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Rongalite-promoted metal-free aerobic *ipso*-hydroxylation of arylboronic acids under sunlight: DFT mechanistic studies

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ABSTRACT

A novel rongalite-promoted metal-free aerobic *ipso*-hydroxylation of arylboronic acids has been developed. This method employs low-cost rongalite as a radical initiator and O_2 as a green oxidizing agent for *ipso*-hydroxylation. This protocol is compatible with a wide variety of functional groups with good to excellent yields at room temperature. Furthermore, mechanistic insight into the role of superoxide radical anions in C-B cleavage has also been provided based on DFT studies.

Introduction

Phenols are some of the most widely available compounds and there is a mounting evidence of its presence in many naturally occurring and biologically active products [1]. Phenols serve as synthons for the construction of wide variety of compounds ranging from pharmaceuticals to agrochemicals, materials and polymers [2]. Naturally occurring phenolic compounds from herbs and dietary plants like flavonoids, coumarins, lignans, tannins etc. exhibit wide range of biological activities including antimicrobial, anti-inflammatory, anti-allergenic, anticancer, anti-oxidant etc [3].

Phenols can be synthesized through the use of a number of processes some of which include a) non-activated aryl halides b) aryl halides activated by transition metal catalysts via aromatic nucleophilic substitution [4]. But the problems associated with the above processes are harsh reaction conditions, longer reaction time and limited substrate scope. In a move to circumvent the problems associated with conventional methods of preparation, chemists have searched for an easily available starting material and green methodologies. Amid arylboronic acids became a versatile starting material for various transformations [5]. Further investigations clearly revealed that the oxidative hydroxylation of arylboronic acids is one of the best methods due to their easy availability and stability. Thus, synthesis of phenols by *ipso*-hydroxylation from arylboronic acids has captivated imagination of researchers all around. However, the process of *ipso*-hydroxylation of arylboronic acids requires the use of transition metal catalysts such as palladium [6], copper [7] or iron salts [8] which are environmentally malignant.

Necessity of green and environment friendly oxidation methods with functional group tolerance, other alternatives such as oxone [9], hydrogen peroxide [10], *N*-oxides [11], hydroxylamine [12], *meta*-chloroperoxybenzoic acid [13], ammonium persulfate [14], organic hypervalent iodine [15] and sodium chlorite [16] are being used, but are required in excess quantities.

Recently, oxidative organic transformations by utilization of green oxidizing agent i.e., molecular oxygen became an emerging research in the field of sustainable chemistry [17]. In addition to this above mentioned protocols, other methods like *ipso*-hydroxylation of arylboronic acids by molecular oxygen catalysed by copper (II) or palladium (II) salts [18]; methylhydrazines [19]; photoredox catalysis by ruthenium or iron [20]; electrocatalytic method that employs methyl viologen as an organic cathodic electrocatalyst to convert arylboronic acids to phenols introduced by liu et al., [21] while Carrillo and co-workers introduced *ipso*-hydroxylation by ascorbate-driven quinone which is further explored by Cozzi and co-workers [22]. Although these new methods help to overcome a majority of issues associated with the reaction, but process inherently have certain limitations such as use of metals, expensive reagents, special reaction setup and long reaction time. In this context, we are developing a metal-free commercially viable rongalite in presence of naturally abundant

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oxygen for oxidative *ipso*-hydroxylation of arylboronic acids to aryl alcohols under sunlight.

Sodium hydroxymethanesulfinate dihydrate (SHM), also called as rongalite is an industrial product that has been used as a bleaching agent in the dye and printing industry [23], it acts as a reducing agent [24], antidote against heavy metal poisoning [25], antioxidant in formulations [26] and a green reagent in organic chemistry [27,28]. In continuation of our efforts on exploring the synthetic utility of rongalite [24a], herein we report metal-free *ipso*-hydroxylation of arylboronic acids.

