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COMMUNICATION

Isopropanol as hydrogen source for single atom cobalt-catalyzed Wacker-type oxidation

Received 00th January 20xx,
Accepted 00th January 20xx

DOI: 10.1039/x0xx00000x

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The first example of the heterogeneous cobalt catalytic system for the Wacker-type oxidation catalyzed by single atom dispersed Co-N/C catalyst using alcohol as hydrogen source under oxygen atmosphere is presented. Combined with the reasonably designed control experiment and various of characterization we finally determined that the single atom cobalt was the active center rather than the nanoparticles or oxides counterparts.

Wacker oxidation, developed by the researchers at Wacker Chemie in 1959,[1] is one of the most important reactions in industrial chemistry, where carbonyl compounds are prepared from olefins with catalytic $PdCl_2$ and stoichiometric $CuCl_2$ under aerobic atmosphere.[2] Although this transformation is one of the most important reactions in industrial chemistry, it still exists some limitations. For example, acetophenone was great difficult to be synthesized by Wacker-type process from styrene owing to their facile polymerization and oxidative cleavage to benzaldehydes and/or benzoic acids.[4] To achieve highly efficient Wacker-type oxidation of styrene derivatives, various methods have been developed. For example, Fernandes and co-workers combined the Pd(II) and Dess–Martin periodinane, simple styrene derivatives are proved to be excellent substrates for the generation of corresponding acetophenones.[5] Ding and co-workers performed the oxidation of the substituted styrenes using the benzoquinone/$NaNO_2$/$HClO_4$ catalytic system.[6] Wang and co-workers used $Pd(OAc)_2$ and trifluoroacetic acid can realize the Tsuji–Wacker oxidation of terminal olefins to methyl ketones under oxygen atmosphere.[7] Very recently, hydrofunctionalizations of olefins can give ketones, but such methods need equivalent hydrogenalkoxysilanes as hydrogen source which highly hindering the development of its industrialization.[8] Isopropanol, as a safe and sustainable source of hydrogen, is widely used in hydrogenation reactions. However, it is rarely reported that that isopropanol provides hydrogen for Wacker-type oxidation reactions.[9] Therefore, the development of sustainable and efficient catalysts to achieve this strategy is highly desirable.

Single atom catalysts (SACs) have attracted extensive attention in the field of catalysis. Due to the lack of metal-metal bond, the single metal sites in SACs more or less resemble the peripheral atoms of metal nanoparticles in supported nanoparticle catalysts. Moreover, single metal sites are found to have cationic character compared to their nanoparticle counterparts. SACs possess unparalleled superiority such as high catalytic activity, stability, selectivity, and 100% atom utilization.[10a] The unique structures of SACs and the favourable interaction between the metal sites and supports make it exhibit the high activity characteristics of homogeneous catalyst. On the basis of the unique electronic properties and our recent investigations on the Co-N_x single atom catalyst in organic reactions,[10b-d] we envisaged the Co single atoms would be made a good candidate for the Wacker-type oxidation. To the best of our knowledge, this is the first heterogeneous cobalt-based catalyst for the target reaction. Herein, we presented an unprecedented strategy for Wacker-type oxidation of aryl alkenes to acetophenones over a nitrogen-doped carbon dispersed with single atom cobalt using isopropanol as hydrogen source. The catalyst showed high activity and exclusive regioselectivity. The satisfactory yields of a broad scope of substrate can be obtained under oxygen atmosphere. Characterizations and control experiments disclose that the single atom cobalt is the active centre rather than the nanoparticles or oxides counterparts. Furthermore, a series of control experiments and free radical capture experiments provide a fundamental understanding of the reaction pathway.

