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Experimental and theoretical study on a one-pot, three-component route to 3,4-dihydropyrimidin-2(1*H*)-ones/thiones $TiCl_3OTf$-[bmim]Cl

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Abstract In this study a synthetic method using $TiCl_3OTf$-ionic liquid was reported for synthesis of 3,4-dihydropyrimidin-2(1*H*)-ones/thiones (3,4-DHPMs). Condensation reactions were carried out for aldehydes, ethyl acetoacetate, and ammonium acetate. In the reaction 1-butyl-3-methylimidazolium chloride ([bmim]Cl) was used as an ionic liquid in the presence of $TiCl_3OTf$ catalyst under solvent-free conditions at 140 °C. The advantages of this method are high yield of product, short reaction time, and reusable catalyst. A mechanism was proposed for this condensation reaction, and all steps of the suggested mechanism were confirmed by density functional theory calculations using the B3LYP/6-311G level of theory.

Keywords Ionic liquid · 3,4-Dihydropyrimidin-2(1*H*)-ones · $TiCl_3OTf$ · [bmim]Cl · DFT · Mechanism

Introduction

In many bioactive natural products and therapeutic compounds, heterocyclic moiety is a very important structure. The preparation method of potential biologically active substances includes multicomponent reactions. For example, the Biginelli type product is very important due to possessing some biological and pharmacological activities. 3,4-DHPMs have appeared as essential pillars of some calcium channel blockers and prevent the binding of HIVgp-120-CD4 cells [1, 2]. A simple one-pot condensation synthesis of an aldehyde, β-ketoester, and urea was reported by Biginelli [3]. The Biginelli type products can be synthesized using different catalysts

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and conditions. [4–8]. One-pot synthesis that includes environmentally friendly chemical processes, and is economically sustainable has received attention as a next policy for 'green' organic syntheses [9].

The growth of very active, stable, friendly to environment, and economically practicable catalysts has been an important objective for chemists in organic synthesis. Lately, ionic liquids have been demonstrated to be an effective method to improve the catalytic activity and its recycling process in organic synthesis. It has been reported that a combinational system of $TiCl_3OTf$-ionic liquid serves as an active catalyst for the synthesis of thioamides and arylnitriles from aldoximes [10, 11]. Here, following further research on this catalytic system, we would like to report a one-pot procedure for the synthesis of some 3,4-dihydropyrimidin-2(1*H*)-ones/thiones using $TiCl_3OTf$-[bmim]Cl (Scheme 2). The advantage of this method is synthesis of Biginelli type product in the green chemistry condition with high yields and short reaction times. Furthermore, the theoretical and experimental data were used to propose the mechanism for this condensation reaction.

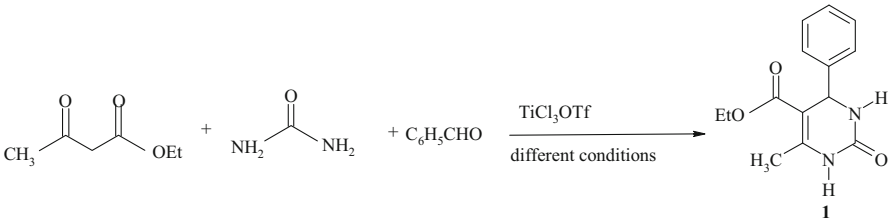
Experimental section

General procedure

In a model reaction (Scheme 1), an equivalent amount of benzaldehyde (1 mmol), ethyl acetoacetate (1 mmol), and urea (1.2 mmol) was studied with different ionic liquids (ILs) in the presence of small amount of the $TiCl_3OTf$ catalyst. The effects of solvents, temperature, time of reaction, and amount of catalyst were studied for the rate of reaction. The results are summarized in Table 1. Ethanol, acetonitrile, and dichloromethane were also used as solvents in this reaction. These solvents made the reaction slow with lower yields. However, the combination of $TiCl_3OTf$ with [bmim]Cl at a reaction temperature of 140 °C displayed the best result (Table 1, entry 6).

