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Efficient Oxidative Dehydrogenation of Dihydropyrimidinones and Thiocyanation of Aromatic Compounds Using 1,1,2,2-Tetrahydroperoxy-1,2-diphenylethane as the Oxidant

K. Khosravi*, A. Azizi and S. Naserifar

Department of Chemistry, Faculty of Science, Arak University, Arak 38156-8-8349, Iran

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A new, efficient and mild approach for the oxidative dehydrogenation of dihydropyrimidinones and thiocyanation of aromatic compounds using 1,1,2,2-tetrahydroperoxy-1,2-diphenylethane (THPDPE) as a terminal oxidant was developed. Initially, various substrates bearing different electron-donating and electron-releasing functionalities were synthesized, and next under the optimized reaction conditions the desired products were yielded after an easy work-up. All of the reactions proceeded in short reaction times, and 1,1,2,2-tetrahydroperoxy-1,2-diphenylethane (THPDPE) proved its potential to yield the desired products in high yields.

Keywords: Dehydropirimidinones, Oxidative dehydrogenation, Thiocyanation, 1,1,2,2-Tetrahydroperoxy-1,2-diphenylethane, Pyrimidinones

INTRODUCTION

Oxidative dehydrogenation has been considered as one of the most important transformations in organic synthesis and industrial productions [1-3]. Various aromatic structures possessing chemical and pharmaceutical applications have been formed through these transformations [4].

In this approach, synthesis of heteroaromatics *via* oxidative dehydrogenation is one of the most fundamental transformations in organic synthesis [5]. A great number of methodologies have been developed to afford the heteroaromatic compounds, howeve, most of which suffer from several drawbacks including stoichiometric reagents requirement and/or harsh reaction conditions [2,6]. Consequently, developing a mild and sustainable catalytic approach, yeilding the desired products, has remained an important challenge.

Oxidative dehydrogenation of numerous heterocycles has been considered as a convenient strategy that affords aromatic structures namely heteroaromatics and phenols [7,8]. Among the heteroaromatic compounds, dihydropyrimidines and dehydropyrimidinones have been a matter of interest since they possess a wide range of biological activities. They serve as antifungal [9], antiproliferative [9], antiviral [9], antitumor [10,11], antiinflammatory [12,13], antihypertensive [14,15], anti-HIV [16], antiepileptic [17], anti-malarial [18], antibacterial [19,20], antitubercular [21], miscellaneous agents [22,23] and potassium [24,25] and calcium channel antagonist [26]. For this reason, dihydrogenation of diydropyrimidines and dehydropyrymidinones owning various functionalities have received much attention due to the facile access *via* Biginelli three-component coupling [27].

Since dihydropyrimidinones are stable structures, their dihydrogenation is not as fast as Hantzsch type dihydropyridines [28]. Various oxidants for instance TBHP/$CuCl_2$/K_2CO_3 (TBHP tert-butyl hydroperoxide) [5],

*Corresponding author. E-mail: k-khosravi@araku.ac.ir

$CAN/NaHCO_3$ (CAN, cerium ammonium nitrate) [29], and $TBHP/PhI(OAc)_2$ [30] have been utilized to accomplish the reaction, though the accompanied difficulties namely products isolation or safety issues have arisen a demand to make much more effort to develop alternative procedures.

Recently, we have applied THPDPE in the oxidation of sulfides to sulfoxides and sulfones and epoxidation of α, β-unsaturated ketones and gained outstanding results [31,32]. Therefore, we decided to evaluate its potential in other oxidative approaches as well. Herein, we report a simple and convenient approach for the oxidative dehydrogenetaion of dihydropyrimidinones using 1,1,2,2-tetrahydroperoxy-1,2-diphenylethane (THPDPE) (Scheme 1) as the oxidant in the presence of CuI as the catalyst (Scheme 2).