The catalysts were prepared by mixing cobalt acetate with phenanthroline in ethanol, addition of the support activated charcoal (DARCO®G-60) followed by removal of the solvent and subsequent pyrolysis at different temperatures. The obtained powders were treated with acid to afford the final

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† Electronic Supplementary Information (ESI) available: See DOI: 10.1039/x0xx00000x

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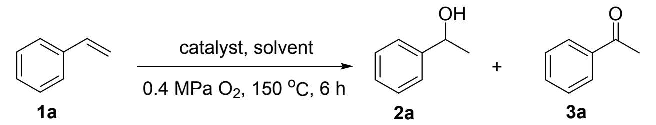
Table 1. Optimization Conditions[a]



Entry	Catalyst	Solvent	Conversion[b] (%)	Yield[b] (%) 2a	3a
1	Co-N/C-600	^{i}PrOH	57.6	12.1	37.8
2	Co-N/C-700	^{i}PrOH	88.9	12.6	71.5
3	Co-N/C-800	^{i}PrOH	99.9	1.2	95.8
4	Co-N/C-900	^{i}PrOH	99.8	1.9	84.8
5[c]	Co-N/C-800	^{i}PrOH	97.4	8.0	79.6
6	Co-N/C-800	MeOH	77.1	trace	53.0
7	Co-N/C-800	EtOH	82.2	12.8	58.2
8	Co-N/C-800	1,4-dioxane	99.7	7.4	48.1
9	Co-N/C-800	CH_3CN	11.8	1.3	2.5
10	Co-N/C-800	^{t}AmOH	10.4	trace	2.8
11[d]	Co-N/C-800	^{i}PrOH	8.8	0	0
12[e]	Co-N/C-800	^{i}PrOH	30.4	0	0

[a] Reaction conditions: 0.25 mmol of styrene, 5 mol% catalyst, 20 mol% K_2CO_3, 4 mL solvent. [b] Conversion and yield were determined by GC using biphenyl as the internal standard. [c] 130 °C. [d] Without K_2CO_3. [e] N_2.

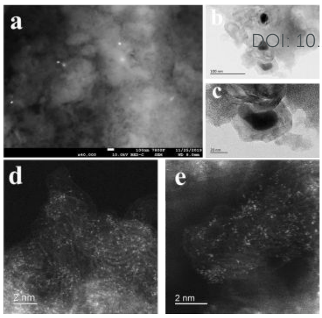


Figure 1. (a) SEM images of Co−N/C-800 under BED mode, (b and c) Nanoparticles of TEM images in Co−N/C-800, (d and e) HADDF-STEM images of Co−N/C-800.

catalysts labelled as Co-N/C-X (X: pyrolysis temperature). More details see Supporting Information.

The obtained dispersed Co-N/C catalyst was evaluated in the Wacker-type oxidation of aryl alkenes to acetophenones. To optimize the reaction conditions, styrene was tested as a model substrate. Typically, this model reaction was performed using ^{i}PrOH as the solvent with catalytic amounts of K_2CO_3 as base under 0.4 MPa O_2 at 150 °C. The results are summarized in Table 1. First, the pyrolysis temperature was investigated (Table 1, entries 1-4). The highest reactivity occurs at 800 °C producing acetophenone in 95.8% yield with a 1.2% 1-phenylethanol as the major by-product (Table 1, entry 3). With the increase of pyrolysis temperature, the activity shows a volcanic lower reaction temperature resulted in the decreasing yields (Table 1, entry 5). Next, different solvents were investigated. Solvents such as methanol, ethanol and dioxane, which are easy to provide protons, can give acceptable yields (Table 1, entries 6-8). The reaction, however, was difficult to proceed when the aprotic solvent acetonitrile was used (Table 1, entry 9). When solvent with larger steric hindrance than isopropanol on -OH (tert-amyl alcohol), the reaction ends with 3.4% of the product (Table 1, entry 10). Based on these results, a hypothesis can be suggested, that is, to make the reaction work, the participation of protons are needed and the further research will be described below. When there was no K_2CO_3 (Table 1, entry 11) or O_2 was replaced with N_2 (Table 1, entry 12), no target product was obtained. It is worth noting that the presence of phenylacetaldehyde is not detected in the product, which demonstrates good regioselectivity.

