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Efficient synthesis of 1,2,3-triazoles catalyzed by copper(I) Schiff base complex

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ABSTRACT

A tricoordinate Cu(I) complex was synthesized employing a neutral bidentate Schiff base (L^{4Cl}), which was prepared by condensing 4-chlorobenzaldehyde with 2,2-dimethylpropane-1,3-diamine, followed by complexation with copper(I) iodide. The structural features of the ligand and its corresponding complex were confirmed by FT-IR, ^{1}H and $^{13}C\{^{1}H\}$ NMR spectroscopy, and elemental (CHN) analysis. The catalytic efficiency of the complex was evaluated in the one-pot synthesis of 1,2,3-triazoles—compounds known for their effectiveness as anticancer agents—*via* a three-component reaction of phenylacetylene, sodium azide, and various benzyl bromides in aqueous medium. The optimized reaction conditions offer significant advantages, including shorter reaction times, high yields, reduced reaction temperature, and a simplified product isolation process. The efficient synthesis of triazoles using this Cu(I) complex highlights its potential as a promising catalyst for developing new drugs that target malignant cells.

1. Introduction

Schiff bases are an important class of organic ligands that are formed by condensing primary amines with aldehydes or ketones. The characteristic feature of a Schiff base is the azomethine linkage (HC=N), which serves as a significant donor site [1−3]. Schiff bases readily form stable complexes with both main-group and transition metals, owing to their structural flexibility and ease of synthesis [4−6]. Additionally, metal complexes exhibit notable biological activity, demonstrating effectiveness against fungi, viruses, and various microorganisms [7–14]. Recently, they have gained attention for their excellent selectivity and high catalytic efficiency in organic reactions—attributes that align with sustainable chemistry principles [15−20].

Copper, a first-row transition metal, plays an essential role in biological systems and often exists in + 1 and + 2 oxidation states, participating in vital enzymatic processes. Copper Schiff base complexes are widely used in catalysis, photoluminescent materials, and light-emitting devices because of their exclusive optoelectronic properties [21].

The electron-rich $3d^{10}$ electronic configuration of Cu(I) affords versatile coordination behavior, enhancing its potential in advanced materials and various catalytic systems [22−24].

Heterocyclic compounds, particularly disubstituted triazoles, imidazoles, and pyridine-based derivatives, exhibit significant potential as pharmaceutical agents [25−28]. The structural flexibility of triazoles allows them to mimic traditional carbocyclic frameworks common in many drugs [29−31]. Modern synthetic techniques increasingly depend on transition metal catalysts, with copper(I) complexes enabling efficient synthesis of triazole derivatives from unconventional precursors such as chalcones and nitroalkenes [32]. A major advancement in molecular assembly is the synthetic accessibility of triazoles *via* click chemistry transformations, notably the copper-catalyzed reactions developed by Sharpless and Meldal [33−35]. Nevertheless, the majority of earlier approaches have relied on basic copper complexes or simple copper salts, which often require harsh conditions and have poor stability.

In contrast, this work employs a copper(I) Schiff base complex as a very effective and stable catalyst, providing a distinct advantage over previous techniques by permitting greater electronic control, enhanced

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performance, and higher yields under moderate reaction conditions.

Therefore, considering the remarkable catalytic potential of Cu(I) Schiff base complexes and as part of our ongoing research in this field [36–38], we synthesized and characterized a bidentate NN Schiff base Cu(I) complex. This study explores its catalytic efficiency in a one-pot aqueous synthesis of 1,2,3-triazole derivatives, using phenylacetylene, sodium azide, and benzyl bromides as starting materials. This study provides a foundation for further exploration in developing triazole-based anticancer drugs.

2. Materials and Methods

All solvents and chemicals were of analytical grade and procured from Sigma-Aldrich and Merck. A Heraeus CHN-O-FLASH EA 1112 analyzer was utilized for elemental analysis. A BRUKER AVANCE 400 MHz spectrometer was used to record NMR spectra, with tetramethylsilane as the internal reference (δ = 0 ppm). Infrared spectra were obtained on a Shimadzu IR Prestige-21 spectrophotometer using KBr pellets to identify functional groups in the synthesized compounds.

