

Synthesis of Ditetrahydrofurfuryl Carbonate as a Fuel Additive Catalyzed by Aminopolycarboxylate Ionic Liquids

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Received: 12 December 2016 / Accepted: 27 March 2017 / Published online: 4 April 2017 © Springer Science+Business Media New York 2017

Abstract A new series of aminopolycarboxylate ionic liquids were designed, synthesized, and applied for efficient and selective synthesis of ditetrahydrofurfuryl carbonate (DTC). Tetraethylammonium nitrilotriacetate

 $([N_{2222}]_3[NTA])$ was demonstrated to show the best catalytic performance, in which DTC could be obtained at a yield of 80% under optimum conditions.



Keywords Fuel additive · Dimethyl carbonate · Transesterification · Ionic liquids

1 Introduction

Organic carbonates (OCs), such as dimethyl carbonate (DMC) and diethyl carbonate (DEC), have numerous applications in lubricating oils, fuel additives, solvents, reaction intermediates, and polymeric materials [1–4]. Particularly, in the field of fuel additives, OCs are expected to improve energy efficiency and reduce particulate matter emissions for decreasing energy consumption and protecting our environment [5, 6]. As a potential oxygenated fuel additive, ditetrahydrofurfuryl carbonate (DTC) is considered to be a better substitute for DMC and DEC, owing to its distinct properties such as high oxygen contents (35 wt%), high boiling point, and good mutual solubility with diesel fuel (Table S1, Electronic supplementary material). In terms of these advantages, the demand of DTC will be growing

Electronic supplementary material The online version of this article (doi:10.1007/s10562-017-2043-3) contains supplementary material, which is available to authorized users.

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¹ College of Chemistry and Chemical Engineering, Jiangxi Inorganic Membrane Materials Engineering Research Centre, Jiangxi Normal University, Nanchang 330022, People's Republic of China fast accompany with the development of facile synthesis of DTC.

Traditionally, the efficient catalytic synthesis of OCs such as DEC and DTC requires highly toxic phosgene as a raw material [7]. Despite the excellent performance of such phosgene technology, the phosgene-free synthesis of OCs with a more environmentally friendly process continues to be appealing. Recently, the transesterification of DMC with alkyl alcohols has attracted much attention as the alternative route for the synthesis of OCs, with the advantages of low pollution, green raw material, and mild reaction conditions [8–11]. Till now, various heterogeneous catalysts such as K₂CO₃/AC (AC, active carbon),[12] CaO,[13] KF/Al_2O_3 ,[14] NaOH/ γ -Al_2O_3,[15] K₂CO₃/ZrO₂,[16] and $TiO_2@SiO_2$,[17] had been reported for efficient synthesis of OCs. For example, Fan and Zhang had found that the supported K₂CO₃/AC catalyst showed higher activity for the transesterification reaction of DMC with propyl alcohol [12]. Bai et al. had studied the synthesis of glycerol carbonate from DMC and glycerol using NaOH/y-Al₂O₃ as catalyst [15]. Tang et al. reported that the transesterification of DMC with phenol in the presence of core-shell $TiO_2@$ SiO₂ could obtain diphenyl carbonate with a yield of 24% at 9 h [17].

However, to our best knowledge, there is no mention of efficient synthesis of DTC from the transesterification of DMC with tetrahydrofurfuryl alcohol (THFA) in any studies. Moreover, those solid basic catalysts usually suffer from many inherent drawbacks such as complex preparation, high mass transfer resistance, easy deactivation, and harsh reaction conditions. There remains a strong need to develop novel catalyst materials with high efficiency and selectivity for facile synthesis of OCs, especially for DTC.

Recently, ionic liquids (ILs) have been received more attention and successfully applied for many catalytic reactions owing to their favorable properties such as environmentally friendly, high thermal stability, nonvolatility, and structural variety [18–20]. Thus, basic ILs possessing certain basicities could present a broad application prospect in the catalytic synthesis of OCs through the transesterification reaction. Herein, we designed and prepared a new series of aminopolycarboxylate ionic liquids (APC-ILs), and they were introduced for the first time into the transesterification of DMC with THFA to obtain high-yielding DTC (Scheme 1). Nuclear magnetic resonance (NMR) spectra investigations and density functional theory (DFT) calculations were further performed to clarify the catalysis of APC-ILs. Moreover, the reaction parameters such as reaction time, temperature, catalyst loading, and molar ratio of reactants were explored in detail to obtain the optimum conditions. The reusability of APC-ILs and the transesterification of DMC with other alcohols were also studied.

