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Topic : DBU as Organocatalyst

ABSTRACT

DBU belongs to amidine class of compounds . It is clear light yellow liquid

Hygroscopic in nature .

Stable at ambient temperature

Hardly soluble in petroleum ether .

But soluble in Water , Ethanol ,
Benzene ,

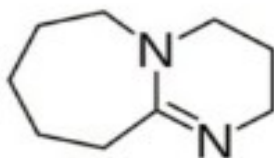
Acetone , Ethyl acetate etc .

Sterically hindered non-nucleophilic
base

The pK_a value

Versatile reagent in organic
synthesis

Structure...

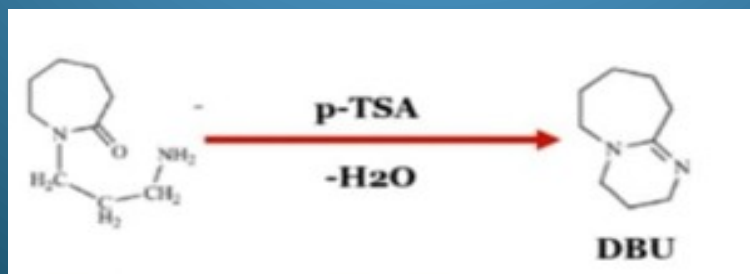
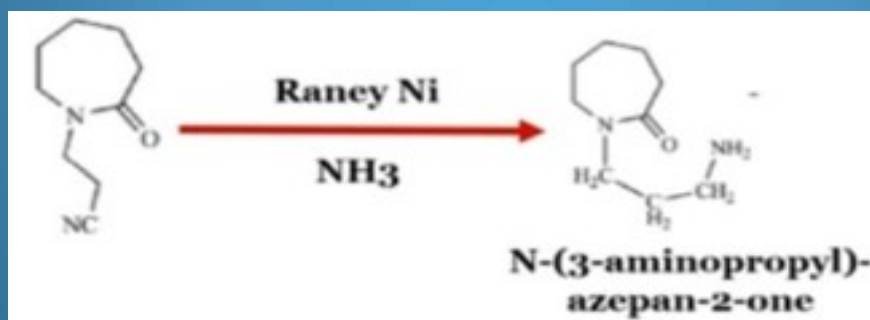


INTRODUCTION

1,8-Diazabicyclo[5.4.0]undec-7-ene (DBU), is a sterically hindered amidine base. It is a liquid with a boiling point of 261°C. It is one of the strongest organic neutral base with a pK_b of 12. The presence of adjacent nitrogen in the molecule stabilizes the protonated species. It is a non-nucleophilic base and due to this it has found to be useful in reactions where side reactions due to inherent nucleophilicity of a basic nitrogen poses problem. Although, traditionally DBU is considered to be a non-nucleophilic base, but there are few reports where DBU has been employed as a nucleophilic base also. It is advantageous to use DBU in organic reactions as it is cheap, commercially available, homogenous and most importantly recoverable. In recent years, DBU has been used as a catalyst, complexing ligand and a nucleophilic/non nucleophilic base in organic reactions.