In continuation of our work, we became interested in thiocyanation reaction since thiocyanate derivatives are significant synthons in organic synthesis [33,34]. These functional groups exist in natural [35] designed compounds with biologically relevant properties [36]. They are key precursors in the synthesis of various sulfur-containing heterocycles [37]. Also, these compounds can be transformed into other sulfur-containing functionalities [38].

Electrophilic thiocyanation is a very popular carbon-heteroatom synthesis route. A multitude number of reagents and catalysis have been participated in electrophilic thiocyanation of arenes such as SCN in cooperation with boron sulfonic acid [39], Br_2 in MeOH [40], silica sulfuric acid/H_2O_2 [41], HCl/H_2O_2 [42] and poly [4-diacetoxyiodo] styrene [43]. However, most of them suffer from harsh reaction conditions, therefore there has been an ever increasing challenge to overcome these deficiencies and introduce new pathways bringing about facile access to the corresponding products.

Accordingly, we developed a new approach for thiocyanation of aromatic compounds using THPDPE in the presence of KSCN and HOAC (Scheme 3).

EXPERIMENTAL

The materials were purchased from Merck and Fluka chemical companies and were used without any additional purification. All reactions were monitored by thin layer chromatography (TLC) on gel F254 plates. Melting points were obtained in open capillary tubes and also were measured on the Electrothermal 9100 apparatus. Nuclear magnetic resonance spectra were recorded on a JEOL FX 90Q and Bruker 300 MHz spectrometer using tetramethylsilane (TMS) as an internal standard. IR spectra were recorded on a Perkin Elmer GX FT IR spectrometer (KBr pellets). Products were characterized on the basis of their melting points, IR, ^{1}H NMR, and ^{13}C NMR spectral analysis.

Caution. We did not encounter any problem with 1,1,2,2-tetrahydroperoxy-1,2-diphenylethane, however, all peroxides are potentially explosive and should be handled with precautions; all reactions should be carried out under a safety shield inside a fume hood and transition metal salts or direct heating should be avoided.

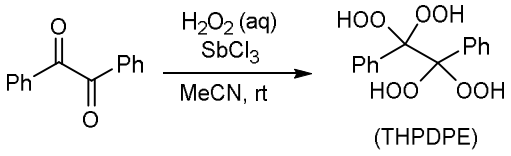
General

General procedures for the Biginelli three-component-coupling for the synthesis of dihydropyrimidinones (1-19). Substrates were prepared according to the literature [44].

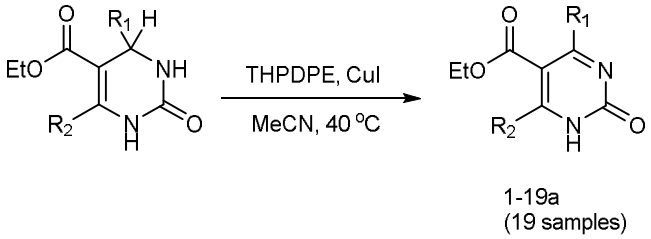
General procedures for synthesis of 1,1,2,2-tetrahydroperoxy-1,2-diphenylethane. 1,1,2,2-Tetrahydroperoxy-1,2-diphenylethane was prepared according to the literature procedure [45].

General procedure for oxidative dihydrogenetaion of dihydropirimidinones. Dihydropyrimidinone derivatives (1 mmol), CuI (0.1 mmol) and MeCN (4 ml) were added to a round bottom flask. THPDPE (0.5 mmol) was then added to the mixtureand the batch was heated at 40 °C for an appropriate time (Table 2). After completion of the reaction as monitored by TLC (n-hexane/ethyl acetate (8:1)), the solution was cooled to room temperature, treated with a mixture of aqueous $Na_2S_2O_3$ (1 M solution, 2 ml), diluted with water (5 ml) and extracted using ethyl acetate (3 × 5 ml). After evaporation of solvent, the residue was recrystallized in ethanol 96% and pure crystalline products were gained. All products were characterized on the basis of their melting points, IR, ^{1}H NMR, and ^{13}C NMR spectral analysis and compared with those reported.