2 Experimental Section

2.1 Materials

Tetraethylammonium hydroxide (25 wt% aqueous solution) was purchased from Sigma-Aldrich. THFA (purity \geq 99%), cyclopentanol (purity \geq 99%), pipecolinic acid (purity \geq 99%), iminodiacetic acid (purity \geq 99%), nitrilotriacetic acid (purity \geq 99%) were purchased from Aladdin Chemical Reagent Co. Ltd. (Shanghai, China). Other reagents such as DMC, alcohol, triethyl amine, sodium carbonate, and sodium hydroxide were of analytical grade and used without any further purification.

2.2 Preparation and Characterization of APC-ILs

The preparation method of three APC-ILs was similar to the procedure described in our previous works [21], as follows. A stoichiometric ratio of $[N_{2222}]$ OH aqueous solution was neutralized with pipecolinic acid, iminodiacetic acid, and nitrilotriacetic acid by stirring at room temperature for 6 h, respectively. After neutralization, water was evaporated under reduced pressure at 60 °C. Then these three APC-ILs were heated to 90 °C in a vacuum oven containing P_2O_5 for 48 h to remove the residual



Scheme 2 Structures of three APC-ILs



water prior to use. The structures of APC-ILs (Scheme 2) were confirmed by NMR, FTIR spectra, CHN elements and thermal analysis. All the detailed characterization results were given in the Supporting Information.

2.3 Typical Procedures for the DTC Synthesis

The transesterification reaction was carried out in a 50 mL round-bottomed flask, equipped with a condenser, thermostat and magnetic stirring. A calculated amount of DMC, THFA, and APC-ILs were added to the reactor, and the reaction mixture was stirred and allowed to proceed for 0.5-2.5 h with the heating at the designed temperature (e.g., 130°C). After the reaction was completed, qualitative analyses of products were examined by a Thermo Trace 1300 GC-ISQ, and quantitative analyses were carried out by a GC-FID (Agilent 7890B) equipped with a capillary column HP-5 (methyl polysiloxane, 30 m \times 0.32 mm \times 1 µm). The detailed analysis conditions were described as follows: The temperatures of injector and detector were 280 and 250 °C, respectively. The column temperature was increased stepwise to 200 °C, holding at 80 °C for 2 min, increasing to 200°C at 40°C min⁻¹, holding at 240 °C for 3 min. Then the conversion of DMC and yield of DTC were calculated according to the area of chromatograph peaks using 1.3.5-trimethylbenzene as an internal standard. After the completion of reaction, the reaction system was cooled down to room temperature and extracted with deionized water, and the system thus forms a liquid-liquid biphase, and the aqueous phase containing APC-ILs could be easily separated by simple decantation. After that, the catalyst APC-ILs were further heated in a vacuum oven at 90 °C for 6 h to remove water and the residual reactants. The water content of recycled APC-ILs was measured prior to the next run and checked to be less than 0.15 wt% by the Karl Fisher titration.

2.4 Quantum Computation

Theoretical calculations were performed at the DFT level using the B3LYP hybrid functional, as implemented in the Gaussian 09 software package [22]. And the 6-31G(d,p) basis set was adopted for all the structural optimizations and natural bond orbital (NBO) charge analysis of each APC-ILs. Frequency calculations were performed to confirm geometries were true minimum and to obtain thermo-dynamic data.

3 Results and Discussion

3.1 Catalytic Performance of APC-ILs

Our work started with the screening of APC-ILs for catalytic synthesis of DTC. The results obtained are presented

 Table 1
 The transesterification of DMC with THFA using various catalysts

Entry	Catalyst	Conversion of DMC (%)	Yield of DTC (%)	Yield of MTC (%)
1	[N ₂₂₂₂] ₃ [NTA]	97	80	17
2	[N ₂₂₂₂] ₂ [IDA]	96	71	25
3	[N ₂₂₂₂][Pipe]	95	65	30
4	NaOH	94	58	36
5	Na ₂ CO ₃	93	55	38
6	Et ₃ N	65	18	47
7	DBU	75	13	62
8	Na ₃ (NTA)	41	Trace	41
9	L-Proline	11	7	4
10	Amberlite-IRA400	47	29	18
11 ^a	K ₂ CO ₃ /ZrO ₂	71	5	66
12 ^b	[N ₂₂₂₂] ₃ [NTA]	89	55	34