Results and discussion

Based on the optimized theoretical results, we studied the substrate scope in a Biginelli reaction. In these reactions various aromatic aldehydes with different substituents were used at the optimized reaction conditions. In order to study the



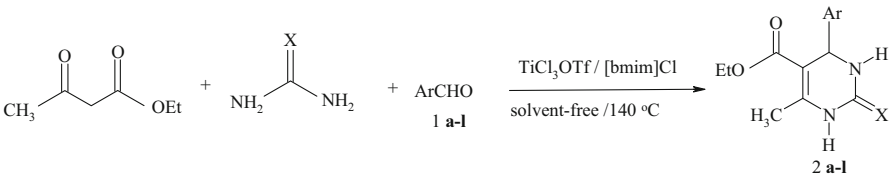
Scheme 1 Synthesis of ethyl 6-methyl-4-phenyl-3,4-dihydropyrimidin-2(1*H*)-one-5-carboxylate using $TiCl_3$ OTf-[bmim]Cl under different conditions

Table 1 Synthesis of ethyl 6-methyl-2-oxo-4-phenyl-1,2,3,4-tetrahydropyrimidin-5-carboxylate **1** in different conditions

Entry	Catalyst (15 % mol)	Solvent (5 mL)/IL (2 mmol)	Temperature (°C)	Time (min)[a]	Yield %[b]
1	$TiCl_3OTf$	CH_3CN	Reflux	120	25
2	$TiCl_3OTf$	C_2H_5OH	Reflux	150	70
3	$TiCl_3OTf$	CH_2Cl_2	Reflux	135	20
4	$TiCl_3OTf$	[bmim]OTf	140	20	45
5	$TiCl_3OTf$	[bmim]Br	140	20	73
6	$TiCl_3OTf$	[bmim]Cl	140	20	90
7	$TiCl_3OTf$	[bmim]Cl	120	45	84
8	$TiCl_3OTf$	[bmim]Cl	90	70	70

[a] The times are given after maximum progression of the reaction

[b] Isolated yield



Scheme 2 The synthesis of Biginelli-type products in the presence of $TiCl_3OTf$ as catalyst and [bmim]Cl as ionic liquid

generality of this procedure, using a similar process, a series of 3,4-dihydropyrimidin-2(1*H*)-ones were synthesized (Scheme 2).The results are shown in Table 2.

The reactions, which were carried out at a temperature of 140 °C, were completed in 15–50 min under the abovementioned conditions. The steric effect of ortho-substituents has relatively little influence on the reaction time and yield. As it is presented in Table 2, 2-chlorobenzaldehyde and 2-bromobenzaldehyde reacted slower than 4-chlorobenzaldehyde and 4-bromobenzaldehyde. A minor electronic effect was also observed. For example, aldehydes with an electron-withdrawing group such as 4-nitrobenzaldehyde enhanced the rate of reaction, while the presence of electron-rich groups such as 4-methyl or 4-methoxy diminished the rate of reaction. Moreover, thiourea was used at similar conditions to prepare the corresponding 3,4-dihydropyrimidin-2(1*H*)-thiones. According to these experimental data and theoretical data (Table 3), the following mechanism was proposed (scheme 3).

*Ethyl 6-methyl-2-oxo-4-phenyl-1,2,3,4-tetrahydropyrimidine-5-carboxylate (**2a**)* mp. 201–203 °C (204–206 °C [7]); UV/Vis (CH_3CN), λ_{max} (log ε_{max}): 274.4 nm (4.01), 228.6 (3.91); IR, $\tilde{\nu}/cm^{-1}$: 1720 ($CO_2C_2H_5$), 1700 (2-CO), 1640 (C=C); ^1H NMR

Table 2 One-pot synthesis of 3,4-dihydropyrimidin-2(1*H*)-ones/thiones using $TiCl_3OTf$-[bmim]Cl under solvent-free conditions at a reaction temperature of 140 °C