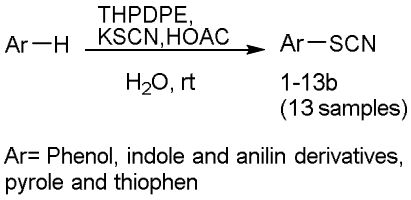
General procedure for thiocyanation of aromatic compounds. KSCN (1 mmol) was added to a mixture of aromatic substrate (1 mmol), peroxide (1 mmol) and HOAc



Scheme 1. Synthesis of 1,1,2,2-tetrahydroperoxy-1,2-diphenylethane



Scheme 2. Oxidative dehydrogenation of dihydropyrimidinones by THPDPE



Scheme 3. Facile thiocyanation of aromatic compounds promoted by 1,1,2,2-tetrahydroperoxy-1,2-diphenylethane

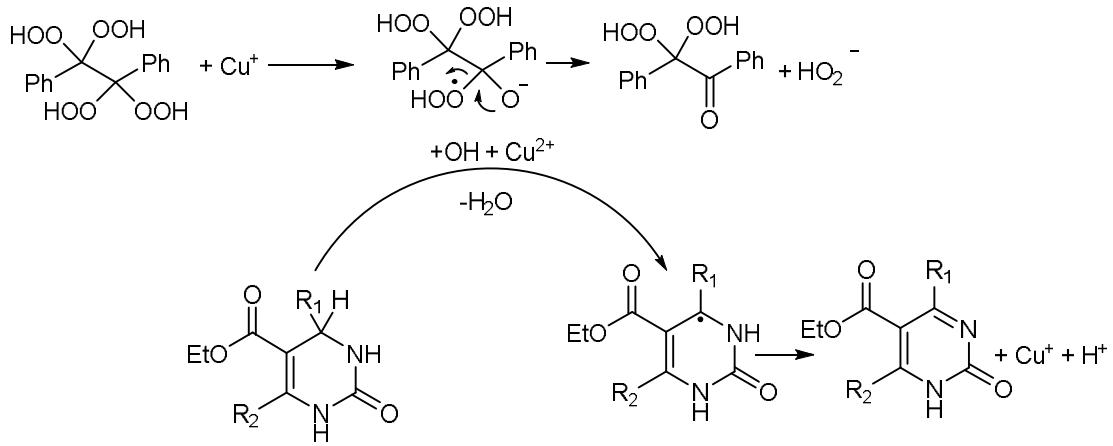
(0.1 mmol) in H_2O (4 ml), and it was stirred at room temperature for an appropriate time monitored by TLC. After completion of the reaction, the mixture was quenched with Na_2SO_3 1 M solution (3 ml) and extracted by $CHCl_3$ (3×5 mL). After evaporation of solvent, the residue was recrystallized in ethanol 96% and purified by chromatography. All products were characterized on the basis of their melting points, IR, ^{1}H NMR, and ^{13}C NMR spectral analyses and compared with those reported.

Spectral Data for the New Compounds

Compound 13a. (Ethyl-4-(2,4-dichlorophenyl)-6-methyl-2-oxo-1,2-dihydropyrimidine-5-carboxylate): M. P.: 280-282 °C. IR ν_{max}/cm^{-1} (KBr pellet): 3360, 3104, 2970, 1699, 1643, 1457, 1226, 1097, 1003, 817; ^{1}H NMR (90 MHz, DMSO-d_6) δ_H: 1.04 (t, 3H, j = 7.2 Hz), 2.32 (s, 3H), 3.97 (q, 2H, j =7.2 Hz), 7.38-7.78 (m, 3H), 9.33 (s, br, 1H). ^{13}C NMR: (22.5 MHz, DMSO-d_6) δ_C: 15.18, 18.96, 60.47, 98.65, 130.06, 131.66, 134.51, 139.21, 142.28, 150.89, 162.58, 166.82; Anal. Calcd. (%) for $C_{14}H_{12}Cl_2N_2O_3$: C, 51.40; H, 3.70; N, 8.56; Found: C: 51.50; H: 3.65; N, 8.70.