2.1. Preparation of bidentate NN Schiff base ligand (L^{4Cl})

A chloroform solution (5 mL) of 2,2-dimethylpropane-1,3-diamine (102 mg, 1 mmol) was added dropwise to a chloroform solution (25 mL) of 4-chlorobenzaldehyde (280 mg, 2 mmol). The resulting mixture was stirred for 3 hours at room temperature, yielding yellow precipitates. The product was filtered, washed with methanol, and finally dried in air.

L^{4Cl}: Yield = 91% (316 mg). Elemental *Anal.* Calcd. (Found) for $C_{19}H_{20}Cl_2N_2$: C, 65.71% (65.93%); H, 5.80% (5.85%); N, 8.07% (7.98%). FT-IR (KBr, cm^{-1}) 1439−1593 (C=C), 1647 (−C=N−), 2878 (−CH=N), 2955 (−CH), 3063 (=CH); ^{1}H NMR (400 MHz, DMSO-d_6, ppm) 1.00 (s, 6 H, CH_3), 3.49 (s, 4 H, CH_2), 7.55 (d, J = 8.48 Hz, 4 H, aromatic), 7.81 (d, J = 8.48 Hz, 4 H, aromatic), 8.36 (s, 2 H, HC=N). ^{13}C{^{1}H} NMR (100 MHz, DMSO-d_6, ppm) 24.81, 37.12, 69.76, 129.26, 129.94, 135.52, 135.58, 160.39.

2.2. Preparation of [Cu(L^{4Cl})I] complex

A THF solution (20 mL) of CuI (190 mg, 1 mmol) was added to a chloroform solution (30 mL) of L^{4Cl} (347 mg, 1 mmol). After stirring for 30 minutes, one-fourth of the solvent was evaporated, and the resulting yellow solid was washed with diethyl ether and air-dried.

[Cu(L^{4Cl})I]: Yield = 68% (366 mg). Elemental *Anal.* Calcd. (Found) for $C_{19}H_{20}Cl_2CuIN_2$: C, 42.44% (42.28%); H, 3.75% (3.79%); N, 5.21% (5.36%). FT-IR (KBr, cm^{-1}) 1628 (−C=N−); ^{1}H NMR (400 MHz, DMSO-d_6, ppm) 0.99 (s, 6 H, CH_3), 3.53 (s, 4 H, CH_2), 7.56 (d, J = 8.44 Hz, 4 H, aromatic), 7.86 (d, J = 8.44 Hz, 4 H, aromatic), 8.53 (s, 2 H, HC=N); ^{13}C{^{1}H} NMR (100 MHz, DMSO-d_6, ppm) 24.77, 37.00, 69.98, 129.28, 130.06, 135.29, 135.73, 160.67.

2.3. Catalytic procedure

In a typical reaction, phenylacetylene (1 mmol) and benzyl bromides (1 mmol), and sodium azide (1.5 mmol) were combined with the catalyst (1 mol%) in water (3 mL). The mixture was heated at 80 °C, and the reaction progress was monitored by TLC using an *n*-hexane:ethyl acetate (5:1) system. Upon completion, the mixture was cooled to room temperature, and the catalyst was subsequently recovered by filtration. The target product was extracted with chloroform (2 × 5 mL), and the combined organic layers were dried over anhydrous calcium chloride. The solvent was then removed under reduced pressure to afford the desired triazole derivative.

2.4. Spectroscopic data

1-Benzyl-4-phenyl-1H-1,2,3-triazole (2a) FT-IR (KBr, cm^{-1}) 3121, 2924, 1609, 1466, 1358, 1223, 1153, 1076; ^{1}H NMR (400 MHz, $CDCl_3$, ppm) 5.54 (s, 2H), 7.27–7.39 (m, 8H), 7.66 (br, 1H), 7.78 (d, J = 7.6 Hz, 2H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$, ppm) 54.15, 119.72, 125.70, 128.08, 128.18, 128.80, 129.17, 130.60, 134.66, 148.62.