Results and discussion

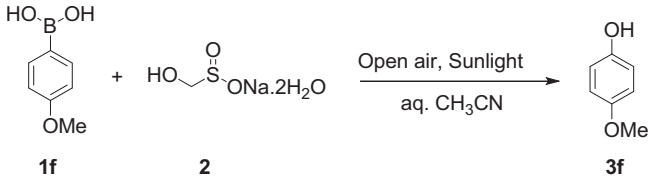
In order to test our hypothesis, a reaction was conducted between 4-methoxyphenylboronic acid **1f** as a model substrate and rongalite **2** in the presence of molecular oxygen as an oxidant in aq. CH_3CN under sunlight to transform into the corresponding phenol **3f**. To our delight the formation of **3f** (60%) was observed in aq. CH_3CN at room temperature (Table 1, entry 1). Then to know the role of components i.e., rongalite, molecular oxygen and sunlight, we have performed a series of reactions and results are shown in Table 1.

Firstly, reaction was conducted in absence of rongalite and observed no phenol formation (Table 1, entry 2), secondly, reaction was conducted under nitrogen atmosphere to avoid presence of atmospheric oxygen then very trace amount of 4-methoxyphenol was formed; this may be due to the dissolved oxygen present in water (Table 1, entry 3).

Finally, reaction was run under dark conditions to avoid sunlight exposure to reaction mixture, here also we got only trace amount of 4-methoxyphenol (Table 1, entry 4). These results clearly demonstrate that rongalite, oxygen and sunlight all are essential components for the conversion of arylboronic acids to aryl alcohols.

Next, attention has been paid to optimize the reaction conditions under sunlight to improve the yield of the product. All the reactions were performed in mixture of solvents at room temperature with 2.0 equiv. of rongalite under sunlight in open-air condition. Among the solvent mixtures tested, CH_3CN:H_2O (3:1) and EtOH:H_2O (3:1) were afforded desired product in good yields (Table 2, entries 7 and 8), however other combinations resulted less yield in more reaction time, this may be attributed to the solubility issues associated with organic substrates (Table 2, entry 9).

Table 1
Optimization of reaction conditions[a].

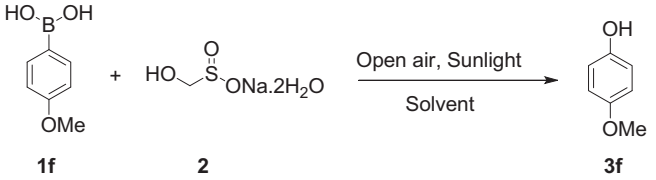


1f **2** **3f**

Entry	Rongalite	Air	Sunlight	Time (h)	Yield[b] (%)
1	+	+	+	8	60
2	–	+	+	8	N.R.[c]
3	+	–	+	8	Trace
4	+	+	–	8	Trace

[a] Reaction conditions: **1f** (0.50 mmol), rongalite (2 equiv., 1.0 mmol), air and sunlight in aq. CH_3CN for 8 h.
[b] Yield of isolated product.
[c] N.R. = No Reaction.

Table 2
Screening of reaction conditions for the hydroxylation of arylboronic acid **1f**[a].



1f **2** **3f**

Entry	Solvent	Rongalite (equiv.)	Time (h)	Yield[b] (%)
1	aq. Dioxane	2	20	55
2	aq. CH_3CN	2	8	74
3	aq. DMSO	2	18	35
4	aq. MeOH	2	8	74
5	aq·THF	2	15	69
6	aq. DMF	2	18	65
7	CH_3CN:H_2O (3:1)	2	6	75
8	**EtOH:H_2O (3:1)**	**2**	**6**	**81**
9	EtOH:H_2O (1:1)	2	10	60
10	EtOH:H_2O (3:1)	3	6	81
11	EtOH:H_2O (3:1)	2	3	81[c]

[a] Reaction conditions: **1f** (0.50 mmol), rongalite (2 equiv., 1.0 mmol), air and sunlight.
[b] Yield of isolated product.
[c] reaction was conducted in presence of oxygen balloon.

Further, increase in amount of rongalite or prolonged time did not improve the yield (Table 2, entry 10). It is worth noting that the reaction time was decreased to 3 h when we use oxygen balloon, which indicates the presence of oxygen is necessary (Table 2, entry 11).