Compound 14a. (Ethyl-6-methyl-4-(naphthalen-1-yl)-2-oxo-1,2-dihydropyrimidine-5-carboxylate): M. P.: 265-267 °C. IR ν_{max}/cm^{-1} (KBr pellet): 3250, 3108, 2975, 1700, 1647, 1431, 1231, 1087, 1024, 777; ^{1}H NMR (90 MHz, DMSO-d_6) δ_H: 0.77 (t, 3H, j = 7.2 Hz), 2.32 (s, 3H), 3.80 (q, 2H, j = 7.2 Hz), 7.32-8.21 (m, 7H), 9.21 (s, 1H). Anal. Calcd. (%) for $C_{18}H_{16}N_2O_3$: C, 70.12; H, 5.23; N, 9.09; Found: C: 70.30; H: 5.25; N, 9.10.

Compound 16a. (Ethyl-6-methyl-2-oxo-4-(thiophen-2-yl)-1,2-dihydropyrimidine-5-carboxylate): M. P.: 238-240 °C. IR ν_{max}/cm^{-1} (KBr pellet): 3241, 3116, 2981, 1705, 1651, 1422, 1290, 1225, 1094, 787, 692; ^{1}H NMR (90 MHz,



Scheme 4. Suggested mechanism for oxidative aromatization of dihydropyrimidinones

DMSO-d_6) δ_H: 1.14 (t, 3H, j = 7.2 Hz), 2.20 (s, 3H), 4.00 (q, 2H, j = 7.2 Hz), 6.88-7.34 (m, 3 H), 9.27 (s, 1 H). ^{13}C NMR: (22.5 MHz, DMSO-d_6) δ_C: 14.86, 18.60, 59.87, 98.86, 121.37, 123.12, 137.42, 150.13, 162.88, 166.07; Anal. Calcd. (%) for $C_{12}H_{12}N_2O_3S$: C, 54.53; H, 4.58; N, 10.60; Found: C: 54.65; H: 4.60; N, 10.60.

Compound 17a. (Ethyl-6-Methyl-2-oxo-4-phenethyl-1, 2-dihydropyrimidine-5-carboxylate): M. P.: 205-208 °C. IR ν_{max}/cm^{-1} (KBr pellet): 3244, 3116, 3031, 2974, 1708, 1652, 1467, 1227, 1249, 1229, 1093, 777; ^{1}H NMR (90 MHz, DMSO-d_6) δ_H: 1.10 (t, 3H, j = 7.2 Hz), 1.71 (m, 2H), 2.16 (s, 3H), 2.50 (m, 2H), 4.04 (q, 2H, j = 7.2 Hz), 7.20 (s, 5H), 8.98 (s, 1H). ^{13}C NMR: (22.5 MHz, DMSO-d_6) δ_C: 15.15, 20.10, 31.56, 51.01, 60.89, 100.42, 126.75, 129.34, 142.79, 149.63, 154.10, 164.10, 166.50; Anal. Calcd. (%) for $C_{16}H_{18}N_2O_3$: C, 67.12; H, 6.34; N, 9.78; Found: C: 67.05; H: 6.30; N, 9.80.