1-(4-Bromobenzyl)-4-phenyl-1H-1,2,3-triazole (2b) FT-IR (KBr, cm^{-1}) 3082, 2928, 1609, 1462, 1350, 1219, 1142, 1076; ^{1}H NMR (400 MHz, $CDCl_3$, ppm) 5.55 (s, 2H), 7.20 (d, J = 8.4 Hz, 2H), 7.35 (t, J = 7.2 Hz, 1H), 7.43 (t, J = 7.2 Hz, 2H), 7.53 (d, J = 8.4 Hz, 2H), 7.72 (br, 1H), 7.83 (d, J = 7.6 Hz, 2H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$, ppm) 53.56, 119.68, 122.96, 125.72, 128.31, 128.87, 129.67, 130.30, 132.48, 133.73, 148.69.

1-(4-Nitrobenzyl)-4-phenyl-1H-1,2,3-triazole (2c) FT-IR (KBr, cm^{-1}) 3082, 2924, 1639, 1589, 1489, 1346, 1219, 1184, 1072; ^{1}H NMR (400 MHz, $CDCl_3$, ppm) 5.56 (s, 2H), 7.21 (d, J = 8.4 Hz, 2H), 7.35 (t, J = 7.2 Hz, 1H), 7.44 (t, J = 7.2 Hz, 2H), 7.55 (d, J = 8.4 Hz, 2H), 7.74 (br, 1H), 7.84 (d, J = 6.8 Hz, 2H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$, ppm) 53.62, 119.86, 122.99, 125.70, 128.31, 128.88, 129.68, 130.43, 132.36, 133.70, 148.60.

1,2-Bis((4-phenyl-1H-1,2,3-triazol-1-yl)methyl)benzene (2d) FT-IR (KBr, cm^{-1}) 3086, 2963, 1609, 1458, 1354, 1223, 1153, 1049; ^{1}H NMR (400 MHz, $CDCl_3$, ppm) 5.74 (s, 4H), 7.30−7.48 (m, 10H), 7.58 (s, 2H), 7.78 (d, J = 5.6 Hz, 4H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$, ppm) 51.38, 119.74, 125.64, 128.33, 128.84, 129.97, 130.15, 130.71, 133.34, 148.42.

1,3-Bis((4-phenyl-1H-1,2,3-triazol-1-yl)methyl)benzene (2e) FT-IR (KBr, cm^{-1}) 3094, 2951, 1609, 1462, 1354, 1219, 1192, 1072; ^{1}H NMR (400 MHz, $CDCl_3$, ppm) 5.62 (s, 4H), 7.34−7.46 (m, 10H), 7.73 (s, 2H), 7.84 (d, J = 5.6 Hz, 4H); ^{13}C{^{1}H} NMR (100 MHz,

$CDCl_3$, ppm) 53.82, 119.44, 125.73, 127.30, 128.28, 128.32, 128.89, 130.08, 130.32, 135.96, 148.44.

3. Results and Discussion

3.1. Synthesis

The NN-donor Schiff base (L^{4Cl}) was synthesized *via* the condensation of 4-chlorobenzaldehyde with 2,2-dimethyl-1,3-propanediamine in chloroform. Subsequent coordination with CuI in tetrahydrofuran afforded the desired copper(I) complex (Scheme 1), which was comprehensively characterized before evaluating its catalytic efficacy in the synthesis of 1,2,3-triazoles (Scheme 2).

3.2. Spectral studies

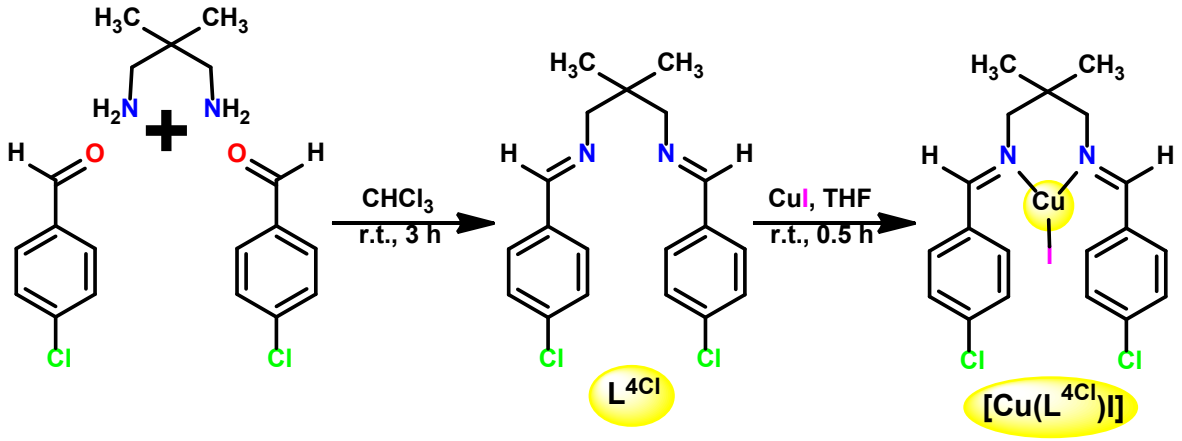
Single-crystal X-ray diffraction analysis was employed to elucidate the molecular structure of the copper complex [39]. Comparative FT-IR analysis (Fig. 1 Supp.) revealed significant spectral changes upon metal coordination. In the ligand spectrum, a distinct absorption band at 1647 cm^{-1} was attributed to the stretching vibrations of the azomethine (HC=N) linkages. Upon complexation with the copper center, this band shifted to a lower wavenumber (1628 cm^{-1}), confirming coordination through the imine nitrogen and indicating a partial reduction in the C=N double-bond character.