Further, we have examined other sulphur-containing radical initiators for *in situ* generation of superoxide radical anion for *ipso*-hydroxylation, results are shown in Table 3. Thiourea dioxide gave desired product with less yield in longer time, whereas sodium dithionite gave inferior results. This data indicates that rongalite is the best radical initiator among the other sulphur-containing radical initiators (Table 3, entry 1).

With optimized reaction conditions (Table 2, entry 8) in hand the applicability of the reaction condition was explored by using various substituted arylboronic acids/pinacol esters and the results are summarized in Table 4 and 5. Electron releasing groups i.e., ethyl, methyl and phenyl substituted arylboronic acids underwent aerobic *ipso*-hydroxylation in good yields (71–92%) within the period of 5–8 h at room temperature under sunlight (Table 4, 3a-3j). Notably, electron withdrawing groups such as nitro, –CHO, –CN and ketone substituted arylboronic acids did not affect the product yield (Table 4, 3m-3p). Interestingly, chloro and bromo substituted arylboronic acids also hydroxylated efficiently with the fore mentioned conditions without undergoing dehalogenation reaction [29].

Table 3
Hydroxylation of arylboronic acids by other sulphur-containing radical initiators.[a-c]

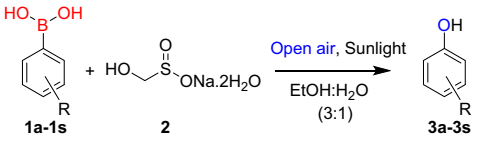
Entry	Radical initiator	Reaction condition	Time (h)	Yield[c](%)
1	Rongalite	Neutral[a]	6	81
2	Thiourea dioxide	Neutral[b]	72	41
3	Sodium dithionite	Neutral[b]	72	trace

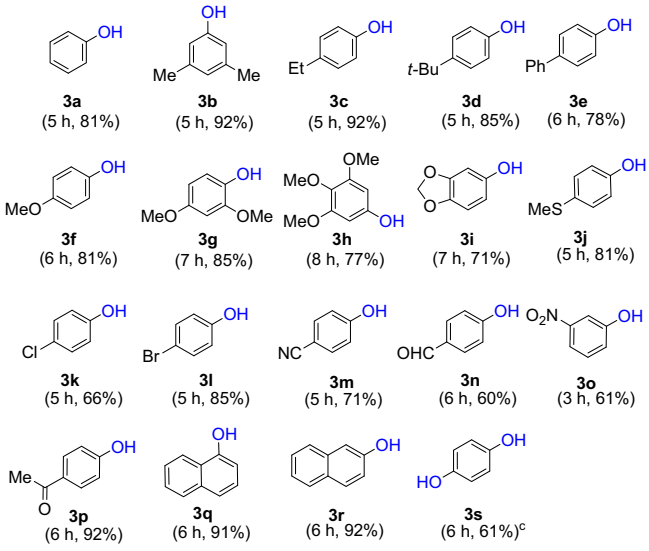
[a] Reaction conditions: **1f** (0.50 mmol), rongalite (2 equiv., 1.0 mmol), air and sunlight in aq. EtOH.
[b] Reaction conditions: **1f** (0.50 mmol), radical initiator (2 equiv., 1.0 mmol), air at RT in aq. EtOH.
[c] Yield of isolated product.

1-Naphthylboronic acid and 2-Naphthylboronic acid also subjected to *ipso*-hydroxylation under the same condition to give corresponding Naphthols (Table 4, 3q-3r). Further, we have applied same optimized reaction conditions to 1,4-phenylenediboronic acid, which was readily gave hydroquinone by oxidative *ipso*-hydroxylation at C-1 and C-4 position (Table 4, 3s).

Next, the scope of this methodology has been extended to phenylboronic acid pinacol esters, which are derivatives of phenylboronic acids. The result obtained from the reaction clearly indicates the formation of desired products in good yields within 2–3 h (Table 5).

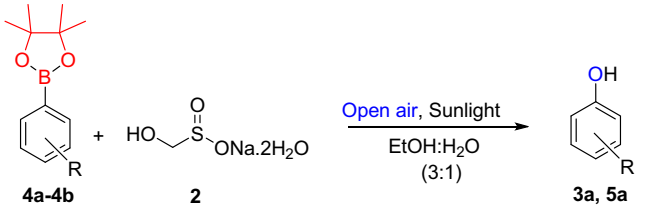
Table 4
Substrate scope of the *ipso*-hydroxylation of arylboronic acids by rongalite in presence of oxygen and sunlight[a–c].