To better understand the origin of catalyst activity, extensive characterizations, such as, SEM, TEM, HAADF-STEM, XPS and XAS techniques, were adopted to study the structure and morphology of our catalysts. Under LED or UED modes of SEM images (Figure S3), it can be clearly seen that the catalyst was composed of amorphous carbon with porous structure, which was in good accordance with the N_2 adsorption-desorption (Figure S14). From SEM images under BED mode, there co-exists a large amount of huge cobalt nanoparticles (150-300 nm) and small counterparts (20-50 nm) before acid treatment (Figure S5) while fewer nanoparticles can be observed after the catalyst was acid leached (Figure 1a and S4). Such nanoparticles were believed to be embedded in the carbon layers. TEM images showed highly graphitized carbon and sporadic cobalt nanoparticles which were shielded by a thick and compact carbon layers (Figure S7-12). These encapsulated nanoparticles can hardly be removed in the acid treatment step (Figure 1b, 1c and S10). HAADF-STEM images from several randomly selected areas are given in Figures 1d, 1e and S13. The support was densely decorated with isolated bright dots, clearly showing the atomic dispersion of Co.

To further determine the local chemical bonding of these isolated Co atoms in the Co–N/C-800 catalyst, the catalyst was analysed using Co K-edge X-ray absorption spectroscopy encompassing both the near-edge and extended energy regions, XANES and EXAFS, respectively. The results are presented in Fig. 2a. From XANES spectra (Fig. 2a), the pre-edge at 7714-7716 eV was regarded as a fingerprint of Co-N_4 square-planar structures.[10e] The position of the white line peak for Co-N/C-800 shifted to Co foil compared to Co-N/C-700A which was passed for only possessing single atom cobalt without any nanoparticles according to the literature.[9] This indicated that the average valence of Co in Co-N/C-800 is situated between that of Co^0 and Co^{II} due to the contribution of Co^0. The peak at 1.88 Å in EXAFS spectra (Fig. 2b) was attributed to the formation of Co^0. The peak at 1.44 Å was assigned to Co-Nx shell which aroused both in Co-N/C-800 and Co-N/C-700A.[11] XPS was used to determine the chemical states of Co and N in the samples (Figure S15). The N 1s spectrum and Co $2P_{3/2}$ spectrum indicated that the Co^{2+} spaces were coordinated with N atoms in Co-N/C-800 (More details see Supporting Information).[12] The XRD patterns of Co-N/C-800 were shown in Figure S17.

After obtaining the optimal reaction conditions, our focus was switched to the substrate scope and functional group tolerance of the catalytic system. As shown in Table 2, the electronegativity of substituents has little effect on the reaction. It can be found that the steric hindrance of substituents has a great influence on the reaction. The substituents with smaller steric hindrance gave higher yields (Table 2, **3b-3i, 3k-3n**). For the substituents with larger steric

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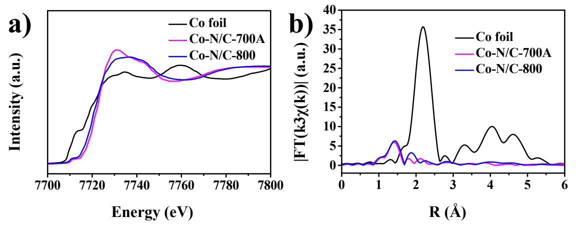
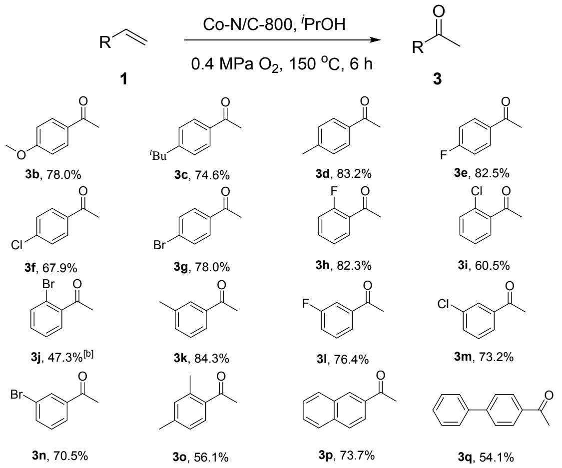


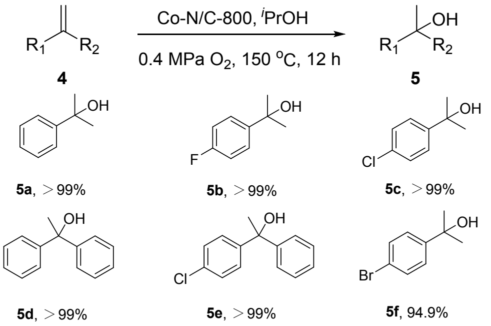
Figure 2. (a) XANES spectra at the Co K-edge of Co-N/C-800, Co foil, and Co-N/C-700A. (b) Fourier transform (FT) at the Co K-edge of Co-N/C-800, Co foil, and Co-N/C-700A.

