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An overview on performance and reaction mechanism of propylene carbonate

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ABSTRACT

The main properties of propylene carbonate have been introduced. Synthetic principles and industry processing of propylene carbonateusing different catalysts such as trans–dichlorotetrapyridineruthenium have been discussed. Furthermore, the reaction mechanism of propylene carbonate has also beenexplained.

KEYWORDS

Overview;
Synthetic methods;
Propylene carbonate.

INTRODUCTION

Propylene carbonate (PC) is one kind of organic solvents witha high performance such as a high boiling point and a high polarity, etc[1]. Propylene carbonate as a major feedstock is widely used in different fields such as organic synthesis[2], gas separation[3] and the battery electrolyte[4], etc. There are four synthetic methods listed as follows, such as phosgenation[5], transesterification method[6], chlorine/propanol method[7] and the synthetic method of carbon dioxide and propylene oxide[8], etc. The synthetic method of carbon dioxide and propylene oxide gradually takes the places of other methods due to poor product performance. These advantages of propylene carbonate instead of carbon dioxide are written as follows, decreasing the greenhouse effect in the atmosphere, high value chemical productsand energy utilization rate, so the synthetic methods of propylene carbonate is gradually focused on.

In the present paper, synthetic principles and industry processing of propylene carbonate using different catalysts such as trans – dichlorotetrapyridineruthenium have been discussed. Furthermore, the reaction mechanism of propylene carbonate has also been introduced.

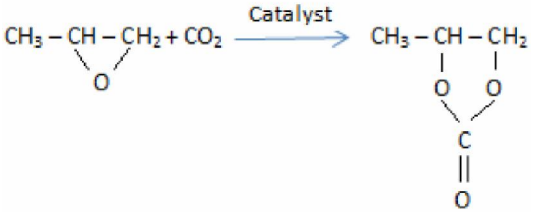
RESULTS AND DISCUSSION

The properties of propylene carbonate

TABLE 1 shows the properties of propylene carbonate[9].

Synthetic principles and industry processing of propylene carbobate

The main reaction of propylene carbonate with carbon dioxide and propylene oxide as feedstocksis listed as follows[9].



(1)

This reaction is an exothermic reaction. Its standard heat of reaction is 106.14kJ/mol. Propylene ox-

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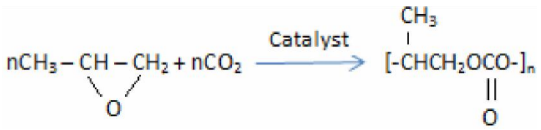
TABLE 1 : The properties of propylene carbonate

Items	Properties
Molecular formula	$C_4H_6O_3$
Molecular weight	102.9
Refractive index	1.4218
Melting point (°C)	-49.2
Boiling point (°C)	238.4
Flash point (°C)	128
Relative density	1.2047
Vapor pressure (20°C /pa)	17.33
Appearance	Colorless and tasteless liquid under the room temperature
Solubility	Easily mix with diethyl ether, acetone, benzene, trichloromethane, ethyl acetate, etc.

ide has three membered ring. An included angle between carbon-oxygen bond and carbon-carbon bond is close to 60 °C. Propylene carbonatemolecules have high activity due to high tension, so its secondary reaction easily happens. These secondary reactions are written as follows.

(1) Propylene oxidereacts withcarbon dioxide to generate poly propylene carbonate.



(2)

(2) Propylene oxideunder the condition of an initiatorreacts by itself to produce bipolymer and polymer.

(3)

(3) Propylene oxide reacts with water in the system to generate propylene glycol.

(4)

Figure 1 shows the industry processing flow chart of propylene carbonate. Carbon dioxide after purification takes the place of air three times in the reactor. Solvent and catalysts are stirred to add into the reactor. Propylene oxide is compressed to pump into the reactor. At the same time carbon dioxide is transported to the reactor. Finally the fine propylene carbonate is gotten from the bottom of the reactor after degasification, getting rid of catalysts and solvent.

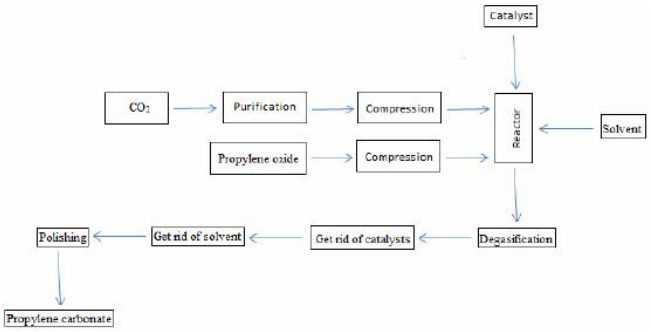


Figure 1: The industry processing flow chart of propylene carbonate

The reaction mechanism of propylene carbonate

Bu Zhanwei[10] introduced the reaction mechanism of carbon dioxide and propylene oxide withtrans – dichlorotetrapyridineruthenium as a catalyst. Figure 2 presents the reaction mechanism of carbon dioxide and propylene oxide. Propylene oxide exchanges with chloridion of trans – dichlorotetrapyridineruthenium. Propylene oxide coordinated with Ru of complex becomes the intermediate (1). At the same time this system can provide chloridion, which as a nucleophile coordinate propylene oxide from less space resistance. Its ring opens to become the intermediate (3). Carbon