Reaction conditions: catalyst loading (0.5 wt%), molar ratio of THFA to DMC (4:1), reaction time (2 h), reaction temperature (130 $^{\circ}$ C)

^aThe catalyst was prepared according to the reference [16]

^b2 wt% water was added into the reaction mixture

in Table 1. It is found that three APC-ILs show different catalytic activities and the sequence of catalytic performance is $[N_{2222}]_3[NTA] > [N_{2222}]_2[IDA] > [N_{2222}][Pipe]$ (entries 1-3). That is to say, the more carboxylate groups the APC-ILs possess, the higher the yield of DTC. Among these APC-ILs, [N₂₂₂₂]₃[NTA] possessing three carboxylate groups catalyzed the reaction to have the highest conversion of DMC (97%) and yield of DTC (80%). This implies that the carboxylate group of APC-ILs is favorable to the synthesis of DTC. Subsequently, several other typical basic catalysts were studied for comparison (entries 4-10). The results showed that four typical inorganic and organic base catalysts had high conversions of DMC but low yields of DTC (entries 4-7). Solid bases Na₃(NTA), L-proline, Amberlite-IRA400 resin, and K₂CO₃/ZrO₂ also showed poor catalytic activity (entries 8-11). This demonstrates that the first step of the transesterification of DMC with THFA to form MTC is easily proceed but the second step of the formation of DTC is hard to perform in the presence of those conventional base catalysts [23]. In addition, the pH values of those three APC-ILs aqueous solution were further explored. As can be seen in Table S2, it is indicated that $[N_{2222}]_3$ [NTA] has a relatively low basicity but shows an excellent catalytic performance. This demonstrates that the basic sites of the APC-IL are not the key active sites in the transesterification of DMC with THFA. In order to clarify the catalysis behavior of APC-ILs, we performed ¹H NMR spectroscopy of THFA and the reaction mixture of THFA and APC-ILs to understand the catalytic mechanism in principle. It can be seen from Fig. 1 that all the OH **Fig. 1** ¹H NMR spectra of (*a*) THFA, (*b*) the mixture of THFA and $[N_{2222}]$ [Pipe], (*c*) the mixture of THFA and $[N_{2222}]_2$ [IDA], (*d*) the mixture of THFA and $[N_{2222}]_3$ [NTA]



signals of THFA became broad and were shifted downfield after adding APC-ILs, revealing that there exists hydrogen bonding interactions between THFA and APC-ILs [24, 25]. For example, the peak of hydroxyl group was observed at 4.42 ppm in the free THFA, while the OH signal in the mixture of THFA and [N₂₂₂₂]₃[NTA] were shifted downfield to 5.21 ppm. This shows that among these three APC-ILs, the hydrogen bonding interaction between THFA and [N₂₂₂₂]₃[NTA] are strongest. [N₂₂₂₂]₃[NTA] can activate THFA well through the hydrogen bond, and thus catalyze the transesterification to have the highest yield of DTC. Furthermore, the effect of water on the catalytic performance of [N₂₂₂₂]₃[NTA] was also studied (entry 12). It is found that the conversion of DMC and the yield of DTC were obviously reduced to 89 and 55%, respectively, when 2 wt% water was added into the reaction system. This demonstrates that water has a significant effect on the catalytic activity of [N2222]3[NTA] and it may remarkably break the intermolecular hydrogen bonding interaction of THFA with $[N_{2222}]_3$ [NTA], resulting in the decrease in DTC yield.

3.2 DFT Study

To get more insight into the catalysis of the carboxylate group of APC-ILs, we further calculated the geometry optimization for the free THFA and the complexes of THFA with APC-ILs, respectively. Then the binding energies of THFA with APC-ILs are given in Table 2, and the corresponding O–H bond lengths of THFA and

