2a**, 10 mol % of PdCl<sub>2</sub>, 40 mol % of Cu(OH)<sub>2</sub>, 0.6 mmol of NH<sub>4</sub>Cl, 3 mL of toluene, 100 °C, air, 16 h. Yields presented are of isolated products.

onic acids with electron-rich substituents such as OEt (**4b**) and electron-poor substituents such as CF<sub>3</sub> (**4c**) on the phenyl ring could be well tolerated, albeit in slightly low yields. Meanwhile, halogen substituents such as F (**4d**) and Cl (**4e**) could survive during the reaction, and the desired products were obtained in excellent yields. Likewise, arylboronic acids with meta substituents on the phenyl ring smoothly delivered the corresponding products in good yields (**4f**). In addition, 2-naphthaleneboronic acid and 4-biphenylboronic acid also proved to be suitable substrates in this reaction (**4g** and **4h**).

Moreover, isocyanide sources were also tested in which phenylboronic acid was utilized as the aryl nucleophile (Scheme 4). Fortunately, different isocyanides could be good C1 sources of the product carbonyl groups. When *t*Bu on isocyanide was

**Scheme 4. Substrate Applicability of Different Isocyanides in Oxidative Carbonylation Reactions To Construct Benzophenones<sup>a</sup>**

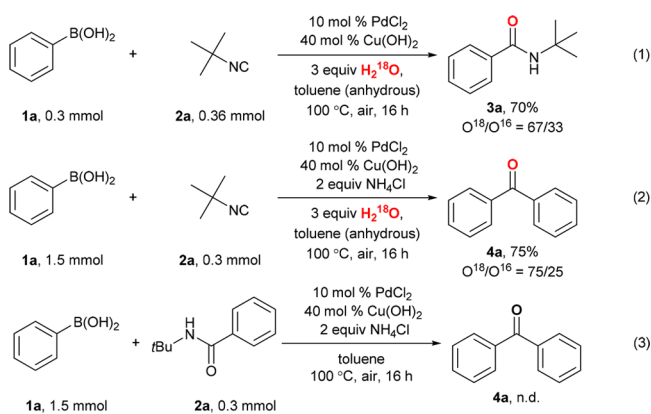


<sup>a</sup>Reaction conditions: 1.5 mmol of **1**, 0.3 mmol of **2a**, 10 mol % of PdCl<sub>2</sub>, 40 mol % of Cu(OH)<sub>2</sub>, 0.6 mmol of NH<sub>4</sub>Cl, 3 mL of toluene, 100 °C, air, 16 h. Yields presented are of isolated products.

changed to other substituents such as cyclohexyl, benzyl, phenyl, or substituted phenyl groups, the desired benzophenone **4a** could still be generated with good efficiency, demonstrating the broad substrate compatibility of this reaction.

Furthermore, in order to gain more insights into the reaction mechanism, the labeling experiments using H<sub>2</sub><sup>18</sup>O was carried out. As shown in Scheme 5, the introduction of a stoichiometric

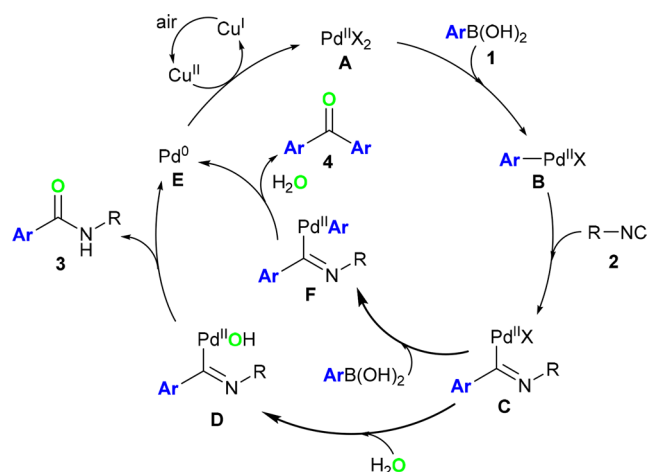
**Scheme 5. Mechanistic Studies**



amount of H<sub>2</sub><sup>18</sup>O furnished the desired benzamide **3a** and benzophenone **4a** in 70% and 75% yields, respectively (eqs 1 and 2), in which the <sup>18</sup>O-labeled products predominated. The small amount of <sup>16</sup>O in the final products was probably from the residual moisture in toluene. These results clearly showed that the products carbonyl oxygen was originated from water. In order to exclude the possibility that diarylketone products were originated from reaction of arylboronic acids with benzamides, we tried to mix **1a** with **3a** under the standard conditions. No benzophenone **4a** was detected after the reaction (Scheme 5, eq 3), clarifying that diarylketones were probably formed directly from arylboronic acids and isocyanides.

On the basis of the above mechanistic studies and previous reports,<sup>6a,b,8</sup> a tentative mechanism of this reaction is demonstrated in Scheme 6. Initial transmetalation of arylboronic acid with Pd<sup>II</sup>X<sub>2</sub> generated Ar–Pd<sup>II</sup>X species **B**. Migratory insertion of B to isocyanide afforded intermediate **C**. At this point, **C** could react with H<sub>2</sub>O to generate a Pd-hydroxyl

**Scheme 6. Plausible Reaction Mechanism**



species **D**, of which further reductive elimination delivered Pd<sup>0</sup> species, and the final benzamide product **3** was obtained via tautomerization. On the other hand, in the presence of an excess amount of **1**, a second transmetalation between **C** and **1** gave intermediate **F**, which further conducts reductive elimination to afford Pd<sup>0</sup> species, and the final benzophenone product **4** was obtained via hydrolysis. At last, Pd<sup>0</sup> could be co-oxidized by Cu<sup>II</sup> and air to finish the catalytic cycle.<sup>9</sup>

In summary, we have successfully developed a palladium-/copper-catalyzed oxidative cross-coupling of arylboronic acids with isocyanides for the selective synthesis of amides and diaryl ketones. Different substituted benzamides and benzophenones could be obtained in good yields. Initial mechanistic studies revealed that the product carbonyl oxygen originated from water. This reaction represents an efficient and alternative strategy for the synthesis of carbonyl compounds. Further studies on reaction mechanism are currently underway.

## ■ ASSOCIATED CONTENT

### Supporting Information

The Supporting Information is available free of charge on the ACS Publications website at DOI: 10.1021/acs.orglett.7b01548.

Experimental procedure, characterization data, and <sup>1</sup>H, <sup>13</sup>C NMR spectra (PDF)

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### Notes

The authors declare no competing financial interest.

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