Nuclear magnetic resonance spectroscopy further confirms the symmetrical nature of both the ligand and its metal complex. The ^1H NMR spectrum of L^{4Cl} exhibits singlets at 1.00 ppm and 3.49 ppm, assigned to the aliphatic methyl (CH_3) and methylene (CH_2) protons, respectively. Aromatic protons appear as two doublets in the region of 7.54-7.82 ppm, while the azomethine proton (CH=N) resonates as a singlet at 8.36 ppm. Upon coordination with the copper center, these signals exhibit only slight chemical shifts, as depicted in (Fig. 2 and 4 Supp.).

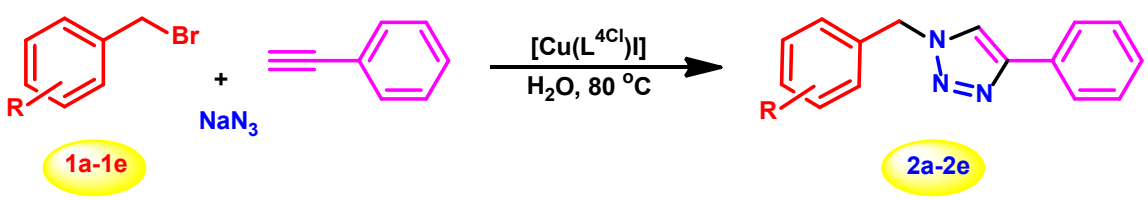
The $^{13}C\{^1H\}$ NMR spectra of L^{4Cl} and [Cu(L^{4Cl})I] are consistent with their proposed structures. The ligand's spectrum displays resonances in the expected regions, with only minor shifts observed in the corresponding complex. Both spectra show 11 distinct carbon signals, confirming the symmetrical framework of these compounds (Fig. 3 and 5 Supp.). Collectively, these spectroscopic results validate the structural integrity of the ligand and its successful coordination with the Cu(I) center.

The UV-Visible spectrum of the [Cu(L^{4Cl})I] complex, recorded in DMF, shows a sharp and intense absorption band at 267 nm, while the other two features at 282 and 291 nm are very small and exhibit low absorption intensities (Fig. 6 Supp.).

The strong band at 267 nm is attributed to $\pi \rightarrow \pi^*$ transitions within the aromatic framework, whereas the weak peak at 282 nm arises from $n \rightarrow \pi^*$ transitions involving the non-bonding electrons of the azomethine linkages. The faint shoulder observed at 291 nm is assigned to a ligand-to-metal charge transfer (LMCT) transition from the Schiff-base donor orbitals to the vacant orbitals of the Cu(I) center. The stable coordination environment surrounding the Cu(I) core is supported by the low intensity of these latter bands, which represent the weak character of the corresponding transitions.



Scheme 1. Preparation of ligand L^{4Cl} and its corresponding complex [Cu(L^{4Cl})I]



Scheme 2. Preparation of 1,2,3-triazoles catalyzed by [Cu(L^{4Cl})I]

3.3. Catalytic activity studies

Following the successful synthesis and characterization of the [Cu(L^{4Cl})I] complex, and as part of our ongoing efforts to develop innovative approaches for heterocyclic synthesis [40–46], we discovered that [Cu(L^{4Cl})I] exhibits remarkable catalytic efficiency in the azide–alkyne cycloaddition, facilitating the formation of 1,2,3-triazoles. For optimization, the reaction between benzyl bromide, phenylacetylene, and sodium azide was selected as a model reaction.