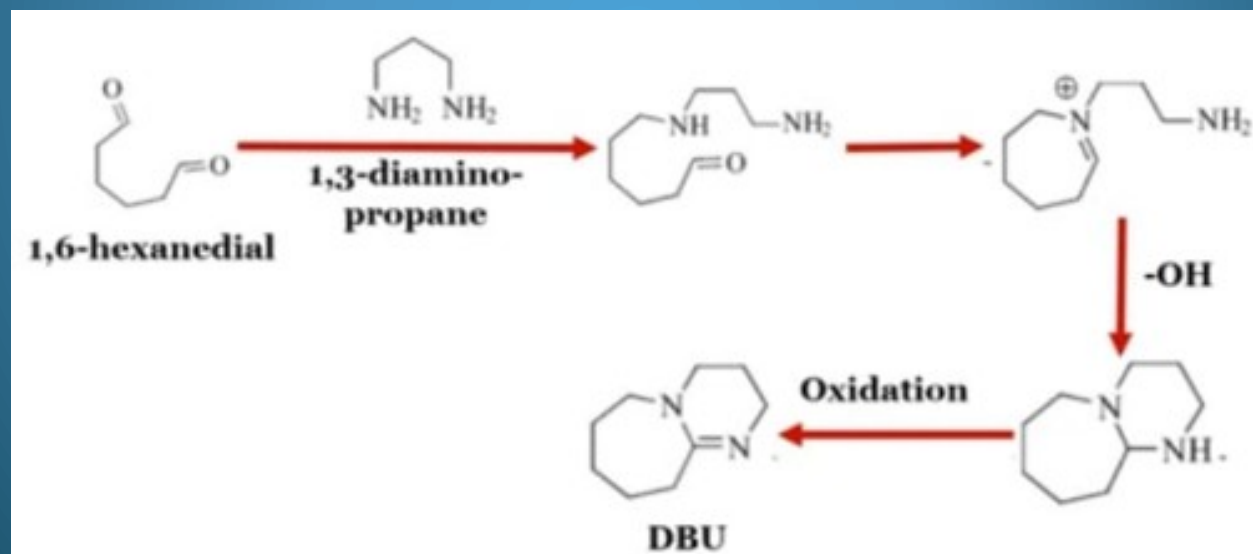
SYNTHESIS OF DBU

Lactam (azepan-2-one) with KOH N – cyanoethylation form and catalytic reduction take place by Raney Ni in presence of NH₃ and finally DBU is form by cyclisation

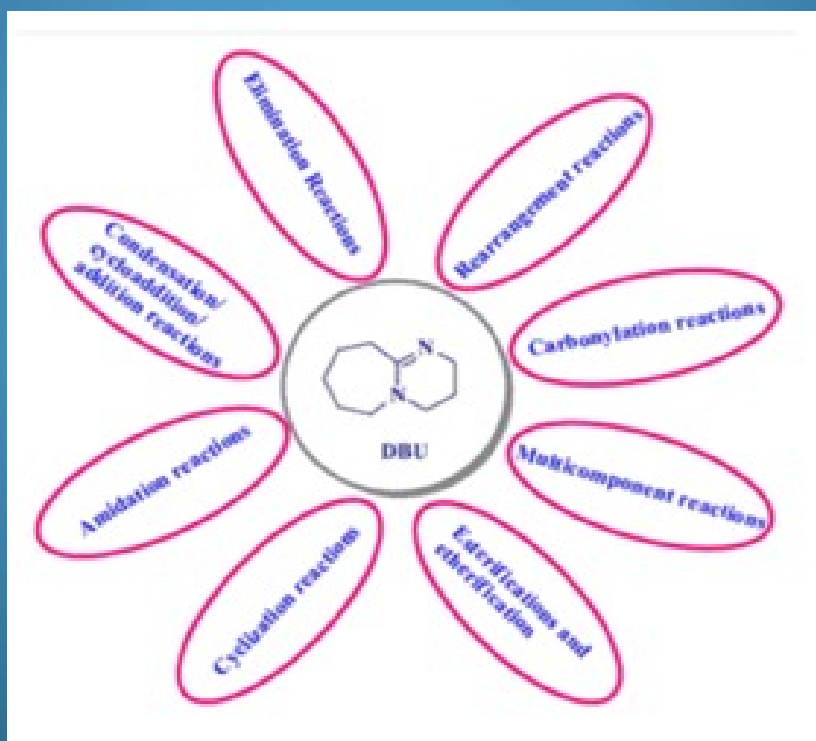


SYNTHESIS OF DBU

1,6-hexanedial react with 1,3-diaminopropane react together to form DBU by oxidation.