Table 2. Wacker-type oxidation of aryl terminal alkenes over Co-N/C-800[a]



[a]Reaction conditions: 0.25 mmol of styrene, 5 mol% catalyst, 20 mol% K_2CO_3, 150 °C, 4 mL ^{i}PrOH. Yields were determined by GC using biphenyl as the internal standard. [b]MeOH, 12 h.

Table 3. Wacker type oxidation of 1,1-disubstituted styrenes over a Co-N/C-800[a]



[a]Reaction conditions: 0.25 mmol of styrene, 5 mol% catalyst, 20 mol% K_2CO_3, 150 °C, 4 mL ^{i}PrOH. Yields were determined by GC using biphenyl as the internal standard.

hindrance (Table 2, **3o-3q**), the yield of the reaction decreased. The larger substituents in the o-position (Table 2, **3i, 3j** and **3o**) may have a negative impact on the reaction. It should be noted that, though the yield was moderate, no aldehydes, obtained by the anti-Markownikov rule addition, were detected which shows great regioselectivity.

To further explore the application scope of the substrates, 1,1-disubstituted styrenes were used as substrates (Table 3). All of the substrates were almost oxidized to the corresponding tertiary alcohol quantitatively (Table 3, **5a-5f**).

Next, a series of control experiments were designed to prove the active sites. The results were shown in Table S2. The reaction cannot occur without Co or N elements (Table S2, entries 1 and 2), as did the physical mixtures of Co/C-800 and N/C-800 or Co/C-800 and N/C-800 (Table S2, entries 3 and 4). When the catalyst was not pyrolyzed (Table S2, entry 5), there was no reactivity, suggesting that the active species should be formed during pyrolysis.

To exclude the active sites of metallic Co or CoO_x nanoparticles, acid-leaching experiments were conducted. After the fresh catalyst was acid treated, the Co content was reduced from 3.6 wt % to 1.8 wt %, but the yield of **2a** increased from 75.1% to 86.6% (Figure 3). It is reported that the graphite wall of carbon nanotubes can activate oxygen by encapsulating iron nanoparticles to regulate the electronic structure.[13] However, in this case, when the graphite walls were more than three layers, the activation effect attenuated significantly with the increase of carbon layer. Although there exist some large nanoparticles when catalysts were acid leached, there were encapsulated by extremely thick graphitic carbon nanoshells and far more than three layers (Figure 2). These results suggested that metallic Co or CoO_x nanoparticles may not be the active sites and even counterproductive.

In order to further confirm the true active sites, SCN^- was introduced into our reaction system as it can block the monodisperse active sites while retain the activity of large nanoparticles.[14] In the presence of KSCN, the performance of the catalyst before and after pickling was first investigated. The results were shown in Figure 3. When SCN^- was introduced into the reaction system to poison the single atom cobalt in Co-N/C-800, the yields of **2a** decreased from 86.6% to 30.8%. This phenomenon indicates that the contribution of single atom cobalt which was survived from being titrated by SCN^- tothe yields. While the Co-N/C-800-non-acid which contains single atom cobalt equal to Co-N/C-800 was exposed to SCN^-, the yield of **2a** was only reached to 15.5%. The experiment carried above clearly shows the side effects of nanoparticles. Then, the effect of the amount of KSCN on the reaction was further investigated. The results were shown in Figure S19. The yield of acetophenone decreased with the increase of SCN^-, and reached the minimum when 3 eqiv. of SCN^- was added into the reaction system. In addition, the relationship between the selectivity and amount of KSCN was also discussed in detail in the Supporting Information (Figure S21). To this, we can deem that the active site of this reaction is the monodisperse cobalt atom instead of metallic Co or CoO_x nanoparticles.

