ChemComm

ROYAL SOCIETY OF CHEMISTRY

COMMUNICATION

View Article Online
View Journal | View Issue

Check for updates

Cite this: *Chem. Commun.*, 2021, 57, 8429

Received 30th June 2021,
Accepted 27th July 2021

DOI: 10.1039/d1cc03496k

rsc.li/chemcomm

Photoinduced transition-metal and external photosensitizer free cross-coupling of aryl triflates with trialkyl phosphites†

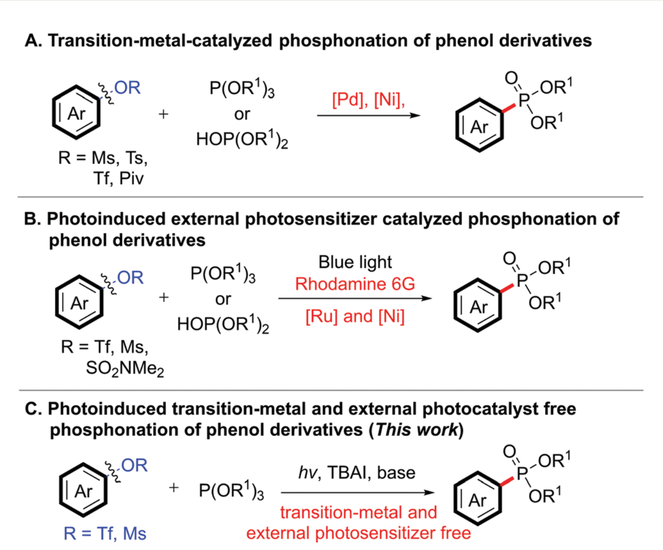
Qian Dou,[ab] Li Geng,[b] Bin Cheng,*[a] Chao-Jun Li *[c] and Huiying Zeng *[b]

Photoinduced phosphonation of aryl triflates with trialkyl phosphites *via* a tandem single-electron-transfer, C–O bond cleavage and Arbuzov rearrangement process in the absence of transition-metal and external photosensitizer is reported herein. The protocol features good functional group compatibility and mild reaction conditions, providing various aryl phosphates in good to high yields. Furthermore, this strategy allows the late-stage phosphonation of complex and biologically active compounds.

Phenols, widely existing in renewable biomasses such as lignin on Earth, are abundant aromatic feedstocks and important fine chemicals.[1] The chemical transformation of phenols has become a hot topic in the field of organic synthesis.[2] However, due to a highly reactive hydroxyl group and a very inert C–O bond with high bond dissociation energy (BDE), it is still a challenge to directly convert phenols *via* C–O bond cleavage. For this reason, pre-activation of phenols into phenol derivatives (*e.g.*, sulfonates, esters, carbamates, ethers and metal salts) fully eliminates the acidity of the hydroxyl group and effectively weakens the C–O bond with transition-metal. Consequently, catalytic C–O bond cleavage has emerged as the powerful strategy for the transformation of pre-activated phenols to high value-added products.[3]

Arylphosphonates, as an important class of organophosphorus compounds, have extensive applications in medicine,[4] material science[5] and organic synthesis.[6] Transition-metal-catalyzed cross-coupling of aryl halides with simple phosphorus reagents including dialkyl phosphites and trialkyl phosphites has been well developed to access arylphosphonates.[7] Phenol derivatives, being a class of aromatic electrophiles, have served as efficient and sustainable alternatives to aryl halides in the transition-metal-catalyzed phosphonation *via* C–O bond cleavage (Scheme 1A).[8] Successively, photoinduced external photosensitizers-catalyzed cross-couplings of phenolic sulfonates with phosphorus reagents *via* SET process have been realized by König's[9] and Yu's groups,[10] respectively (Scheme 1B).