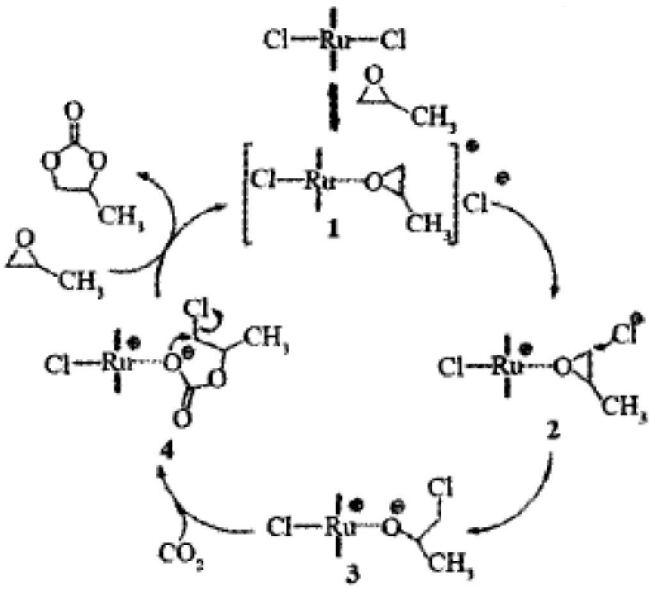


Figure 2 : The reaction mechanism of carbon dioxide and propylene oxide by using trans – dichlorotetrapyridineruthenium as a catalyst

dioxide is inserted the Ru-O bond to become the intermediate (4), which becomes propylene carbonate after the cyclization and the elimination reaction.

Bu Zhanwei[11] explained why $RuCl_3$(22'-bipy) (CH_3OH)used as a catalysthas no catalytic ability by itself. Figure 3 showsthe reaction mechanism of carbon dioxide and propylene oxide by using$RuCl_3$(22'-bipy) (CH_3OH)/hexadecyltrimethyl ammonium chloride. CH_3OH atom is released from this system and cannot provide enough strong nucleophile. Hexadecyltrimethyl ammonium chloride not only activate carbon dioxide but also provides enough chloridion in the system of $RuCl_3$(22'-bipy) (CH_3OH)/hexadecyltrimethyl ammonium chloride. Its catalytic ability is greatly improved.

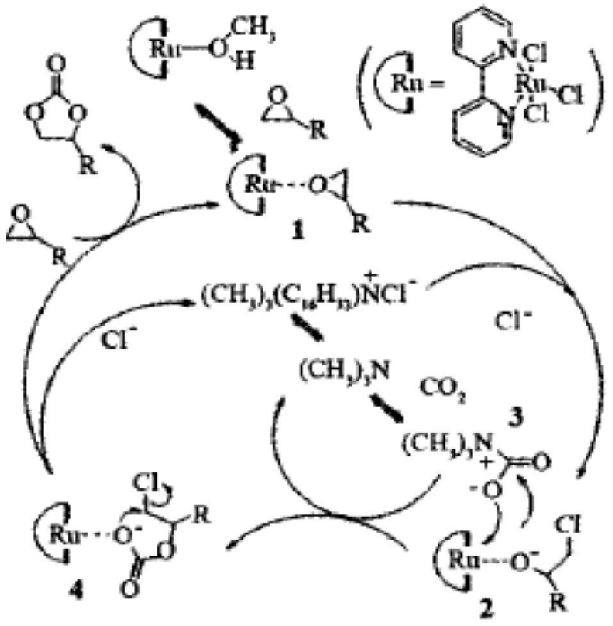


Figure 3 : Shows the reaction mechanism of carbon dioxide and propylene oxide by using $RuCl_3$(22'-bipy) (CH_3OH)/ hexadecyltrimethyl ammonium chloride

CONCLUSION

The reaction mechanism of carbon dioxide and propylene oxide points out that adeeply comprehending reaction mechanism of propylene carbonate not only has a very importantsignificance, but also provides a theoretical foundation forthe chemical plantbased on the above discussion and review. It is important for the chemical plant to design and operate rightly and optimizes the reaction processing and may increase theplant's benefits.

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