Comp.	X	Time (min)	Yield %
2a	O	20	90
2b	O	50	70
2c	O	25	90
2d	O	20	95
2e	O	40	80
2f	O	35	85
2g	O	35	90
2h	O	15	90
2i	O	20	95
2j	O	20	80
2k	O	30	85
2l	O	30	80
2a	S	30	65
2d	S	35	75
2l	S	40	70

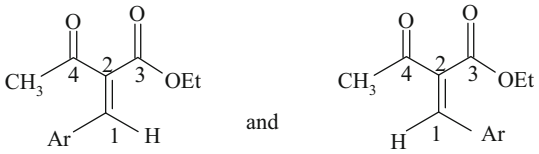
Table 3 Calculation of the Mullikan's charges on the different atoms *Z* and *E* isomers with a B3LYP/6-31G level

Comp.	*Z* isomer Atoms			*E* isomer Atoms		
	C1	C3	C4	C1	C3	C4
Ia	−2.108	−1.480	0.278	0.041	−0.697	0.227
Ib	−0.161	0.440	0.323	−0.140	0.485	0.286
Ic	−0.147	0.384	0.346	−0.168	0.470	0.346
Id	−0.168	0.432	0.343	−0.170	0.467	0.347
Ie	−2.294	−2.001	0.370	−0.116	−0.642	0.200
If	−2.432	−1.818	0.232	−0.043	−0.789	0.265
Ig	−2.225	−1.805	0.193	−0.057	−0.847	0.285
Ih	−2.182	−2.143	0.234	−0.013	−0.71	0.197
Ii	−2.308	−1.868	0.084	0.208	−0.723	0.245
Ij	−0.170	0.428	0.341	−0.173	0.465	0.345
Ik	−1.564	−1.796	0.261	−0.164	−0.588	0.161
Il	−2.313	−1.575	0.177	0.206	−0.687	0.259

(DMSO-d_6), δ: 1.08 (t, 3H, $J = 7.07$ Hz, OCH_2CH_3), 2.24 (s, 3H, CCH_3), 3.97 (q, 2H, $J = 7.07$ Hz, OCH_2CH_3), 5.14 (d, $J = 3$ Hz, 1H, C*CH*NH), 7.22–7.34 (m, 5H, Ar), 7.72 (s, 1H, NH), 9.17 (s, 1H, NH).

*Ethyl 6-methyl-4-(4-methylphenyl)-2-oxo-1,2,3,4-tetrahydropyrimidine-5-carboxylate (**2b**)* mp. 211–214 °C (212–215 °C [12]); UV/Vis (CH_3CN), λ_{max} (log ε_{max}): 276 nm (3.45), 232 (3.70); IR, $\tilde{\nu}/cm^{-1}$: 1710 ($CO_2C_2H_5$), 1700 (2-CO), 1650

Scheme 3 *E* and *Z* isomers of different benzylidenes of ethyl acetoacetate



E (I a-l) **Z (I a-l)**

(C=C); ^{1}H NMR (DMSO-d_6), δ: 1.12 (t, 3H, J = 7.5 Hz, OCH$_2$*CH$_3$*), 2.28, 2.30 (s, 3H), 4.00 (q, 2H, J = 7.5 Hz, O*CH$_2$*CH$_3$), 5.11 (d, 1H, J = 3.0 Hz, C*CH*NH), 7.25 (m, 4H), 7.70 (br s, 1H, NH), 9.19 (br s, 1H, NH).

Ethyl 6-methyl-4-(3-methylphenyl)-2-oxo-1,2,3,4-tetrahydropyrimidine-5-carboxylate ***(2c)*** mp. 211–214 °C (210–212 °C [13]); UV/Vis (CH$_3$CN), λ_{max} (log ε_{max}): 274 nm (3.47), 230 (3.75); IR, $\tilde{\nu}$/cm^{-1}: 1725 ($CO_2C_2H_5$), 1700 (2-CO), 1650 (C=C).