On the other hand, in terms of greenness, operational simplicity and product purification, photoinduced transition-metal and external photosensitizer free cross-coupling reactions provide a more attractive strategy for carbon–carbon and carbon–heteroatom bond cross-couplings.[11] Recently, our group reported light-enabled borylation and iodination of aryl triflates *via* direct C–O bond cleavage in absence of catalyst.[12] Herein, as a part of our ongoing research on transformation of phenol derivatives *via* C–O bond activation,[13] photo-induced transition-metal and external photosensitizer free phosphonation of aryl triflates is reported (Scheme 1C).



Scheme 1 Methods for phosphonation of phenol derivatives *via* C–O bond cleavage.

---

[a] *Institute of Marine Biomedicine, Shenzhen Polytechnic, Shenzhen 518055, China. E-mail: chengbin@szpt.edu.cn*

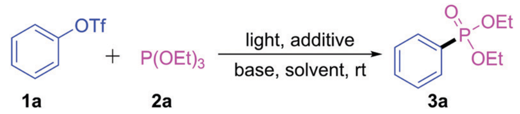
[b] *The State Key Laboratory of Applied Organic Chemistry and College of Chemistry and Chemical Engineering, Lanzhou University, 222 Tianshui Road, Lanzhou, 730000, China. E-mail: zenghy@lzu.edu.cn*

[c] *Department of Chemistry and FQRNT Centre for Green Chemistry and Catalysis, McGill University, 801 Sherbrooke St. West, Montreal, Quebec H3A 0B8, Canada. E-mail: cj.li@mcgill.ca*

† Electronic supplementary information (ESI) available. See DOI: 10.1039/d1cc03496k

To investigate the conceived phosphonation of aryl triflates *via* photo-induced C–O bond cleavage, phenyl triflate (**1a**) and triethyl phosphate (**2a**) were selected as standard substrates. Our preliminary attempt with a mixture of 0.1 mmol **1a**, 0.4 mmol **2a** and NaI (0.5 equiv.) in acetonitrile (1.0 mL) under argon, which was irradiated by 254 nm light, gave the desired product **3a** in 16% yield (Table 1, entry 1). Encouraged by this result, various bases were tested. When organic bases, such as Et_3N, DIPEA and DBU were used, the yield of **3a** was enhanced to 30% (entries 2–4). Compared to organic bases, inorganic bases provided superior yields of **3a**, up to 63% yield when K_2CO_3 was used (entries 5–8). Conducting the reaction without NaI caused a significant inhibition on the product formation, which indicated that iodide salt was crucial for this reaction (entry 9). Thus, other iodide salts, such as KI, LiI and TBAI, were explored (entries 10–12), increasing the yield to 67% with TBAI (entry 12). Then, other solvents including DMF, EtOAc and THF were examined, and all showed lower efficiency than CH_3CN (entries 13–15). Increasing or reducing the amount of TBAI did not improve the formation of **3a** (entries 16 and 17). Adjusting the loading of K_2CO_3 resulted in a slightly lower yield (entries 18 and 19). When the reaction of **1a** (0.1 mmol) and **2a** (0.3 mmol) was performed in CH_3CN (0.5 mL), the C–P bond formation product **3a** was obtained in 71% NMR yield and 66% isolated yield (entry 20). No product was detected when the reaction mixture was either irradiated by blue LED or run in the dark, suggesting that the light (254 nm) is indispensable in this phosphonation process (entries 21 and 22). Notably, when 5.0 μL H_2O was added into the reaction system, we obtained 68% yield indicating that this reaction is not sensitive to water (entry 23). However, the yield was reduced to 52% when the reaction was performed under air atmosphere (entry 24).