The main factors affecting the model reaction for the synthesis of 1-benzyl-4-phenyl-1*H*-1,2,3-triazole (2a) are shown in Table 1. The control experiment (Entry 1) clarifies the need for the [Cu(L^{4Cl})I] catalyst, since its absence resulted in just a small amount of product, even at a high temperature of 100 °C and with an excess of sodium azide. This confirms that the cycloaddition is catalyzed by the Cu(I) complex and does not proceed *via* an uncatalyzed pathway. We initially compared the performance of our freshly synthesized [Cu(L^{4Cl})I] complex to that of commercially available copper(I) halides to demonstrate its worth (Entries 2−4). After two hours under the same circumstances (1 mol% catalyst, 2 mmol NaN_3, 100 °C), the product was obtained in moderate yields of 45%, 51%, and 55% for CuCl, CuBr, and CuI, respectively. In a shorter amount of time (1 hour), our [Cu(L^{4Cl})I] complex (Entry 5) produced a noticeably greater yield of 94%. The Schiff base ligand has a beneficial role in stabilizing the Cu(I) center, preventing aggregation, and facilitating the production of the crucial copper-acetylide intermediate in the catalytic cycle. It emerged that selecting the right solvent was crucial to attaining high efficiency (Entries 5−9). In organic solvents like toluene (30%), ethyl acetate (43%), acetonitrile (38%), and even ethanol (65%), the reaction did not progress well. In contrast, water afforded the highest yield of 94%, aligning with green chemistry principles by eliminating volatile organic solvents and simplifying the separation process. Additionally, the sodium azide stoichiometry was examined. Its decrease to 1.5 mmol (Entry 11) remained a good yield of 93%, suggesting that this was the ideal quantity of NaN_3, even if a greater amount (2 mmol, Entry 5) produced a 94% yield. A further reduction to 1.2 mmol decreased the yield to 75% (Entry 12), most likely as a result of inadequate concentration of the immediately produced benzyl azide that accelerated the cycloaddition to completion. At last, the impact of temperature was assessed.

A small amount of product was generated at ambient temperature, indicating a considerable temperature dependency of the reaction (Entry 13). At 60 °C (Entry 14), a modest yield of 80% was obtained; however, raising the temperature to 80 °C (Entry 15) produced the best results, yielding 93% in just one hour. This temperature provides the activation energy required by the catalytic cycle without consuming a significant amount of heat energy. Thus, according to Table 1's data, the ideal reaction conditions are as follows: a 1:1:1.5 molar ratio of phenylacetylene:benzyl bromide:NaN_3 in water at 80 °C, and a 1 mol% catalyst loading (Entry 15). These conditions afforded excellent yields while maintaining mild and sustainable reaction parameters.

We reacted a variety of benzyl bromides (1 mmol) with NaN_3 (1.5 mmol) and phenylacetylene (1 mmol) under ideal circumstances (1 mol% catalyst, H_2O, 80 °C). In 45–60 minutes, we obtained the respective 1,2,3-triazoles (2a–2e) with a substantial yield (89–93%) (Table 2). The catalytic system's efficiency with different benzyl bromides was impressive. Within an hour, the parent benzyl bromide produced the intended product 2a in an outstanding 93% yield. Significantly, benzyl bromides containing powerful electron-withdrawing species, including bromo (2b) and nitro (2c) substituents in the *para*-position, underwent even faster conversion, generating high yields of 90% and 92% in 45 minutes, respectively. This accelerated rate is due to the increased electrophilicity of the benzylic carbon, which facilitates the initial nucleophilic substitution by the azide ion to form benzyl azide. This observation suggests that the formation of benzyl azide is the rate-determining step.