Ethyl 6-methyl-4-(2-methylphenyl)-2-oxo-1,2,3,4-tetrahydropyrimidine-5-carboxylate ***(2d)*** mp. 207–210 °C (208–209 °C [12]); UV/Vis (CH$_3$CN), λ_{max} (log ε_{max}): 276.5 nm (3.52), 227 (3.36); IR, $\tilde{\nu}$/cm^{-1}: 1700 ($CO_2C_2H_5$), 1645 (2-CO), 1595 (C=C).

Ethyl 4-(4-methoxyphenyl)-6-methyl-2-oxo-1,2,3,4-tetrahydropyrimidine-5-carboxylate ***(2e)*** mp. 201–202 °C (201–205 °C [7]); UV/Vis (CH$_3$CN), λ_{max} (log ε_{max}): 274 nm (3.47), 230 (3.75); IR, $\tilde{\nu}$/cm^{-1}: 1725($CO_2C_2H_5$), 1700 (2-CO), 1650 (C=C); ^{1}H NMR (DMSO-d_6), δ: 1.10 (t, 3H, J = 7.08 Hz, OCH$_2$*CH$_3$*), 2.23 (s, 3H, C*CH$_3$*), 3.71 (s, 3H, O*CH3*), 3.97 (q, 2H, J = 7.07 Hz, O*CH$_2$*CH$_3$), 5.09 (d, 1H, J = 2.9 Hz, C*CH*NH), 6.87 (d, 2H, J = 8.5 Hz, Ar), 7.14 (d, 2H, J = 8.5 Hz, Ar), 7.66 (s, 1H, NH), 9.15 (s, 1H, NH).

Ethyl 4-(3-methoxyphenyl)-6-methyl-2-oxo-1,2,3,4-tetrahydropyrimidine-5-carboxylate ***(2f)*** mp. 207–209 °C (207–208 °C [7]); UV/Vis (CH$_3$CN), λ_{max} (log ε_{max}): 276.5 nm (3.52), 227 (3.36); IR, $\tilde{\nu}$/cm^{-1}: 1700 ($CO_2C_2H_5$), 1645 (2-CO), 1595 (C=C); ^{1}H NMR (DMSO-d_6), δ: 1.10 (t, 3H, J = 7 Hz, OCH$_2$*CH$_3$*), 2.24 (s, 3H, C*CH$_3$*), 3.72 (s, 3H, O*CH$_3$*), 3.99 (q, 2H, J = 7 Hz, O*CH$_2$*CH$_3$), 5.11 (d, 1H, J = 2.2 Hz, C*CH*NH), 6.77–6.83 (m, 3H, Ar), 7.24 (t, 1H, J = 7.8 Hz, Ar), 7.73 (s, 1H, NH), 9.19 (s, 1H, NH).

Ethyl 4-(2-methoxyphenyl)-6-methyl-2-oxo-1,2,3,4-tetrahydropyrimidine-5-carboxylate ***(2g)*** mp. 259–260 °C (262–263 °C [7]); UV/Vis (CH$_3$CN), λ_{max} (log ε_{max}): 276.5 nm (3.52), 227 (3.36); IR, $\tilde{\nu}$/cm^{-1}: 1700 ($CO_2C_2H_5$), 1645 (2-CO), 1595 (C=C); ^{1}H NMR (DMSO-d_6), δ: 1.06 (t, 3H, J = 7.04 Hz, OCH$_2$*CH$_3$*), 2.07 (s, 3H, C*CH$_3$*), 3.87 (s, 3H, O*CH$_3$*), 4.04 (q, 2H, J = 7.04 Hz, O*CH$_2$*CH$_3$), 5.58 (s, 1H, C*CH*NH), 6.57–6.93 (m, 1H, Ar), 7.01–7.07 (m, 2H, Ar), 7.24–7.33 (m, 1H, Ar), 7.56 (s, 1H, NH), 9.12 (s, 1H, NH).