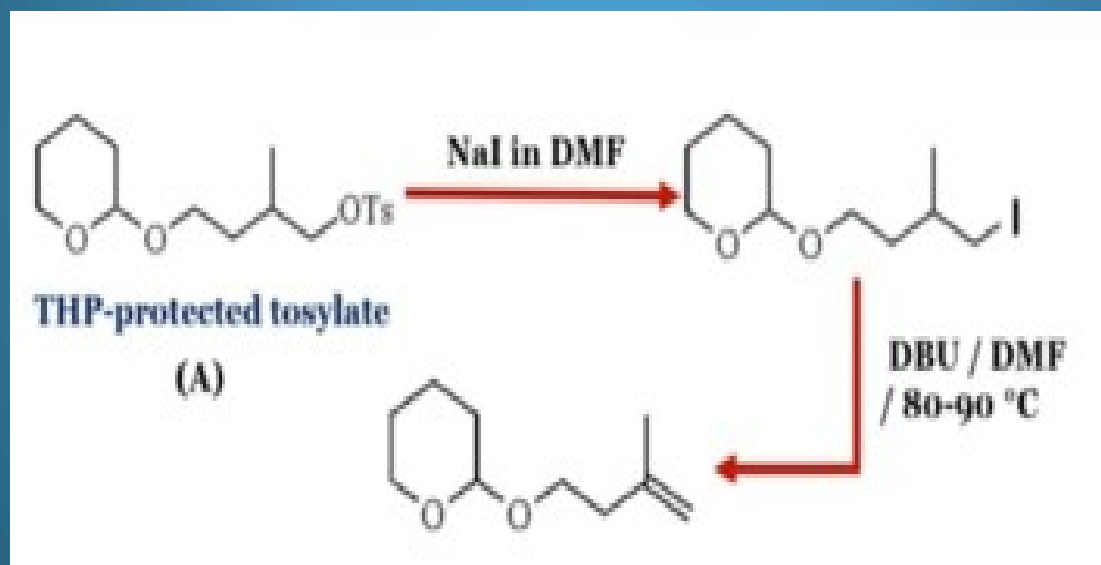
DBU is effective under relatively mild conditions for a variety of base mediated organic transformation viz elimination, isomerization, esterification, amidation, condensation, and some multicomponent reaction



Elimination

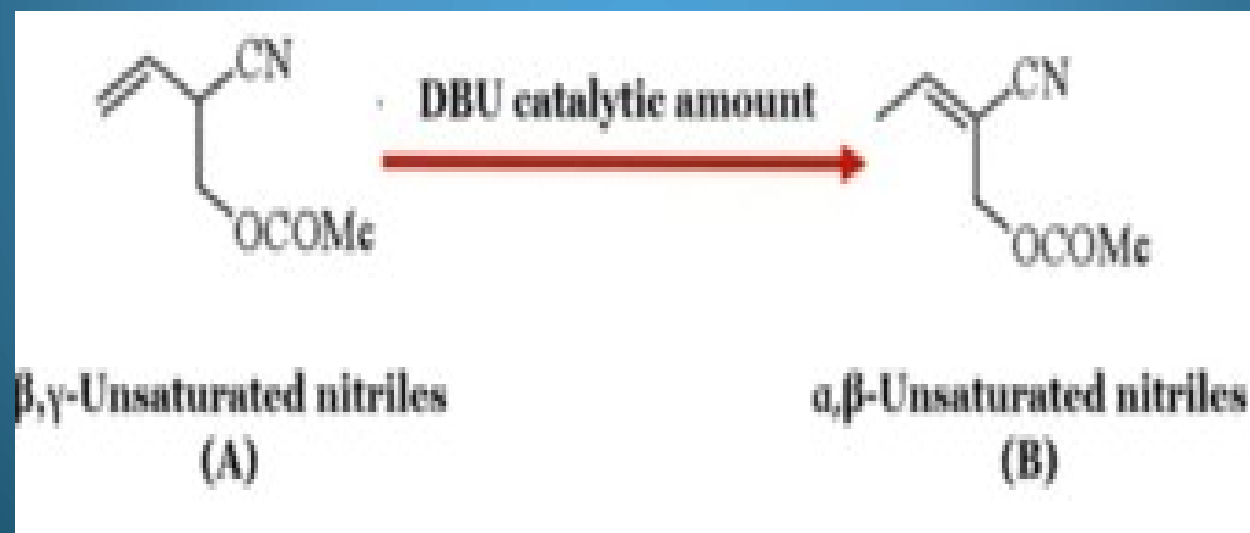
THP-protected tosylate convert into iodide which then heating with DBU at 80 °C for 3-4 h