Compound 19a. (Ethyl-4-ethyl-6-methyl-2-oxo-1,2-dihydropyrimidine-5-carboxylate): M. P.: 186-188 °C. IR ν_{max}/cm^{-1} (KBr pellet): 3248, 3122, 2962, 2934, 1724, 1644, 1467, 1290, 1249, 1229, 1115, 1095, 779; ^{1}H NMR (90 MHz, DMSO-d_6) δ_H: 0.70 (t, 3H, j = 4.2 Hz), 1.17 (t, 3H, j = 7.2 Hz), 1.40 (t, 2H, j = 7.2), 2.16 (s, 3H), 4.09 (q, 2H, j = 7.2 Hz), 8.90 (s, 1 H). ^{13}C NMR: (22.5 MHz, DMSO-d_6) δ_C: 9.90, 15.66, 19.15, 31.13, 60.63, 100.58, 149.87, 154.67, 160.75, 167.19; Anal. Calcd. (%) for $C_{10}H_{14}N_2O_3$: C, 57.13; H, 6.71; N, 13.33; Found: C: 57.20; H: 6.59; N, 13.41.

RESULTS AND DISCUSSION

Dehydrogenation of Dihydropyrimidinones

Initially, 5-acetyl-6-methyl-4-phenyl-3,4-dihydropyrimidin-2(1*H*)-one was selected as the substrate to optimize the reaction conditions. A variety of solvents were examined though only MeCN led to higher yields. Next, an investigation on optimal catalyst revealed that Cu(I) salts particularly CuI enhanced the reaction completion significantly. Further examinations on the required amount of the oxidant showed that 0.5 mmol of oxidant caused a noticeable rate acceleration and therefore the best conversion and yield were afforded. According to the results, any increase in the amount of the oxidant had no influence on the reaction. Also, it was noticed that in absence of catalyst and peroxide the reaction almost stopped (entries 15 and 16, Table 1). Finally, several peroxides were tested to carry out the reaction and THPDPE was proved to possess the best potential to yield the desired product. (Table 1, entries 17-19). Consequently, the results gathered within the evaluated parameters confirmed the completion of the procedure *via* a moderate reaction conditions. The optimum reaction conditions were found as follows: dihydropyrimidinone (1 mmol), THPDPE (0.5 mmol), CuI (0.1 mmol), MeCN (4 ml), and 40 °C.

It seems that the mechanism included radicals and it is similar to other reported mechanisms [5,30]. The suggested

Table 1. Optimization of Reaction Condition for the Oxidative Dehydrogenation of Ethyl-6-methyl-2-oxo-4-phenyl-1,2,3,4-tetrahydropyrimidine-5-carboxylate[a]

Entry	Oxidant (mmol)	Catalyst	Catalyst (mmol)	Solvent	Time (h)	Yield (%)[b]
1	THPDPE (0.5)	$CuSO_4$	0.10	MeCN	5	45
2	THPDPE (0.5)	CuCl	0.10	MeCN	5	65
3	THPDPE (0.5)	$CuCl_2$	0.10	MeCN	5	82
4	THPDPE (0.5)	CuI	0.10	MeCN	4	91
5	THPDPE (0.5)	CuI	0.05	MeCN	8	50
6	THPDPE (0.5)	CuI	0.12	MeCN	4	87
7	THPDPE (0.5)	CuI	0.10	$CHCl_3$	6	55
8	THPDPE (0.5)	CuI	0.10	CH_3OH	1.2	53
9	THPDPE (0.5)	CuI	0.10	THF	5	40
10	THPDPE (0.5)	CuI	0.10	CH_2Cl_2	5	88
11	THPDPE (0.3)	CuI	0.10	MeCN	8	80
12	THPDPE (0.4)	CuI	0.10	MeCN	7	86
13	THPDPE (0.7)	CuI	0.10	MeCN	3.5	84
14	THPDPE (1)	CuI	0.10	MeCN	3	63
15	THPDPE (0.5)	-	-	MeCN	10	10
16	-	CuI	0.10	MeCN	10	0
17	UHP (0.5)	CuI	0.10	MeCN	4	25
18	H_2O_2 (0.5)	CuI	0.10	MeCN	4	20
19	TBHP (0.5)	CuI	0.10	MeCN	4	60

[a]Conditions: Dihydropyrimidinone derivatives (1 mmol), CuI (0.1 mmol) THPDPE (0.5 mmol), and MeCN (4 ml), at 40 °C. [b]Isolated yields.

mechanism is started by generation of hydroxyl radical, which is similar to Haber-Weiss reaction. [46,47]. Then, the formed radical dihydropyrimidinone is oxidized to aromatic product rapidly (Scheme 4).