As shown in Scheme 3, the copper(I)-catalyzed azide-alkyne cycloaddition (CuAAC) reaction follows a known route [47, 48]. A copper-acetylide complex (I) is formed when the Cu(I) species coordinates with the terminal alkyne, starting the catalytic cycle. The binding of the organic azide to the copper core occurs after this activation phase, producing an essential intermediate (II) that positions the reactants for cyclization. Ring closure results from the nucleophilic addition of the azide to the activated alkyl, producing intermediate (III). Following its conversion to intermediate (IV), this molecule is protonated in an aqueous environment, which regenerates the copper catalyst and yields the required 1,4-disubstituted 1,2,3-triazole [49−52].

Additionally, this procedure worked well for the synthesis of bis-triazoles 2d and 2e using different substrates, specifically *ortho*- and *meta*-xylylene dibromides. These reactions proceeded effectively in spite of the increased steric demand and functionality, producing the intended products in 89% and 91% yields, respectively, within 60 minutes. The durability and excellent efficiency of the [Cu(L^{4Cl})I] catalyst are demonstrated by the effective production of these bis-triazoles. To evaluate the catalyst's performance, the reaction parameters were analyzed and outcomes for producing 2a alongside previously reported methods (Table 3).

The findings demonstrate that our method is efficient for triazole synthesis, offering advantages regarding catalyst loading, reaction time, conditions, and product yield [47−52]. These findings demonstrate the importance of our study as the developed approach

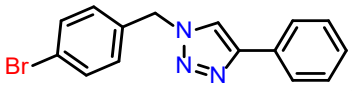
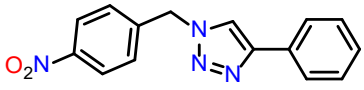
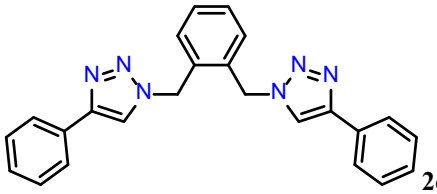
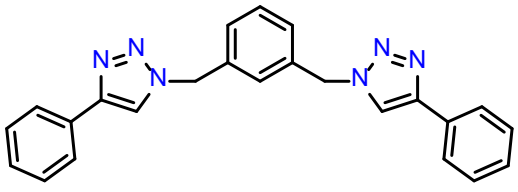
surpasses current protocols in terms of sustainability, operational ease, and overall performance, in addition to guaranteeing high efficiency in the synthesis of 1,2,3-triazoles.

Table 1. Optimized conditions

Entry	NaN_3 (mmol)	Catalyst (mol%)	Solvent	Conditions	Time (h)	Yield (%)
1	2	-	H_2O	Reflux	2	Trace
2	2	CuCl (1)	H_2O	Reflux	2	45
3	2	CuBr (1)	H_2O	Reflux	2	51
4	2	CuI (1)	H_2O	Reflux	2	55
5	2	[Cu(L^{4Cl})I] (1)	H_2O	Reflux	1	94
6	2	[Cu(L^{4Cl})I] (1)	MeCN	Reflux	1	38
7	2	[Cu(L^{4Cl})I] (1)	EtOAc	Reflux	1	43
8	2	[Cu(L^{4Cl})I] (1)	EtOH	Reflux	1	65
9	2	[Cu(L^{4Cl})I] (1)	PhMe	Reflux	1	30
10	2	[Cu(L^{4Cl})I] (0.5)	H_2O	Reflux	2	60
11	1.5	[Cu(L^{4Cl})I] (1)	H_2O	Reflux	1	93
12	1.2	[Cu(L^{4Cl})I] (1)	H_2O	Reflux	2	75
13	1.5	[Cu(L^{4Cl})I] (1)	H_2O	25 °C	2	Trace
14	1.5	[Cu(L^{4Cl})I] (1)	H_2O	60 °C	2	80
15	1.5	[Cu(L^{4Cl})I] (1)	H_2O	80 °C	1	93

[a] Conditions: phenylacetylene (1 mmol), benzyl bromide (1 mmol), NaN_3 (1.2–2 mmol), catalyst (0–1 mol%), solvent (3 mL)

Table 2. Preparation of 1,2,3-triazoles using [Cu(L^{4Cl})I][a]