Ethyl 4-(4-chlorophenyl)-6-methyl-2-oxo-1,2,3,4-tetrahydropyrimidine-5-carboxylate ***(2h)*** mp. 209–211 °C (210–212 °C [14]); UV/Vis (CH_3CN), λ_{max} (log ε_{max}): 280 nm (3.46), 233 (3.27); IR, $\tilde{\nu}/cm^{-1}$: 1720 ($CO_2C_2H_5$), 1690 (2-CO), 1615 (C=C); ^1H NMR (DMSO-d_6), δ: 1.15 (t, 3H, $J = 7.2$ Hz, OCH_2CH_3), 2.33 (s, 3H, CCH_3), 4.10 (q, 2H, $J = 7.8$ Hz, OCH_2CH_3), 5.30 (s, 1H, C*CH*NH), 7.26–7.33 (m, 4H, Ar), 7.69 (s, 1H, NH), 9.17 (s, 1H, NH).

Ethyl 4-(3-chlorophenyl)-6-methyl-2-oxo-1,2,3,4-tetrahydropyrimidine-5-carboxylate ***(2i)*** mp. 193–195 °C (197–198 °C [7]); UV/Vis (CH_3CN), λ_{max} (log ε_{max}): 278.5 nm (3.52), 229 (3.36); IR, $\tilde{\nu}/cm^{-1}$: 1710 ($CO_2C_2H_5$), 1690 (2-CO), 1650 (C=C); ^1H NMR (DMSO-d_6), δ: 1.08 (t, 3H, $J = 7.0$ Hz, OCH_2CH_3), 2.24 (s, 3H, CCH_3), 3.98 (q, 2H, $J = 7.0$ Hz, OCH_2CH_3), 5.14 (s, 1H, C*CH*NH), 7.36–7.17 (m, 4H, Ar), 7.7 (s, 1H, NH), 9.24 (s, 1H, NH).

Ethyl 4-(2-chlorophenyl)-6-methyl-2-oxo-1,2,3,4-tetrahydropyrimidine-5-carboxylate ***(2j)*** mp. 216–218 °C (218–219 °C [7]); UV/Vis (CH_3CN), λ_{max} (log ε_{max}): 278.5 nm (3.52), 229 (3.36); IR, $\tilde{\nu}/cm^{-1}$: 1705 ($CO_2C_2H_5$), 1690 (2-CO), 1635 (C=C); ^1H NMR (DMSO-d6), δ 0.98 (t, 3H, $J = 6.9$ Hz, OCH_2CH_3), 2.28 (s, 3H, CCH_3), 3.87 (q, 2H, $J = 6.9$ Hz, OCH_2CH_3), 5.61 (d, 1H, $J = 2.98$ Hz, C*CH*NH), 7.28–7.33 (m, 3H, Ar), 7.36–7.39 (m, 1H), 7.70 (s, 1H, NH), 9.25 (s, 1H, NH).

Ethyl 4-(4-bromophenyl)-6-methyl-2-oxo-1,2,3,4-tetrahydropyrimidine-5-carboxylate ***(2k)*** mp. 210–212 °C (213–215 °C [15]); UV/Vis (CH_3CN), λ_{max} (log ε_{max}): 285 nm (3.35), 230 (3.30); IR, $\tilde{\nu}/cm^{-1}$: 1710 ($CO_2C_2H_5$), 1685 (2-CO), 1610 (C=C); ^1H NMR (DMSO-d6), δ: 1.13 (t, 3H, $J = 7.0$ Hz, OCH_2CH_3); 2.29 (s, 3H, CCH_3), 4.02 (q, 2H, OCH_2CH_3, $J = 7.0$ Hz,), 5.17 (d, 1H, J = 2.2 Hz, C*CH*NH), 7.23 (d, 2H, $J = 8.2$ Hz,), 7.56 (d, 2H, $J = 8.2$ Hz,), 7.80 (s, 1H), 9.28 (s, 1H).