As shown in Table 2, all of the starting materials were transformed into their corresponding products in high yields. The nature of the substituents and also their positions on the phenyl ring had a significant role in reaction times. For instance, electron-donating functionalities 2-methoxy, 4-methoxy (Table 2, entries 1h and 1i) or 4-methyl (Table 2, entry 1o) enhanced the reaction rates and must have stabilized the intermediate while the electron-withdrawing species such as 2-NO_2 (Table 2, entry 1c) decelerated it. Moreover, substituents causing steric hindrance namely 1-naphtyl (Table 2, entry 1n) and also *ortho* substitutions

Table 2. Oxidative Dihydrogenetaion of DDihydropirimidinone

Entry	R_1	R_2	Time (h)	Yield (%)	Ref.
1a	C_6H_5	Me	4	91	[30]
1b	4-F-C_6H_4	Me	7	85	[1]
1c	2- NO_2-C_6H_4	Et	10	74	[48]
1d	3- NO_2-C_6H_4	Me	6	85	[30]
1e	4- NO_2-C_6H_4	Me	7	81	[30]
1f	2-Cl-C_6H_4	Me	8	80	[48]
1g	4-Cl-C_6H_4	Me	6	83	[30]
1h	2-MeO-C_6H_4	Me	4	85	[48]
1i	4-MeO-C_6H_4	Me	3	90	[48]
1j	2-Br-C_6H_4	Me	8	70	[48]
1k	3-Br-C_6H_4	Me	6	82	[30]
1l	4-Br-C_6H_4	Me	6	81	[48]
1m	2,4-Cl_2-C_6H_3	Me	9	70	New
1n	1-Naphtyl	Me	10	72	New
1o	4-Me-C_6H_4	Me	4	92	[30]
1p	2-Thiophen	Me	6	88	New
1q	2-Phenylethyl	Me	10	76	New
1r	C_7H_{15}	Et	12	70	[1]
1s	C_2H_5	Me	12	70	New

Conditions: Substrate (1 mmol), oxidant (0.5 mmol), CuI (1 mmol), MeCN (4 ml), 40 °C.

(Table 2, entries 1c, 1f, 1j and 1m) destabilize the intermediate and as a result decrease the reaction rate. In addition, aliphatic groups were also applied and since no stabilization effects were caused by these substitutions, the reactions were accomplished in longer reaction times.

Thiocyanation of Aromatic Compounds (Scheme 5)

In order to study the thiocyanation reaction, 3-thiocyanato-1*H*-indole was used as the model reaction to evaluate various parameters for instance solvents, the amounts of KSCN, HOAC and THPDPE. The collected data led to the optimized reaction conditions; aromatic substrate (1 mmol), peroxide (1 mmol), KSCN (1 mmol), HOAC (0.2 mmol), and H_2O (4 m1) (Table 3).

To understand the scope of the reaction, various substrates were applied to the optimized reaction conditions. Some anilines and phenols underwent selectively *p*-thiocyanated (Table 4, entries 2g, 2i-2k). As presented in Table 4, substrates containing electron donating functionalities are involved in the reactions in shorter