Table 2 The binding energy of THFA interaction with APC-ILs

Complex	THFA-[Pipe]	THFA-[IDA]	THFA-[NTA]
ΔE (KJ/mol)	-65.88	-92.30	-127.96
	E E		

 $\Delta E = E_{\text{complex}} - E_{\text{THFA}} - E_{\text{APC-IL}}$

hydrogen bonding lengths between THFA and APC-ILs are shown in Fig. 2. It can be seen that the binding energies between THFA and APC-ILs are calculated to be more than -60 kJ/mol, and all the O-H bond lengths in the complexes of THFA and APC-ILs are predicted to be stretched and are longer than that in the free THFA. This indicates that the intermolecular hydrogen bonding interactions between THFA and APC-ILs are strong, and result in an increase in the O-H bond length. [N₂₂₂₂]₃[NTA] enables THFA to have the longest O-H bond length compared with the other two APC-ILs, owing to its larger binding energies. Moreover, Fig. 3 shows the natural bond orbital (NBO) charges of carbon, hydrogen, and oxygen atoms in the free THFA and the complexes of THFA with APC-ILs. It is obvious that compared with the free THFA counterpart, the NBO negative charge of the oxygen atom O (1) increases from 0.452 to 0.629 in the presence of $[N_{2222}]_3$ [NTA]. This means that the nucleophilicity of THFA could improve effectively by interacting with [N₂₂₂₂]₃[NTA], and then it is favorable to make a nucleophilic attack to DMC. As a result, a high DTC yield can be obtained catalyzed by $[N_{2222}]_3[NTA].$



3.3 Optimization of Reaction Conditions

In order to obtain the optimum conditions, reaction parameters such as reaction time, temperature, catalyst amount, and initial molar ratio of reactants were studied in detail in the system of $[N_{2222}]_3$ [NTA]. Figure 4 shows the effect of reaction temperature on the synthesis of DTC at different temperatures ranging from 100 to 150 °C. It can be seen that the conversion of DMC and selectivity of DTC remarkably increase with the elevated temperature from 110 to 130 °C. However, when the temperature further increased to 150 °C, a slight drop in the selectivity of DTC was observed and the corresponding yield of DTC was reduced to 74%. It could be reasoned that the transesterification reaction of DMC with THFA is slightly exothermic and reversible. High reaction temperature would decrease the equilibrium constant and is favorable to the reverse of transesterification reaction, resulting in a decrease in the selectivity of DTC [20]. These indicating that the excessive high reaction temperature was not beneficial to the selectivity of DTC. Thus, an optimized reaction temperature would choose at 130 °C. Figure 5 shows the effect of reaction time on the reaction. It is found that the yield of DTC increases notably to 80% in the first 2 h but remains almost unchanged as reaction proceeds. Hence further increase in the reaction time is not very necessary. As a result, 2 h is identified as the optimal reaction time.

The effect of catalyst loading on the reaction was evaluated, and the results are shown in Fig. 6. The yield of DTC increases rapidly by increasing the amount of



Fig. 4 Effect of reaction temperature on the reaction. Reaction conditions: reaction time (2 h), molar ratio of THFA to DMC (4:1), catalyst (0.5 wt%)



Fig. 5 Effect of reaction time on the reaction. Reaction conditions: reaction temperature (130 °C), molar ratio of THFA to DMC (4:1), catalyst (0.5 wt%)

catalyst. The yields increased from 19 to 80% with the rise of catalyst loadings from 0.1 to 0.5 wt%. This shows that with an increase in the dosage of ILs, the total number of catalytic sites available for the reaction increases and thus the rate of transesterification is enhanced, resulting in a higher yield of DTC. However, as the catalyst loading further increases from 0.5 to 0.9 wt%, the conversion of DMC and yield of DTC remain almost unchanged. This means that too large catalyst loading is not favorable to this reaction, and 0.5 wt% is regarded as the optimal catalyst loading. Figure 7 shows the effect of



Fig. 6 Effect of catalyst loading on the reaction. Reaction conditions: reaction temperature $(130 \,^{\circ}\text{C})$, reaction time (2 h), molar ratio of THFA to DMC (4:1)



Fig. 7 Effect of molar ratio on the reaction. Reaction conditions: reaction temperature $(130 \,^{\circ}\text{C})$, reaction time (2 h), catalyst (0.5 wt%)

the THFA/DMC molar ratio from 1:1 to 5:1 on the reaction. The yield of DTC was obviously increased from 33 to 80% in 2 h, while the initial THFA/DMC molar ratio increased from 1:1 to 4:1. The reason for this phenomenon is that excess amount of THFA can shift the reaction equilibrium towards products. Nevertheless, the reaction rates in the initial molar ratio of 5:1 was just comparable to the case of 4:1, indicating that a further increase in the amount of THFA can not continue to improve the yield. Thus, the optimal THFA/DMC molar ratio for the production of DTC is 4:1.



