

Formal Insertion of Imines (or Nitrogen Heteroarenes) and Arynes into the C–Cl Bond of Carbon Tetrachloride

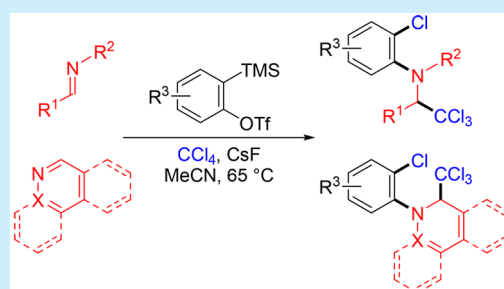
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S Supporting Information

ABSTRACT: The formal insertion of double and triple bonds into the C–Cl bond of carbon tetrachloride has enabled the full utilization of carbon tetrachloride in chemical synthesis. A range of unactivated imines and electron-deficient nitrogen heteroarenes served as effective sources of C=N bonds to react with arynes and carbon tetrachloride to afford functionalized anilines whose core structures are present in some valuable arthropodocides. Control experiments and DFT calculations suggest the involvement of a trichloromethyl anion intermediate.



Carbon tetrachloride is an inexpensive bulk chemical that was formerly used in fire extinguishers, as a dry cleaning solvent, and as a precursor to refrigerants.¹ Although carbon tetrachloride frequently serves as a solvent in chemical reactions and spectroscopic analysis, it is capable of participating in some chemical reactions under certain conditions. Carbon tetrachloride serves as a chlorinating agent in the Appel reaction² or as a source of dichloromethylene group in carbonyl olefination³ as well as in olefin cyclopropanation.⁴ In addition, both the chlorine and trichloromethyl groups of carbon tetrachloride can be incorporated into the target compounds through the formal insertion of olefins^{5,6} or strained rings⁷ into the C–Cl bond (Scheme 1a). Such a transformation greatly facilitates the

nitrogen heteroarenes, providing convenient access to structurally diverse polychlorinated aniline derivatives whose core structures are present in some arthropodocides for both agricultural and home applications (Figure 1).⁹

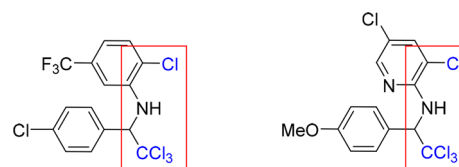
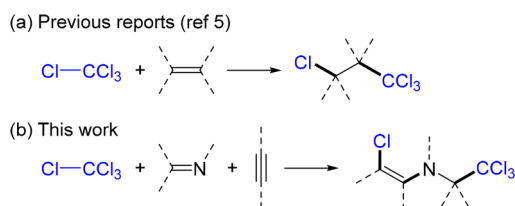


Figure 1. Representative arthropodocides for both agricultural and home applications.

Scheme 1. Formal Insertion of Unsaturated Bonds into the C–Cl Bond of Carbon Tetrachloride

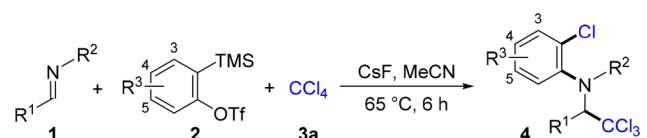


preparation of polychlorinated compounds with broad-spectrum bioactivities.⁸ Herein, we report a new strategy for the full utilization of carbon tetrachloride in chemical synthesis through the formal insertion of C=N and C≡C bonds into the C–Cl bond under mild conditions (Scheme 1b). Importantly, the three-component reaction is applicable to various C=N bonds in both unactivated imines and electron-deficient

During our recent exploration of the chemistry of imines activated by arynes,^{10–13} we unexpectedly found that a three-component mixture of imine **1a**, 2-(trimethylsilyl)phenyl triflate (**2a**) (as a benzyne precursor), and carbon tetrachloride (**3a**) in the presence of CsF proceeded in acetonitrile at 65 °C to afford polychlorinated compound **4a** in 87% yield (Table 1, entry 1). This three-component reaction involves an unprecedented formal insertion of an imine and an aryne into the C–Cl bond of carbon tetrachloride. The reaction did not occur when replacing CsF with other fluoride sources (e.g., NaF, KF, ZnF₂, NH₄F, and tetrabutylammonium fluoride) or replacing acetonitrile with some other solvents such as tetrahydrofuran, 1,4-dioxane, 1,2-dichloroethane, dimethyl sulfoxide, and *N,N*-dimethylformamide.