Ethyl 4-(3-bromophenyl)-6-methyl-2-oxo-1,2,3,4-tetrahydropyrimidine-5-carboxylate ***(2l)*** mp. 190–193 °C (196–197 °C [16]); UV/Vis (CH_3CN), λ_{max} (log ε_{max}): 275 nm (3.45), 235 (3.25); IR, $\tilde{\nu}/cm^{-1}$: 1700 ($CO_2C_2H_5$), 1680 (2-CO), 1615 (C=C).

Ethyl 4-(2-bromophenyl)-6-methyl-2-oxo-1,2,3,4-tetrahydropyrimidine-5-carboxylate ***(2m)*** mp. 198–200 °C (205–207 °C [16]); UV/Vis (CH_3CN), λ_{max} (log ε_{max}): 280 nm (3.40), 228 (3.32); IR, $\tilde{\nu}/cm^{-1}$: 1720 ($CO_2C_2H_5$), 1680 (2-CO), 1600 (C=C).

Ethyl 6-methyl-4-(4-nitrophenyl)-2-oxo-1,2,3,4-tetrahydropyrimidine-5-carboxylate ***(2n)*** mp. 207–209 °C (207–208 °C [7]); UV/Vis (CH_3CN), λ_{max} (log ε_{max}): 264 nm (3.31), 225 (3.17); IR, $\tilde{\nu}/cm^{-1}$: 1725 ($CO_2C_2H_5$), 1700 (2-CO), 1640 (C=C); ^1H NMR (DMSO-d6), δ: 1.09 (t, 3H, $J = 6.9$ Hz, OCH_2CH_3), 2.26 (s, 3H, C*CH3*), 3.98 (q, 2H, $J = 7.2$ Hz, OCH_2CH_3), 5.27 (d, 1H, $J = 3.3$ Hz, C*CH*NH), 7.49–7.52 (m, 2H, Ar), 7.89 (s, 1H, NH), 8.20–8.23 (m, 2H, Ar), 9.36 (s, 1H, NH).

Ethyl 6-methyl-4-(3-nitrophenyl)-2-oxo-1,2,3,4-tetrahydropyrimidine-5-carboxylate ***(2o)*** mp. 223–225 °C (226–227 °C [17]); UV/Vis (CH_3CN), λ_{max} (log ε_{max}): 264 nm (3.31), 225 (3.17); IR, $\tilde{\nu}/cm^{-1}$: 1720 ($CO_2C_2H_5$), 1690 (2-CO), 1640 (C=C); ^1H NMR (DMSO-d6), δ: 1.09 (t, 3H, $J = 7.0$ Hz, OCH_2CH_3), 2.26 (s, 3H, CCH_3),

3.98 (q, 2H, $J = 7.0$ Hz, OCH_2CH$_3$), 5.30 (d, 1H, $J = 2.5$ Hz, C*CH*NH), 7.62–7.71 (m, 2H, Ar), 7.90 (s, 1H, NH), 8.08–8.15 (m, e)

Theoretical section

Structural and electronic characteristics of the abovementioned compounds were calculated using B3LYP/6-311G. The optimized geometries were analyzed in the following sections. All computations were carried out using the Gaussian 98 package [18].