Fig. 8 Recycle test of [N₂₂₂₂]₃[NTA] catalyst



Fig. 9 FTIR spectra of (a) fresh $[N_{2222}]_3[NTA]$ catalyst, and (b) used $[N_{2222}]_3[NTA]$ catalyst after five times run

3.4 Catalyst Recycles

The reusability of catalysts is very important for their industrial applications. Thus, the catalyst $[N_{2222}]_3$ [NTA] was recycled for five times in order to test its activity as well as stability. The results obtained in five consecutive runs are shown in Fig. 8. It is indicated that no obvious drop in both the conversion of DMC and selectivity of DTC was observed during these five successive recycles, which shows that the catalyst [N₂₂₂₂]₃[NTA] is stable enough. The slight decrease in the activity may be ascribed to the slight loss of the catalyst $[N_{2222}]_3$ [NTA] due to the transferring of samples during the regeneration. Moreover, compared with the fresh [N₂₂₂₂]₃[NTA] catalyst, these above characteristic bands also appeared in the reused [N₂₂₂₂]₃[NTA] catalyst (Fig. 9). This further showed that $[N_{2222}]_3$ [NTA] could be very stable in the synthesis of DTC for several runs. In addition, supported ionic liquid catalyst [N2222]3[NTA]/AC (AC, active carbon) was prepared by impregnating 20 wt%

 $[N_{2222}]_3[NTA]$ into active carbon and employed to test its reaction performance and recyclability. The results listed in Table S3 indicated that even though $[N_{2222}]_3[NTA]/AC$ catalyst can be separated from the reaction system effortlessly by filtration, the catalytic activity of $[N_{2222}]_3[NTA]/AC$ catalyst decreased obviously from 60 to 42% DTC yield after three recycle times. This implies that $[N_{2222}]_3[NTA]$ may be lost during the reaction process because of active carbon loaded with $[N_{2222}]_3[NTA]$ using physical impregnation. Therefore, we believe that the homogeneous catalysis of APC-ILs is still a good strategy for highly efficient synthesis of DTC, although its separation and recycle is tedious.

3.5 Reaction of DMC with Other Alcohols

To obtain more information about other dialkyl carbonate, the transesterification reaction of DMC with other alcohols such as ethanol, propanol, pentanol, cyclopentanol, benzyl alcohol and phenol was studied and the results are listed in Table 3. It is indicated that both DMC conversion and dialkyl carbonate yield improve with the increase of carbon chain length of fatty alcohol (entries 1-4). This shows that long chain fatty alcohol has the better nucleophilicity to form corresponding dialkyl carbonate, and the reverse reaction of higher dialkyl carbonate is suppressed [26, 27]. Moreover, a low yield was obtained and resulted from the steric effect of cyclopentanol. Diphenyl carbonate was also not detected in the transesterification of DMC with phenol because of its very high reaction activation energy. Thus, the catalyst [N₂₂₂₂]₃[NTA] was demonstrated to display considerable catalytic performance for the transesterification of DMC with many alkyl alcohols, implying the wide applicability of APC-ILs in the production of various OCs.

4 Conclusions

In summary, a new methodology based on using APC-ILs as catalysts for high-yielding synthesis of DTC was developed in this work. It is found the catalytic performance of APC-ILs can be related to their carboxylate groups in anions, and the more carboxylate groups the APC-ILs possess, the higher the catalytic activity. The best APC-IL $[N_{2222}]_3[NTA]$ displays excellent activity in the catalytic synthesis of DTC, with the conversion of DMC of 97% and yield of DTC of 80%, being superior to traditional base catalysts. $[N_{2222}]_3[NTA]$ is also featured with fairly good reusability and wide applicability in the synthesis of other OCs. The strategy introduced herein opens up a new opportunity to improve the efficiency of current industrial process for the production of OCs.

 Table 3
 Results of transesterification of DMC with other alcohols

Entry	Alcohols	Product	Conversion of DMC (%)	Yield (%)
1	∕ОН		95	54
2	∕∕ОН		96	59
3	∕∕∕ОН		99	66
4	OH		97	61
5	ОН	$\bigcirc_0^0 \bigcirc_0^{-1} \odot_0^{-1} \odot_0^{-1} \bigcirc_0^{-1} \odot_0^{-1} \bigcirc_0^{-1} \odot_0^{-1} \odot_0^$	86	47
6	OH		trace	trace

Reaction conditions: reaction temperature $(130 \,^{\circ}\text{C})$, reaction time (2 h), molar ratio of alcohol to DMC (4:1), catalyst (0.5 wt%)

Acknowledgements This work was supported by the National Natural Science Foundations of China (Nos. 21566011, 31570560), the Natural Science Foundations of Jiangxi Province (No. 20151BAB213016), and the Jiangxi Province Sponsored Program for Distinguished Young Scholars (20162BCB23026).

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