Table 1 Optimization of the reaction conditions[a]



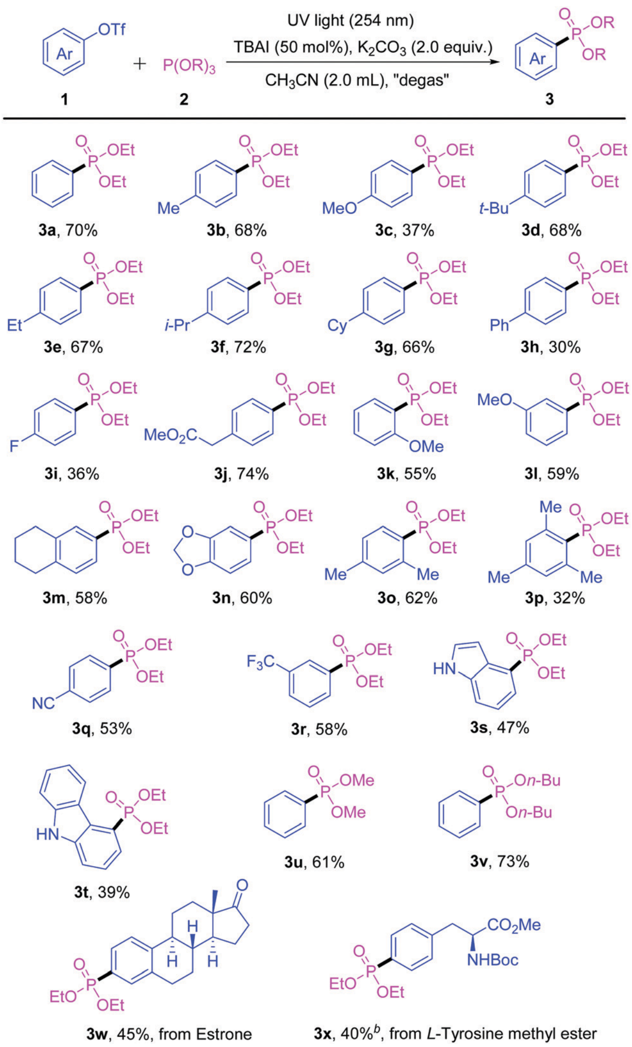
Entry	Base	Solvent	Additive	Yield[b] (%)
1	—	CH_3CN	NaI	16
2	Et_3N	CH_3CN	NaI	19
3	DIPEA	CH_3CN	NaI	29
4	DBU	CH_3CN	NaI	30
5	KF	CH_3CN	NaI	37
6	CsF	CH_3CN	NaI	48
7	Cs_2CO_3	CH_3CN	NaI	57
8	K_2CO_3	CH_3CN	NaI	63
9	K_2CO_3	CH_3CN	—	7
10	K_2CO_3	CH_3CN	KI	63
11	K_2CO_3	CH_3CN	LiI	60
12	K_2CO_3	CH_3CN	TBAI	67
13	K_2CO_3	DMF	TBAI	35
14	K_2CO_3	EtOAc	TBAI	16
15	K_2CO_3	THF	TBAI	37
16[c]	K_2CO_3	CH_3CN	TBAI	54
17[d]	K_2CO_3	CH_3CN	TBAI	60
18[e]	K_2CO_3	CH_3CN	TBAI	61
19[f]	K_2CO_3	CH_3CN	TBAI	63
20[g]	**K_2CO_3**	**CH_3CN**	**TBAI**	**71(66)**
21[gh]	K_2CO_3	CH_3CN	TBAI	n.r.
22[gi]	K_2CO_3	CH_3CN	TBAI	n.r.
23[gj]	K_2CO_3	CH_3CN	TBAI	68
24[gk]	K_2CO_3	CH_3CN	TBAI	52

[a] General conditions: **1a** (0.1 mmol), **2a** (0.4 mmol), base (2.0 equiv.), additive (0.5 equiv.), and solvent (1.0 mL) were irradiated by UV light (254 nm) for 24 h under argon atmosphere. [b] Yields were determined by ^{31}P NMR using trimethyl phosphate as an internal standard; isolated yield was shown in parentheses. [c] TBAI (0.25 equiv.). [d] TBAI (1.0 equiv.). [e] K_2CO_3 (1.5 equiv.). [f] K_2CO_3 (3.0 equiv.). [g] **2a** (0.3 mmol), CH_3CN (0.5 mL). [h] Blue LED. [i] In the dark. [j] 5.0 μL H_2O was added. [k] Under air atmosphere.