Electronic parameters

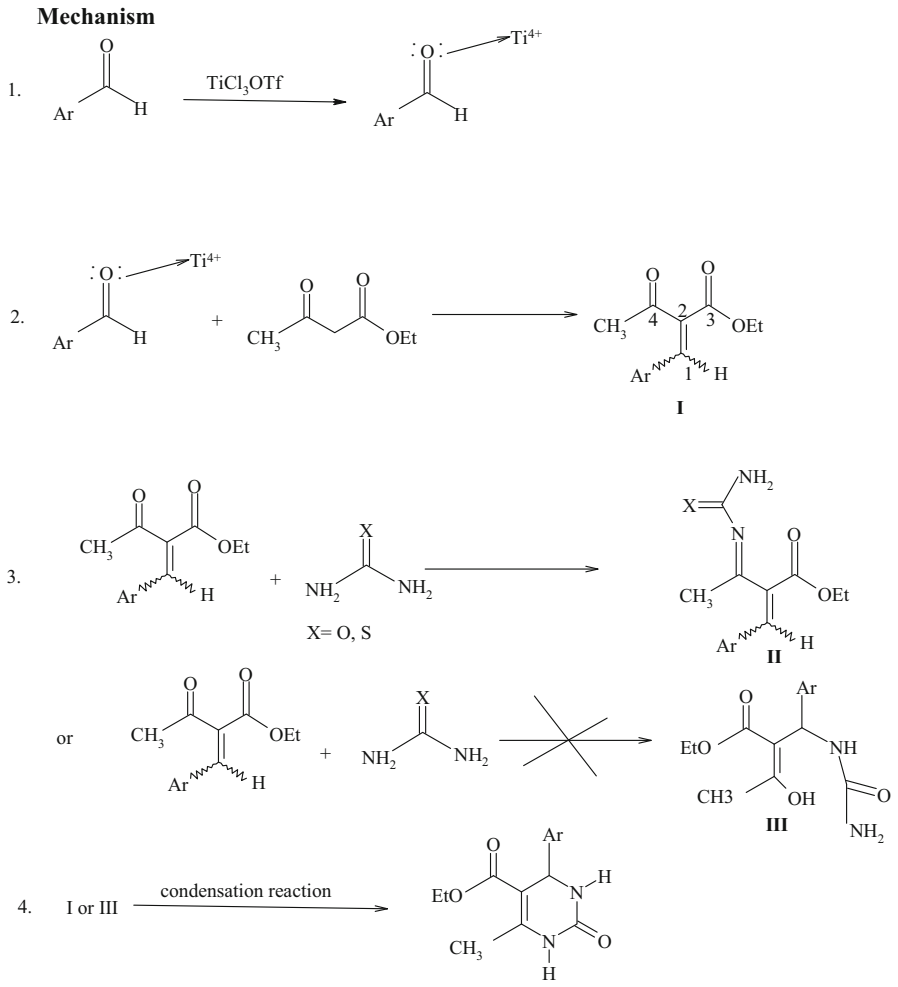
Currently, numerous attempts have been made to study molecules from theoretical point of views. Among different quantum mechanical methods, density functional theory (DFT) provides a reasonable theoretical framework for the study of both reactivity and selectivity of molecular systems [19]. In this study the Mullikan's charges were calculated on the different atoms of some benzylidene derivatives and aldehydes (Scheme 3), (Tables 3, 4).

Analysis of data reported in the Table 3, shows that nucleophilic attachment on the C4 atom is times as fast as C1 atom in two isomers. (Scheme 4 entry 3) Furthermore, Mullikan's charges on the N atom on the urea and thiourea are −0.594 and −0.484, respectively. These data are in agreement with time reactions for synthesis of Biginelli type products.

Comparison of the Mullikan's charges on carbon atoms of aldehydes demonstrated that the charge densities on the carbon atom of carbonyl groups are more positive. However, nucleophilic attachment can be carried out on the carbonyl group of aldehydes is times as fast as C1 atom of benzylidene compounds.

Table 4 Calculation of the Mullikan's charges on the carbonyl group of some different aldehydes with a B3LYP/6-31G level

Comp.	CHO
1a	0.160
1b	0.160
1c	0.163
1d	0.174
1e	0.159
1f	0.155
1g	
1h	0.348
1i	0.174
1j	0.259
1k	0.239
l	0.244



Scheme 4 Proposed mechanism for synthesis of DHPMs by using $TiCl_3$ OTf-[bmim]Cl

Conclusion

We have introduced a new procedure for preparation of 3,4-dihydropyrimidin-2(1*H*)-ones/thiones using $TiCl_3$OTf-[bmim]Cl as catalyst. High yield, short time of reaction, easy work-up, and no use of toxic solvents are the advantages of this method. Furthermore, comparative results of the experimental and theoretical investigation were reported for some 3,4-dihydropyrimidin-2(1*H*)-one. Finally a mechanism was proposed for this synthetic reaction.

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