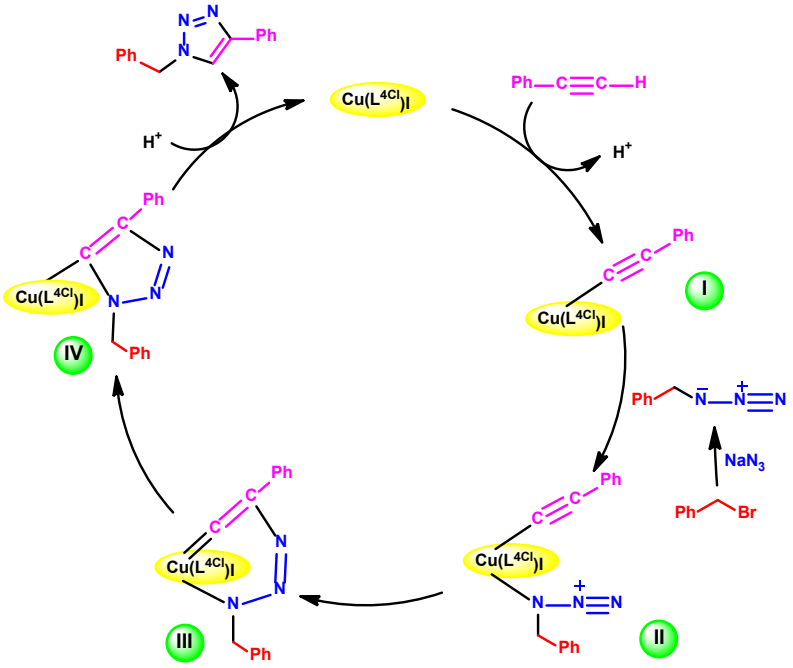
Entry	Triazole	Time (min.)	Yield (%)	TOF (h^{-1})[b]
1	 **2a**	60	93	93
2	 **2b**	45	90	120
3	 **2c**	45	92	123
4	 **2d**	60	89	89
5	 **2e**	60	91	91

[a] Conditions: phenylacetylene:benzyl bromides:NaN_3 (1:1:1.5), [Cu(L^{4Cl})I] (1 mol%), H_2O (3 mL), 80 °C
[b] TOF = (mmol of product) / [(mmol of catalyst) × (time)]

Table 3. Performance evaluation of **[Cu(L^{4Cl})I]** versus alternative catalysts in producing **2a**

Entry	Catalyst (mol%)	Solvent	Conditions	Time (h)	Yield (%)	TOF (h^{-1})	Ref.
1	Cu@βCD-PEG-mesoGO (5)	H_2O	r.t.	1	90	18	[47]
2	[$C_{20}H_{20}N_2$)PPh_3Cl] (15)	H_2O	45 °C	1	95	6.3	[48]
3	[$C_{20}H_{20}N_2$)PPh_3Br] (15)	H_2O	45 °C	1	92	6.1	[48]
4	GO-CO-NH-IA-Cu(I) (40)	EtOH:H_2O (1:1)	US, r.t.	0.13	94	18.1	[49]
5	[Cu(PN^{NTPh}–Ph)Cl] (0.25)	EtOH:H_2O (1:1)	60 °C	0.5	97	776	[50]
6	LCu (2)	H_2O	70 °C	0.33	98	148.5	[51]
7	Cu^{II}-Schiff base/SBA-15 (0.2)	H_2O	70 °C	12	97	40.4	[52]
8	[Cu(L^{4Cl})I] (1)	H_2O	80 °C	1	93	93	-[a]

[a] This work



Scheme 3. Proposed mechanism for the preparation of 1,2,3-triazoles mediated by [Cu(L^{4Cl})I]

4. Conclusion

In the conclusion section, you remind the reader of wh In this study, a copper(I) complex was successfully synthesized by reacting a bidentate Schiff base ligand (L^{4Cl}) with CuI. The ligand and its corresponding complex were characterized using elemental analysis, FT-IR, and NMR spectroscopy, confirming their structural integrity. The catalytic efficiency of the complex was assessed for the synthesis of 1,2,3-triazole derivatives *via* azide-alkyne cycloaddition under mild conditions. The findings suggest that this Cu(I) complex is a highly active and economical catalyst for click chemistry. Importantly, the current method overcomes key limitations associated with traditional, expensive catalysts, such as low yields, excessive catalyst loading, and harsh reaction conditions. In the future, this approach could be further explored for the scalable synthesis of biologically active triazole derivatives and their potential application in drug development.

Supplementary files

Supplementary file 1.

Acknowledgements

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