With the optimized reaction conditions established, the scope of this phosphonation was explored with 0.2 mmol scale of aryl triflates **1** and 3.0 equiv. of trialkyl phosphites under argon using 2.0 equiv. of K_2CO_3 as base and 0.5 equiv. of TBAI as additive in CH_3CN (1.0 mL), irradiated by light (254 nm). The phosphonation product **3a** was obtained in 70% isolated yield. A variety of aryl triflates equipped with different substituents on the aryl ring realized the phosphonation smoothly. The substrates bearing electron-donating groups including methyl, methoxyl, *tert*-butyl, ethyl, isopropyl and cyclohexyl were efficiently converted to the desired products **3b–3g** in moderate to high yields. Notably, π-extended aryl triflate **1h** was also found to successfully engage in this photoinduced phosphonation, affording the corresponding product **3h** with moderate yield. Besides halogen group such as F, the ester group was also tolerated, and the desired products **3i–3j** were formed in 36% and 74% yields, respectively. The phosphonation proceeded with similar efficiency when methoxyl substituted at *ortho*- or *meta*-position of aromatic ring, and the desired products **3k–3l** were generated in good yields. Tetrahydronaphthol derivative, as well as sesamol derivative, could be phosphonated under standard conditions, providing the corresponding products **3m–3n** in good yields. The reaction showed marked steric effect when 2,4-dimethyl and 2,4,6-trimethyl substituted substrates were investigated, generating the phosphonated product **3o** in good yield for the former but only moderate yield for the latter (**3p**). Aryl triflates bearing strong electron-withdrawing groups (CF_3 or CN) also gave the corresponding products **3q** and **3r** with moderate to good yields. Hetero-aromatic triflates, such as indole or carbazole triflate derivatives, could also be cross-coupled with triethyl phosphite, giving the phosphonated products **3s–3t** in moderate yields. For trialkyl phosphites, trimethyl phosphite and tributyl phosphite also reacted well, generating the desired aryl phosphates **3u–3v** in good yields under standard conditions. Furthermore, we further explored this transition-metal and external photocatalyst free process on the late-stage modification of biologically active phenolic compounds to avoid trace metal residues. Aryl triflate **1w** derived from estrone was efficiently converted into phosphonated product **3w** with 45% yield under standard conditions. The L-tyrosinate derivative, bearing an ester group and an amino group, also successfully generated the desired product **3x** in a moderate yield when 4.0 equiv. of K_2CO_3 was used (Table 2).

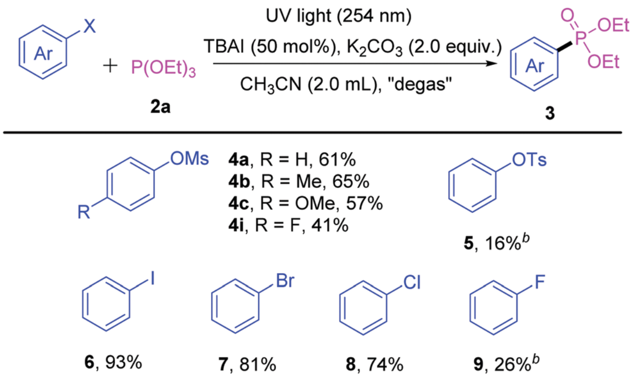
In addition, the reactivity of other aryl electrophiles was also investigated under standard conditions (Table 3). Aryl mesylates (**4a–4c**, **4i**) have similar reactivity to aryl triflates, and

Table 2 Photo-induced Arbuzov-type reaction of aryl triflates with trialkyl phosphites[a]

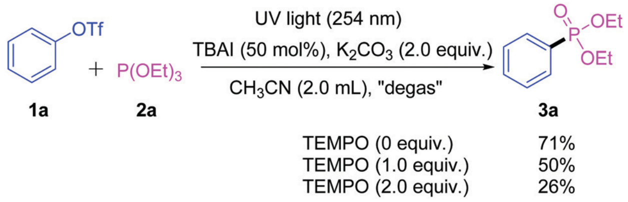


[a] General conditions: **1** (0.2 mmol), **2** (0.6 mmol), K_2CO_3 (2.0 equiv.), TBAI (0.5 equiv.), and CH_3CN (1.0 mL) were irradiated by UV light (254 nm) for 24 h under argon atmosphere; isolated yields were given. [b] K_2CO_3 (4.0 equiv.).