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Table 1. Three-Component Reaction of Imines, Arynes, and Carbon Tetrachloride^a


entry	1, R ¹ , R ²	2, R ³	4	yield (%) ^b
1	1a, PMP, Me	2a, H	4a	87
2 ^c	1b, Ph, Me	2a, H	4b	86
3	1c, 4-FC ₆ H ₄ , Me	2a, H	4c	95
4	1d, 4-ClC ₆ H ₄ , Me	2a, H	4d	85
5	1e, 4-BrC ₆ H ₄ , Me	2a, H	4e	86
6	1f, 3-MeOC ₆ H ₄ , Me	2a, H	4f	68
7	1g, 2-MeOC ₆ H ₄ , Me	2a, H	4g	59
8	1h, cyclohexyl, Me	2a, H	4h	74
9	1i, PMP, ^t Bu	2a, H	4i	81
10	1j, PMP, allyl	2a, H	4j	76
11	1k, PMP, propargyl	2a, H	4k	66
12	1l, PMP, ⁱ Pr	2a, H	4l	75
13	1m, PMP, PMP	2a, H	4m	65
14	1a, PMP, Me	2b, 3-OMe	4n	91
15 ^d	1a, PMP, Me	2c, 4-Me	4o + 4o'	87
16	1a, PMP, Me	2d, 4,5-(OMe) ₂	4p	81
17	1a, PMP, Me	2e, 4,5-F ₂	4q	40

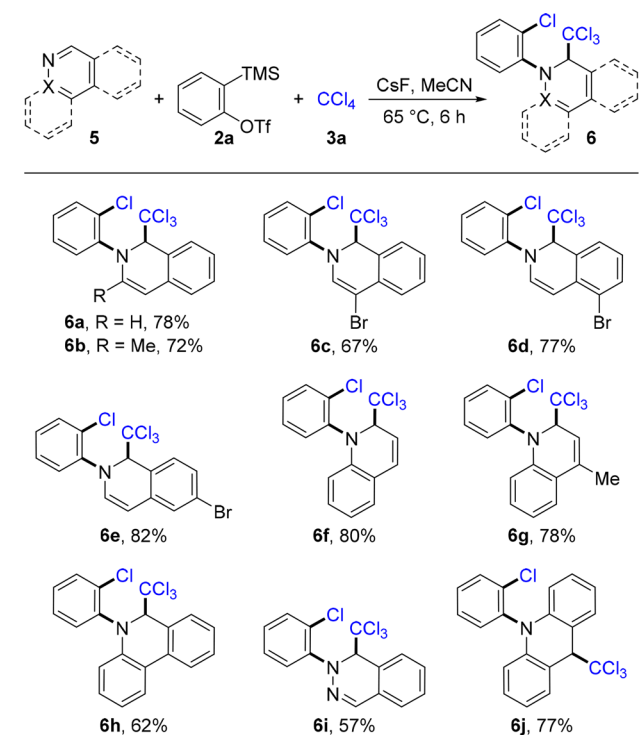
^aReaction conditions: **1** (0.10 mmol), **2** (0.15 mmol), **3a** (0.15 mL), CsF (0.30 mmol), acetonitrile (0.20 mL), 65 °C, 6 h. ^bIsolated yield.

^cThe structure of **4b** was unambiguously confirmed by X-ray crystallography (CCDC 1840926). ^dRatio **4o** (R³ = 4-Me)/**4o'** (R³ = 5-Me) = 43:57.

Then, we investigated the reaction scope under the optimized reaction conditions (Table 1). A range of aromatic and aliphatic imines smoothly underwent the three-component reaction with benzyne precursor **2a** and carbon tetrachloride (**3a**) to afford structurally diverse 2-chloro-*N*-(2,2,2-trichloroethyl)anilines in good to excellent yields (entries 1–13). It is noteworthy that the *N*-substituents could be alkyl groups, an allyl group, a propargyl group, and an aryl group. The reaction was successfully extended to a few 2-(trimethylsilyl)aryl triflates bearing either electron-donating or -withdrawing groups (entries 14–17). The regioselectivity was found to depend highly on the nature and position of the substituents in the in situ-generated unsymmetrical aryne. In line with previous studies,^{12d} the reaction with 4-methylbenzyne gave poor regioselectivity (entry 15), and in sharp contrast, a single regioisomer was obtained from the reaction with 3-methoxybenzyne (entry 14).

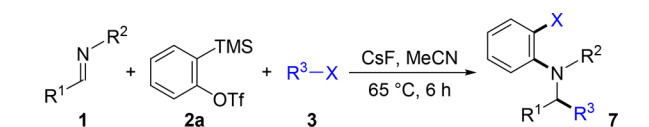
In addition to the unactivated imines, electron-deficient nitrogen heteroarenes also served as effective sources of C=N bonds in the three-component reaction through dearomatization under the standard conditions.¹⁴ As demonstrated by the results shown in Scheme 2, isoquinoline, quinoline, phenanthridine, and phthalazine smoothly participated in the three-component reaction with benzyne precursor **2a** and carbon tetrachloride (**3a**) to afford a range of functionalized nitrogen-containing heterocycles in moderate to good yields. Interestingly, acridine participated in the three-component reaction through the 1,4-addition rather than the 1,2-addition (Scheme 2, **6j**).