Table 3. Optimization of the Reaction Condition for Thioyanation of Indole

Entry[a]	Oxidant (mmol)	Solvent (4 ml)	HOAc (mmol)	Time (min)	Yield (%)[b]
1	THPDPE (0.5)	H_2O	0.2	25	92
2	THPDPE (0.8)	H_2O	0.2	10	93
3	THPDPE (1)	H_2O	0.2	4	95
4	THPDPE (1.2)	H_2O	0.2	4	91
5	THPDPE (1)	H_2O	-	12	94
6	THPDPE (1)	H_2O	0.1	10	95
7	THPDPE (1)	H_2O	0.3	4	95
8	THPDPE (1)	MeCN	0.1	15	93
9	THPDPE (1)	CCl_4	0.1	60	70
10	THPDPE (1)	1,4-Dioxane	0.1	40	75
11	UHP (1)	H_2O	0.1	100	40
12	H_2O_2 (1)	H_2O	0.1	120	10

[a]Conditions: aromatic substrate (1 mmol), room temperature. [b]Isolated yields.

Table 4. Thiocyanation of Aromatic Compounds Promoted by THPDPE

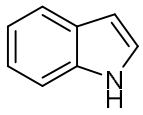
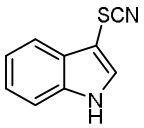
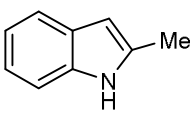
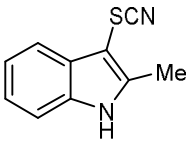
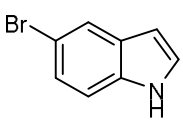
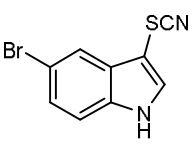
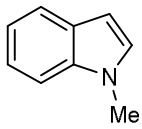
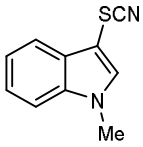
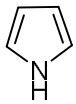
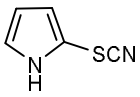
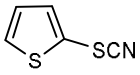
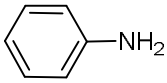
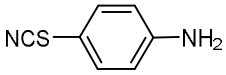
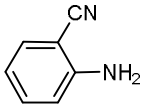
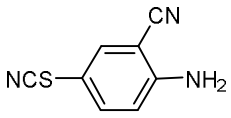
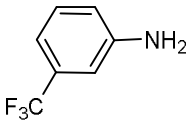
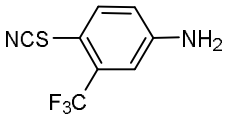
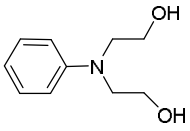
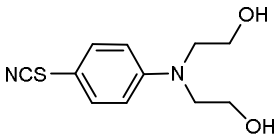
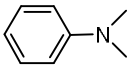
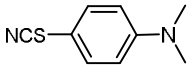
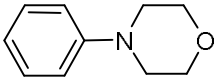
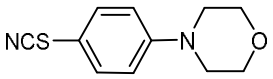
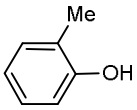
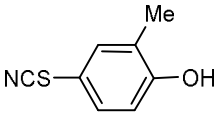
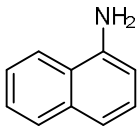
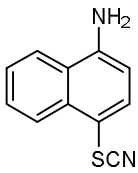
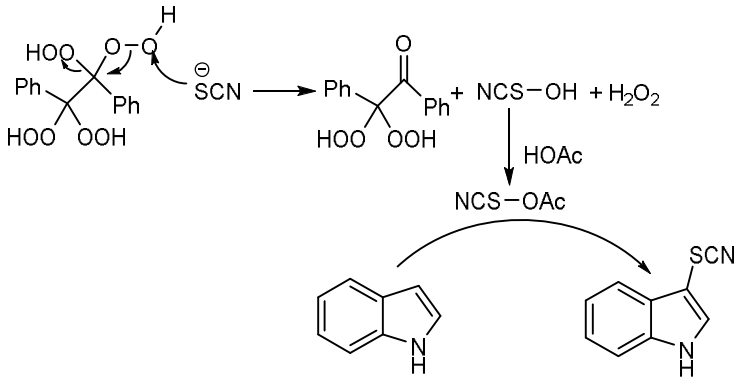
Entry	Substrate	Product	Time (min)	Yield (%)	Ref.
2a			4	95	[41]
2b			10	87	[41]
2c			12	89	[41]