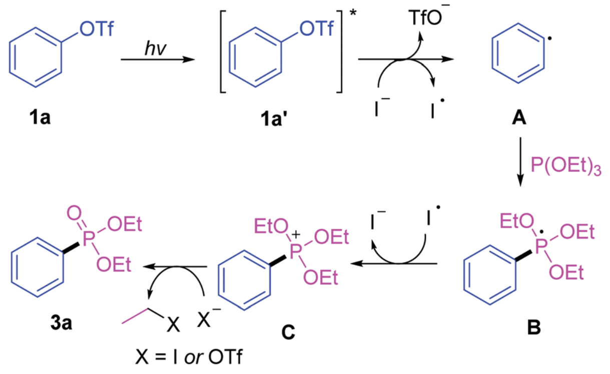
Table 3 Photo-induced Arbuzov-type reaction of various aryl electrophiles with triethyl phosphate[a]



[a] General conditions: aryl electrophile (0.2 mmol), **2a** (0.6 mmol), K_2CO_3 (2.0 equiv.), TBAI (0.5 equiv.), and CH_3CN (1.0 mL) were irradiated by UV light (254 nm) for 24 h under argon atmosphere; isolated yields were given. [b] Yields were determined by ^{31}P NMR using trimethyl phosphate as an internal standard.



Scheme 2 Radical trapping experiments.



Scheme 3 Tentative mechanism.

could also be phosphonated *via* C–O bond activation by this photoinduced strategy. When phenyl tosylate (**5**) was applied as aryl electrophile, it gave the product **3a**. It is interesting to note that aryl halides, such as iodobenzene (**6**), bromobenzene (**7**) and chlorobenzene (**8**), showed excellent reactivity, affording the product **3a** up to 93% yield. Despite high bond dissociation energy of unactivated C(sp^2)–F, fluorobenzene (**9**) was also phosphonated with 26% yield *via* C–F bond cleavage.[11r]

To gain insight into the reaction mechanism, radical trapping experiments were carried out with 2,2,6,6-tetramethylpiperidin-1-oxyl (TEMPO) as radical quencher under standard conditions (Scheme 2). The yield of phosphonated product **3a** was gradually decreased with increasing the amount of TEMPO.

Based on the above results of radical trapping experiments and reported work,[12] a plausible mechanism was proposed in Scheme 3. The phenyl triflate **1a** is irradiated by light to form excited-state **1a′**, which undergoes SET process with iodine anion to form phenyl radical **A** and iodine free radical. The radical **A** is captured by triethyl phosphite, providing an unstable P-centered radical **B**,[14] followed by further oxidation by iodine free radical to form phosphorous cation **C**. The cation **C** undergoes Arbuzov-type rearrangement[15] to generate the desired product **3a** and ethyl iodide or ethyl trifluoromethane-sulfonate.

In conclusion, we have developed a photoinduced catalyst-free transformation of pre-activated phenols into arylphosphonate *via*

C–O cleavage. This aromatic Arbuzov-type reaction proceeded at room temperature with broad substrate scope in moderate to good yields in the absence of transition-metal and external photosensitizer. In addition, the method has been successfully employed in the late-stage phosphonation of biologically active phenolic compounds. The mechanistic investigations show that the reaction involves SET process, radical formation and Arbuzov-type rearrangement. This method provides a promising pathway for green synthesis of arylphosphorous compounds without external transition-metal catalysts or photosensitizer under mild conditions. The chemical transformations of other aryl electrophiles are underway in our laboratory.