Replacing carbon tetrachloride with some other organohalides was surveyed in the three-component reaction with

Scheme 2. Three-Component Reaction of Nitrogen Heteroarenes, Benzyne, and Carbon Tetrachloride^{a,b}

^aReaction conditions: **5** (0.10 mmol), **2a** (0.15 mmol), **3a** (0.15 mL), CsF (0.30 mmol), acetonitrile (0.20 mL), 65 °C, 6 h. ^bIsolated yields.

imines and benzyne precursor **2a** under the standard conditions (Table 2). We found that the C–Cl bond of

Table 2. Three-Component Reaction of Imines, Benzyne, and Organohalides^a


entry	1, R ¹ , R ²	3, R ³ , X	7	yield (%) ^b
1 ^c	1a, PMP, Me	3b, CCl ₂ CN, Cl	7a	23
2 ^d	1a, PMP, Me	3c, CBr ₃ , Br	7b	30
3	1h, cyclohexyl, Me	3d, CF ₂ CO ₂ Et, Br	7c	32

^aReaction conditions: **1** (0.10 mmol), **2a** (0.15 mmol), **3** (0.30 mmol), CsF (0.30 mmol), acetonitrile (0.20 mL), 65 °C, 6 h.

^bIsolated yield. ^cUsing **3b** (1.0 mmol). ^dReaction carried out at rt.

trichloroacetonitrile (**3b**) and the C–Br bonds of carbon tetrabromide (**3c**) and ethyl bromodifluoroacetate (**3d**) were subjected to the formal insertion of C=N and C≡C bonds. The yields are far from satisfactory due to the low conversion of the imines. Moreover, the three-component reaction failed to occur with some other organohalides such as BrCCl₃, C₂Cl₆, PhC≡CX (X = Cl, Br, I), and *N*-halosuccinimides (NXS, X = Cl, Br, I).

When 2 and 10 equiv of 2,2,6,6-tetramethyl-1-piperidinyloxy (TEMPO) were added to the reaction mixture of imine **1a**, benzyne precursor **2a**, and carbon tetrachloride (**3a**) under the standard conditions, desired product **4a** was obtained in 62 and 50% yields, respectively (Scheme 3). Considering that a large excess of the radical scavenger (TEMPO) failed to

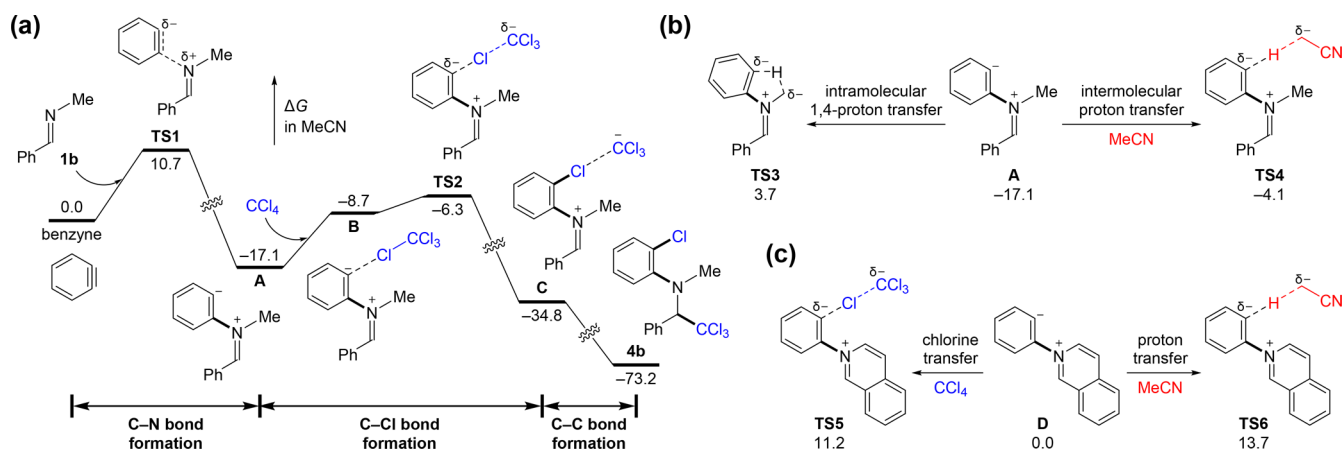
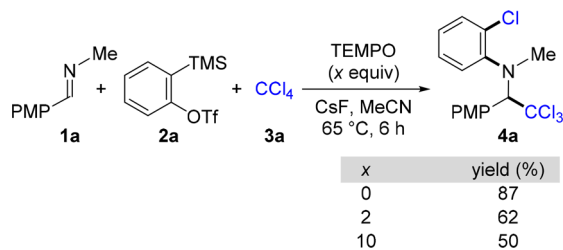