To gain more insights into the reaction process of this transformation, some possible intermediates originate from reaction were examined. The results were shown in Scheme S1, when possible intermediates **6a** and **7a** were subjected to the standard conditions, no target products were detected. It is obvious that **3a** can be obtained from **2a**. A kinetic study of the oxidation of styrene was carried out (Figure S20), which showed that styrene was oxidized to **3a** and minor amounts of **2a**, rapidly. With increasing reaction time, **2a** can also be oxidized to **3a**. It's worth noting that the reaction of **3a** under the standard conditions did not give **2a** which was different from the previous work.[10,15] These results suggested that **2a**

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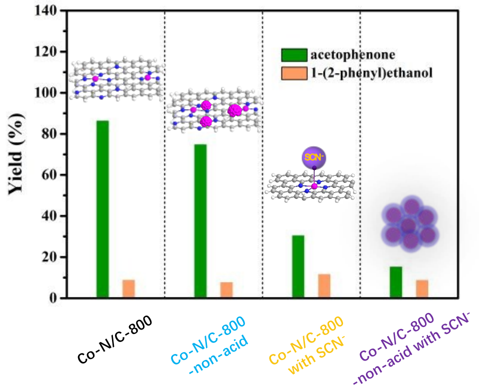

Figure 3. Titration experiment of active sites with KSCN. For the Co-N/C-800-non-acid, 5 mol% of catalyst (20 mg) was added to the reaction system. In order to eliminate the influence of the supporter on the reaction, 2.5 mol% of Co-N/C-800 (20 mg) was added.

may be an intermediate rather than a by-product. Isotopic labelling experiments indicate that the H adds across the olefin stems from 2-propanol-d_8. The reaction was failed when O_2 was replaced with N_2, which indicated that the oxygen in **3a** comes from O_2 instead of other resources.

Based on the above experiments and literature, the reaction process can be proposed and was shown in the supporting information (Scheme S2). First, it was reported that in ORR, the superoxide species were formed by the electron transfer from Co-3d orbitals to O_2, where O_2 was chemically adsorbed on the single cobalt centres (A).[16,17a-b] According to the report of literature, with the help of K_2CO_3, the ^{i}PrOH was deprotonated to form **E**.[17c-d] Intermediate **B** formed through intermediated **F** by abstracting proton by **A** from **E**.[17a-b] Second, intermediate **C** was obtained via synergistic addition of **1a** and intermediate **B**, intermediate **C** can be further decomposed into **3a** and **2a**. **3a** can also be generated from the oxidation of **2a**.[9] Finally, the whole catalytic cycle can be completed by continuous oxidation of solvent to remove one water molecule.[16]

In summary, the first heterogeneous cobalt catalyst used in Wacker-type oxidation has been reported. This strategy features the characteristics of high efficiency and good environment. Catalysed by single atom dispersed Co-N/C catalyst using isopropanol as hydrogen source, styrene was oxidized to acetophenone with excellent yield (95%) and regioselectivity (100%). Extensive characterization and control experiments show that the active site of Wacker-type oxidation reaction is monodisperse cobalt atom rather than their nanoparticles counterparts. This work would provide an alternative catalyst for the Wacker-type oxidation of aryl alkenes to high-value-added chemicals.

Financial support from the Department of Science and Technology of Liaoning Province (No. 2019-ZD-0470) and he National Natural Science Foundation of China (No. 21773227, 21403219, 21773232, and 21902151).

Conflicts of interest

There are no conflicts to declare.

Notes and references

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Isopropanol as hydrogen source for single atom cobalt-catalyzed Wacker-type oxidation

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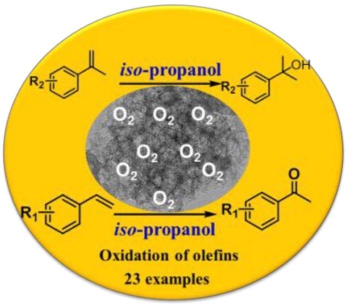

The first example of Wacker-type oxidation catalyzed by single atom cobalt catalyst under dioxygen using isopropanol as hydrogen source was established.

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