We thank the NSFC (21971093), the International Joint Research Centre for Green Catalysis and Synthesis (grant no. 2016B01017 and 18JR4RA003), the 111 project and Post-doctoral Foundation Project of Shenzhen Polytechnic (6021330006K) for support of our research. We also thank the Canada Research Chair (Tier I) foundation, the E. B. Eddy Endowment Fund, the CFI, NSERC, and FQRNT to C.-J. Li.

Conflicts of interest

There are no conflicts to declare.

Notes and references

1 (*a*) J. Zakzeski, P. C. A. Bruijnincx, A. L. Jongerius and B. M. Weckhuysen, *Chem. Rev.*, 2010, **110**, 3552–3599; (*b*) W. Schutyser, T. Renders, S. Van den Bosch, S. F. Koelewijn, G. T. Beckham and B. F. Sels, *Chem. Soc. Rev.*, 2018, **47**, 852–908.

2 (*a*) H. Zeng, Z. Qiu, A. Domínguez-Huerta, Z. Hearne, Z. Chen and C.-J. Li, *ACS Catal.*, 2017, **7**, 510–519; (*b*) Z. Qiu, H. Zeng and C.-J. Li, *Acc. Chem. Res.*, 2020, **53**, 2395–2413.

3 (*a*) D.-G. Yu, B.-J. Li and Z.-J. Shi, *Acc. Chem. Res.*, 2010, **43**, 1486–1495; (*b*) B. M. Rosen, K. W. Quasdorf, D. A. Wilson, N. Zhang, A.-M. Resmerita, N. K. Garg and V. Percec, *Chem. Rev.*, 2011, **111**, 1346–1416; (*c*) J. Cornella, C. Zarate and R. Martin, *Chem. Soc. Rev.*, 2014, **43**, 8081–8097; (*d*) B. Su, Z.-C. Cao and Z.-J. Shi, *Acc. Chem. Res.*, 2015, **48**, 886–896; (*e*) M. Tobisu and N. Chatani, *Acc. Chem. Res.*, 2015, **48**, 1717–1726.

4 (*a*) K. Yoshino, T. Kohno, T. Morita and G. Tsukamoto, *J. Med. Chem.*, 1989, **32**, 1528–1532; (*b*) E. A. Wydysh, S. M. Medghalchi, A. Vadlamudi and C. A. Townsend, *J. Med. Chem.*, 2009, **52**, 3317–3327; (*c*) X. Chen, D. J. Kopecky, J. Mihalic, S. Jeffries, X. Min, J. Heath, J. Deignan, S. Lai, Z. Fu, C. Guimaraes, S. Shen, S. Li, S. Johnstone, S. Thibault, H. Xu, M. Cardozo, W. Shen, N. Walker, F. Kayser and Z. Wang, *J. Med. Chem.*, 2012, **55**, 3837–3851; (*d*) G. Németh, Z. Greff, A. Sipos, Z. Varga, R. Székely, M. Sebestyén, Z. Jászay, S. Béni, Z. Nemes, J.-L. Pirat, J.-N. Volle, D. Virieux, Á. Gyuris, K. Kelemenics, É. Áy, J. Minarovits, S. Szathmary, G. Kéri and L. Őrfi, *J. Med. Chem.*, 2014, **57**, 3939–3965.

5 T. Baumgartner and R. Réau, *Chem. Rev.*, 2006, **106**, 4681–4727.

6 (*a*) P. E. Goudriaan, P. W. N. M. van Leeuwen, M.-N. Birkholz and J. N. H. Reek, *Eur. J. Inorg. Chem.*, 2008, 2939–2958; (*b*) J. C. Zhang, S. X. Cao, X. L. Yang and Y. F. Zhao, *Chin. Chem. Lett.*, 2004, **15**, 646–648; (*c*) W. Yang, B. Li, M. Zhang, S. Wang, Y. Ji, S. Dong, J. Feng and S. Yuan, *Chin. Chem. Lett.*, 2020, **31**, 1313–1316; (*d*) Y.-C. Wang, L.-Q. Liu, G.-M. Wang, H. Ouyang and Y.-J. Li, *Green Chem.*, 2018, **20**, 604–608; (*e*) Y.-Y. Xie, Y.-C. Wang, Y. He, D. C. Hu, H. S. Wang and Y.-M. Pan, *Green Chem.*, 2017, **19**, 656–659.