Table 4. Continued

2d			5	90	[41]
2e			10	91	[41]
2f			15	80	[49]
2g			15	89	[49]
2h			65	87	[41]
2i			70	85	[41]
2j			25	82	[41]
2k			15	89	[49]
2l			35	88	[41]
2m			10	92	[49]
2n			40	90	[41]

[a]Conditions: Aromatic substrate (1 mmol), peroxide (1 mmol), KSCN (1 mmol), HOAC (0.2 mmol), H_2O (4 ml), at room temperature. [b]Isolated yields.



Scheme 5. Suggested mechanism for thiocyanation

Table 5. Efficiency Comparison of the Present Work with some Reported Methodologies for the Synthesis of 3-Thiocyanato-1*H*-indole

Entry	Reagent	Conditions	Time	Yield	Ref.
1	THPDPE	KSCN/HOAc/H_2O/rt	4	95	This work
1	Oxone	NH_4SCN/MeOH/rt	43	98	[50]
2	UHP	SSA/KSCN/H_2O/rt	40	95	[41]
3	H_2O_2	SBSA/KSCN/H_2O/rt	19	90	[41]
4	I_2O_5	NH_4SCN/MeOH/rt	19.8	93	[51]
5	I_2	NH_4SCN/MeOH/rt	50	85	[52]
6	Diethyl azodicarboxylate	NH_4SCN/CH_3CN/rt	45	85	[53]
7	H_2O_2	SiO_2-$VO(OH)_2$/ KSCN/H_2O/rt	45	96	[54]

reaction times and higher yields (Table 4, entries 2b, 2d and 2m). Investigation through the effect of halogens such as Br (Table 4, entry 2c) revealed that the reaction takes place in a longer time, however it affords the desired product in a high yield. The effects of inductive and resonance withdrawing groups were also studied. As shown in Table 4, in the presence of CF_3 and CN (Table 4, entries 2h and 2i) the reactions were carried out in longer reaction times but with fairly high yields. In the case of *N*-substituted amines (Table 4, entries 2j, 2k and 2l), the products were yielded in the short reaction time and excellent yields. Other functional groups such as alcoholic hydroxyl group (Table 4, 2j and 2m) remained intact under the reaction conditions.

A proposed reaction mechanism is shown in Scheme 5. Initially, THPDPE reacts with SCN^- and generates benzophenone, hydrogen peroxide and SCNOH which in the presence of HOAC as the acid is able to produce SCN^+ and water. In the last step, SCN^+ attacks to indole and produces the corresponding thiocyanated derivative. The suggested mechanism, shown in Scheme 4, is an approval to this observation, as in the last step substrates with high electron content facilitate the nucleophilic attack to SCN^+.

Hence, electron-releasing substitutions accelerate the rates of the reactions.

Finally, in order to investigate the potential of THPDPE, the collected results toward the synthesis of 3-thiocyanato-1*H*-indole in the present work were compared with several reported methodologies. As shown in Table 5, in comparison with other applied reagents such as oxone, UHP, H_2O_2, I_2O_5, I_2 and diethyl azodicarboxylate in the presence of some catalysts, TDHPE has proved its potential to carry out the reaction in a shorter reaction time and higher yield under mild and catalyst free reaction conditions.

CONCLUSIONS

In conclusion, this work demonstrated a facile, efficient, simple and convenient methodology for the oxidative dehydrogenation of dihydropyrimidinones and thiocyanation of aromatic compounds using 1,1,2,2-tetrahydroperoxy-1,2-diphenylethane. Short reaction times, easy work-up, and good to high yields of the products are the notable advantages of the presented methodology. Also, THPDPE as a stable solid comparatively non-toxic oxidant which can be stored for several months without any loss in its activity proved its potential to carry out the reactions under mild reaction conditions.

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