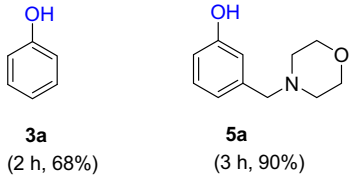




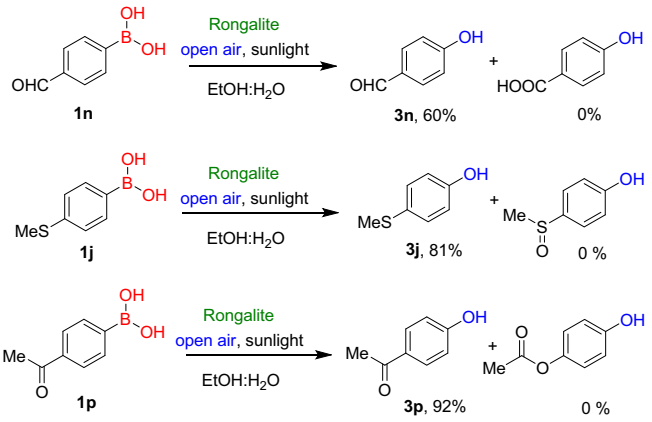
[a]Reaction conditions: substrate (0.50 mmol), rongalite (2 equiv., 1.0 mmol), air and sunlight in 1 mL of EtOH:H_2O (3:1).
[b]Yield of isolated product.
[c]4 equiv. of rongalite used.

Table 5
Rongalite mediated hydroxylation of phenylboronic acid pinacol esters[a,b].





[a]Reaction conditions: substrate (0.50 mmol), rongalite (2 equiv., 1.0 mmol), air and sunlight in 1 mL of EtOH:H_2O (3:1).
[b]Yield of isolated product.



Scheme 1. Chemoselectivity of the proposed method.

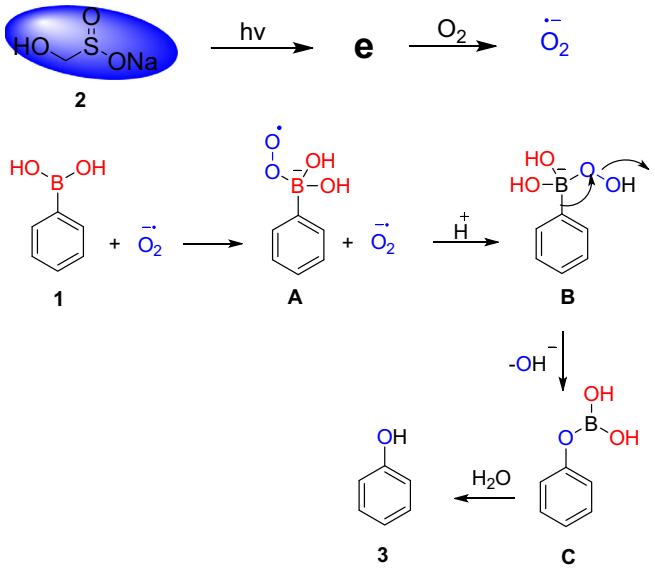
To validate the proposed mechanism, a few mechanistic studies have been carried out. First, whether Ultraviolet light or Visible light is responsible for electronic transitions in the rongalite, we have recorded UV-VIS spectrum of rongalite and showed λ_{max} at 202 and 227 nm in water as solvent, these absorption bands may be attributed to $\pi \rightarrow \pi^*$ and $n \rightarrow \pi^*$ electronic transitions of SO_2 group in the rongalite (Fig. S1). Later, we carried the same reaction under 400 W Hg immersion lamp. The reaction was completed within 1 h 15 min. It clearly indicates that the Ultraviolet light is responsible for moving the reaction under sunlight irradiation.

Controlled reactions were conducted to probe role of free-radical involvement in the reaction. The model reaction under optimal reaction condition was completely inhibited after the addition of free radical capturing agent (2,2,6,6-Tetramethylpiperidin-1-yl) oxyl (TEMPO).