7 (*a*) T. Hirao, T. Masunaga, Y. Ohshiro and T. Agawa, *Synthesis*, 1981, 56–57; (*b*) M. Kalek, A. Ziadi and J. Stawinski, *Org. Lett.*, 2008, **10**, 4637–4640; (*c*) D. Gelman, L. Jiang and S. L. Buchwald, *Org. Lett.*, 2003, **5**, 2315–2318; (*d*) A. J. Bloomfield and S. B. Herzon, *Org. Lett.*, 2012, **14**, 4370–4373; (*e*) E. L. Deal, C. Petit and J.-L. Montchamp, *Org. Lett.*, 2011, **13**, 3270–3273; (*f*) X. Zhang, H. Liu, X. Hu, G. Tang, J. Zhu and Y. Zhao, *Org. Lett.*, 2011, **13**, 3478–3481; (*g*) C. Huang, X. Tang, H. Fu, Y. Jiang and Y. Zhao, *J. Org. Chem.*, 2006, **71**, 5020–5022; (*h*) J.-L. Montchamp and Y. R. Dumond, *J. Am. Chem. Soc.*, 2001, **123**, 510–511; (*i*) Y.-L. Zhao, G.-J. Wu, Y. Li, L.-X. Gao and F.-S. Han, *Chem. – Eur. J.*, 2012, **18**, 9622–9627; (*j*) K. Xu, F. Yang, G. Zhang and Y. Wu, *Green Chem.*, 2013, **15**, 1055–1060.

8 (*a*) G. Yang, C. Shen, L. Zhang and W. Zhang, *Tetrahedron Lett.*, 2011, **52**, 5032–5035; (*b*) J. Yang, J. Xiao, T. Chen and L.-B. Han, *J. Org. Chem.*, 2016, **81**, 3911–3916; (*c*) W. C. Fu, C. M. So and F. Y. Kwong, *Org. Lett.*, 2015, **17**, 5906–5909; (*d*) Y.-L. Zhao, G.-J. Wu and F.-S. Han, *Chem. Commun.*, 2012, **48**, 5868–5870; (*e*) J. Yang, T. Chen and L.-B. Han, *J. Am. Chem. Soc.*, 2015, **137**, 1782–1785; (*f*) M. Kalek, M. Jezowska and J. Stawinski, *Adv. Synth. Catal.*, 2009, **351**, 3207–3216.

9 R. S. Shaikh, S. J. S. Düsel and B. König, *ACS Catal.*, 2016, **6**, 8410–8414.

10 L.-L. Liao, Y.-Y. Gui, X.-B. Zhang, G. Shen, H.-D. Liu, W.-J. Zhou, J. Li and D.-G. Yu, *Org. Lett.*, 2017, **19**, 3735–3738.