Figure 2. (a) Gibbs energy profile for the reaction of imine **1b**, benzyne, and carbon tetrachloride in MeCN at 298 K. (b) Intra- and intermolecular proton transfer pathways for intermediate **A**. (c) Chlorine and proton transfer pathways for intermediate **D**. Relative Gibbs energies are reported in kcal/mol. Computed at the SMD(MeCN)/M06-2X/maug-cc-pVTZ//SMD(MeCN)/M06-2X/6-31+G(d,p) level.

Scheme 3. Control Experiments^{a,b}



^aReaction conditions: **1a** (0.10 mmol), **2a** (0.15 mmol), **3a** (0.15 mL), CsF (0.30 mmol), TEMPO (0.10x mmol, x = 0, 2, 10), acetonitrile (0.20 mL), 65 °C, 6 h. ^bIsolated yield.

completely inhibit the desired three-component reaction, we ruled out the radical mechanism, which was proposed previously in the formal insertion of olefins into the C–Cl bond of carbon tetrachloride.⁵

To shed more light on the reaction mechanism, we performed DFT (M06-2X¹⁵) calculations on the reaction of imine **1b**, benzyne, and carbon tetrachloride (Figure 2a).¹⁶ The reaction starts with the nucleophilic addition of imine **1b** to benzyne via transition state **TS1**, generating aryl anion intermediate **A**. Then, **A** may interact with carbon tetrachloride to form transient halogen-bonded complex **B**.¹⁷ Subsequently, an S_N2 process takes place at the chlorine center via transition state **TS2**, generating ion pair **C** consisting of an iminium cation and a trichloromethyl anion.¹⁸ The Gibbs energy of activation for such a chlorine transfer process is 10.8 kcal/mol. Finally, a barrierless nucleophilic addition of the trichloromethyl anion to the iminium cation occurs, leading to the formation of final product **4b**.

In addition to the reaction pathway mentioned above, there are two competing pathways for aryl anion **A** (Figure 2b). One is the intramolecular 1,4-proton transfer via transition state **TS3** (the Gibbs energy of activation is 20.8 kcal/mol).^{11,12h} The other is the intermolecular proton abstraction from MeCN via transition state **TS4** (the Gibbs energy of activation is 13.0 kcal/mol).^{10,11} In comparison to the chlorine transfer, these two proton transfer processes¹⁹ are both kinetically disfavored.¹⁶ To verify whether the same conclusions hold for nitrogen heteroarenes, we performed additional DFT calculations by using isoquinoline as a representative example of

nitrogen heteroarenes (Figure 2c). In this case, we found that the chlorine transfer from CCl₄ via transition state **TS5** is also kinetically favored over the proton transfer from CH₃CN via transition state **TS6** (by 2.5 kcal/mol). Because of the ease of these chlorine transfer processes, we envision that the reaction of carbanions with carbon tetrachloride may be used to design new synthetic methodologies.

In summary, we have established a new strategy for the full utilization of carbon tetrachloride in chemical synthesis through the formal insertion of C=N and C≡C bonds into the C–Cl bond under mild conditions. With 2-(trimethylsilyl)aryl triflates as arylene precursors, a range of unactivated imines smoothly reacted with arynes and carbon tetrachloride to afford structurally diverse 2-chloro-*N*-(2,2,2-trichloroethyl)anilines in moderate to excellent yields. Moreover, electron-deficient nitrogen heteroarenes could serve as alternative sources of C=N bonds in the three-component reaction through dearomatization. DFT calculations indicate that the reaction takes place through successive C–N, C–Cl, and C–C bond formations.

■ ASSOCIATED CONTENT

Supporting Information

The Supporting Information is available free of charge on the ACS Publications website at DOI: 10.1021/acs.orglett.8b01845.

Experimental procedures, characterization data, copies of ¹H and ¹³C NMR spectra, X-ray crystallographic data, and computational details (PDF)

Accession Codes

CCDC 1840926 contains the supplementary crystallographic data for this paper. These data can be obtained free of charge via www.ccdc.cam.ac.uk/data_request/cif, or by emailing data_request@ccdc.cam.ac.uk, or by contacting The Cambridge Crystallographic Data Centre, 12 Union Road, Cambridge CB2 1EZ, UK; fax: +44 1223 336033.

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Notes

The authors declare no competing financial interest.

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