Based on the controlled experiments, previous reports [32] we proposed a possible reaction mechanism involving radical pathway (Scheme 2) and has been validated using density functional theory calculations (Figs. 1 and S2-3). Initially, on irradiation of rongalite **2** under sunlight releases electron which is trapped by molecular oxygen to form superoxide radical anion. Later, superoxide radical anion attacks on the electrophilic boron atom of the phenylboronic acid **1** to form tetrahedral intermediate **A**, which in turn converts to **B** upon protonation. Subsequently, phenyl group in tetrahedral intermediate **B** undergoes Baeyer-Villiger type of migration onto peroxy oxygen atom to form intermediate **C** and followed by hydrolysis to afford phenol **3** as a product.

Density functional theory (DFT) calculations

To gain insight into the reaction mechanism, density functional theory (DFT) calculations were performed. Geometries of reactants, transition structures (TSs), and intermediates were fully optimized using UB3LYP/6–311 + G(d,p) level of theory [33,34]. Detailed computational methodology is given in supplementary information. Calculated relative energy profile shown in Fig. 1 along with important geometry.



Scheme 2. A possible reaction mechanism.

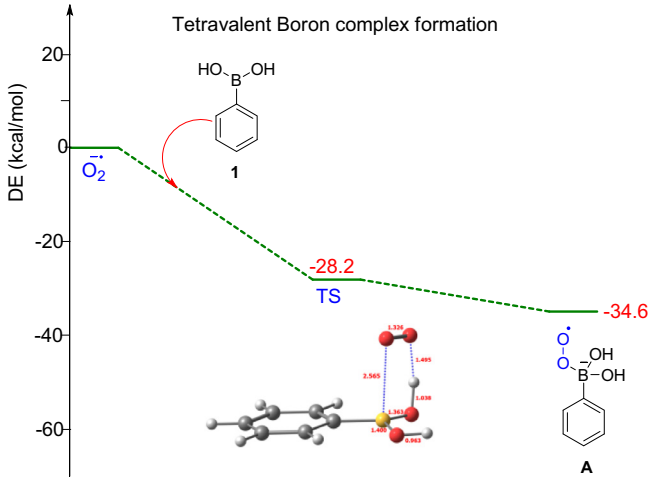


Fig. 1. Relative energy profile of tetravalent boron intermediate formation. (Color key: White = Hydrogen, Yellow = Boron, Grey = Carbon and Red = Oxygen).

Formation of superoxide radical anion described elsewhere [35]. Close analysis of relative energy of formation of transition state (TS) is −28.2 kcal/mol, which clearly indicates that the super oxide radical anion readily reacts with phenylboronic acid to form the intermediate structure **A** (Fig. 1). It is also interesting to note from the optimized geometry of TS that phenylboronic acid forms hydrogen bond interaction with the incoming super oxide radical anion. Therefore, it is worth to mention that the low energy barrier of this reaction may be attributed to the additional stabilization of TS arises due to the formation of hydrogen bond. Furthermore, it can also be noted that relative energy of formation of tetravalent boron complex is less when compared to that of TS and reactant. Therefore, it is worth to mention that the reaction initiation (i.e. creation of super oxide radical anion) step only requires the energy and other intermediate steps effortlessly involve in the changes. Detailed description of complete reaction and energetics are given in supplementary information (Figs. S2–S3).

In summary, we have developed a green protocol using Rongalite:molecular oxygen reagent, which generates superoxide radical anion *in situ* provides the *ipso*-hydroxylation of arylboronic acids to their corresponding phenols in good yields with relatively short reaction times. Additionally, this protocol allows to a wide range of functional groups on arylboronic acids. Notably, this protocol is chemoselective and functional groups which are sensitive to oxidation are well tolerated. Further DFT calculations were performed to gain insight into the reaction mechanism.

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Appendix A. Supplementary data

Supplementary material that include synthetic procedures, characterization data, DFT calculations and NMR (^{1}H & ^{13}C) of the compounds **3a-3s & 5a** described in this article. Supplementary data to this article can be found online at https://doi.org/10.1016/j.tetlet.2019.151539.

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