11 (*a*) M. Fagnoni and A. Albini, *Acc. Chem. Res.*, 2005, **38**, 713–721; (*b*) W. Liu, J. Li, C.-Y. Huang and C.-J. Li, *Angew. Chem., Int. Ed.*, 2020, **59**, 1786–1796; (*c*) Y. Lang, C.-J. Li and H. Zeng, *Org. Chem. Front.*, 2021, **8**, 3594–3613; (*d*) D. Cao, P. Pan, C.-J. Li and H. Zeng, *Green Synth. Catal.*, 2021, DOI: 10.1016/j.gresc.2021.04.006; (*e*) Y. Lang, X. Peng, C.-J. Li and H. Zeng, *Green Chem.*, 2020, **22**, 6323–6327; (*f*) L. Li, W. Liu, X. Mu, Z. Mi and C.-J. Li, *Nat. Protoc.*, 2016, **11**, 1948–1954; (*g*) H. Zeng, Q. Dou and C.-J. Li, *Org. Lett.*, 2019, **21**, 1301–1305; (*h*) D. Cao, C. Yan, P. Zhou, H. Zeng and C.-J. Li, *Chem. Commun.*, 2019, **55**, 767–770; (*i*) L. Li, W. Liu, H. Zeng, X. Mu, G. Cosa, Z. Mi and C.-J. Li, *J. Am. Chem. Soc.*, 2015, **137**, 8328–8331; (*j*) V. Dichiarante, M. Fagnoni and A. Albini, *Chem. Commun.*, 2006, 3001–3003; (*k*) A. M. Mfuh, J. D. Doyle, B. Chhetri, H. D. Arman and O. V. Larionov, *J. Am. Chem. Soc.*, 2016, **138**, 2985–2988; (*l*) M. Fagnoni, M. Mella and A. Albini, *Org. Lett.*, 1999, **1**, 1299–1301; (*m*) M. De Carolis, S. Protti, M. Fagnoni and A. Albini, *Angew. Chem., Int. Ed.*, 2005, **44**, 1232–1236; (*n*) V. Dichiarante, M. Fagnoni and A. Albini, *Angew. Chem., Int. Ed.*, 2007, **46**, 6495–6498; (*o*) S. Protti, M. Fagnoni and A. Albini, *Angew. Chem., Int. Ed.*, 2005, **44**, 5675–5678; (*p*) D. Cao, Z. Chen, L. Lv, H. Zeng, Y. Peng and C.-J. Li, *iScience*, 2020, **23**, 101419; (*q*) Y. Kim and C.-J. Li, *Green Synth. Catal.*, 2020, **1**, 1–11; (*r*) Q. Dou, Y. Lang, H. Zeng and C.-J. Li, *Fundam. Res.*, 2021, DOI: 10.1016/j.fmre.2021.06.018.

12 W. Liu, X. Yang, Y. Gao and C.-J. Li, *J. Am. Chem. Soc.*, 2017, **139**, 8621–8627.

13 (*a*) J. Yu, C.-J. Li and H. Zeng, *Angew. Chem., Int. Ed.*, 2021, **60**, 4043–4048; (*b*) Q. Dou, C.-J. Li and H. Zeng, *Chem. Sci.*, 2020, **11**, 5740–5744; (*c*) D. Cao, J. Yu, H. Zeng and C.-J. Li, *J. Agric. Food Chem.*, 2020, **68**, 13200–13205; (*d*) Z. Wang, J. Niu, H. Zeng and C.-J. Li, *Org. Lett.*, 2019, **21**, 7033–7037; (*e*) H. Zeng, D. Cao, Z. Qiu and C.-J. Li, *Angew. Chem., Int. Ed.*, 2018, **57**, 3752–3757; (*f*) Z. Chen, H. Zeng, S. A. Girard, F. Wang, N. Chen and C.-J. Li, *Angew. Chem., Int. Ed.*, 2015, **54**, 14487–14491; (*g*) H. Zeng, D. Cao, Z. Qiu and C.-J. Li, *ACS Catal.*, 2018, **8**, 8873–8878; (*h*) H. Zeng, Z. Wang and C.-J. Li, *Angew. Chem., Int. Ed.*, 2019, **58**, 2859–2863; (*i*) Z. Wang, H. Zeng and C.-J. Li, *Org. Lett.*, 2019, **21**, 2302–2306; (*j*) H. Zeng, J. Yu and C.-J. Li, *Chem. Commun.*, 2020, **56**, 1239–1242; (*k*) Y. Lang, C.-J. Li and H. Zeng, *Synlett*, 2021, 429–435.

14 J.-J. L. Fu, W. G. Bentrude and C. E. Griffin, *J. Am. Chem. Soc.*, 1972, **94**, 7717–7722.

15 A. Arbuzov, *J. Russ. Phys. -Chem. Soc.*, 1906, **38**, 687.