Afforded terminal alkene in 82% yield



isomerization

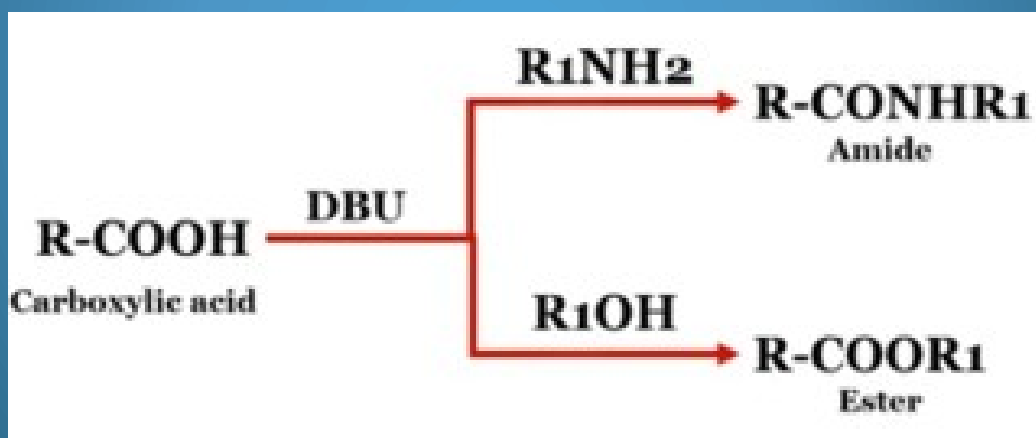
DBU catalyzes isomerization of a β, γ - unsaturated nitriles get converted into thermodynamically favoured α, β - unsaturated nitriles



Carboxylic acid get converted into amide in presence of DBU

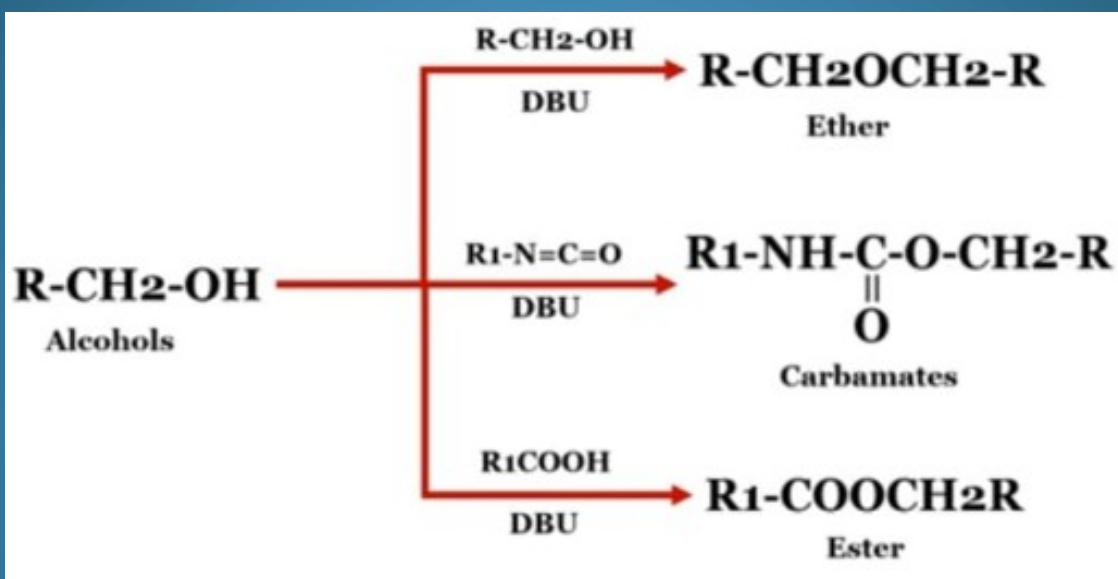
Carboxylic acid react with OH to form ester in presence of DBU

Carboxylic acid perform estrification and amidation simultaneously with the help of DBU

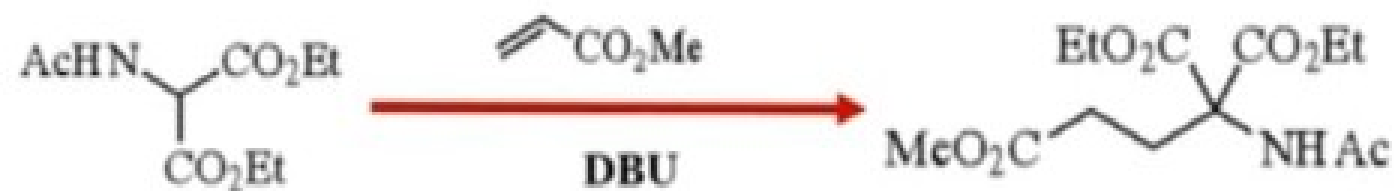


Just like above ;

Alcohol get converted into ether,
ester as well as carbamates are
catalysed by DBU.



In condensation , DBU found to be an effective base for the michael reaction

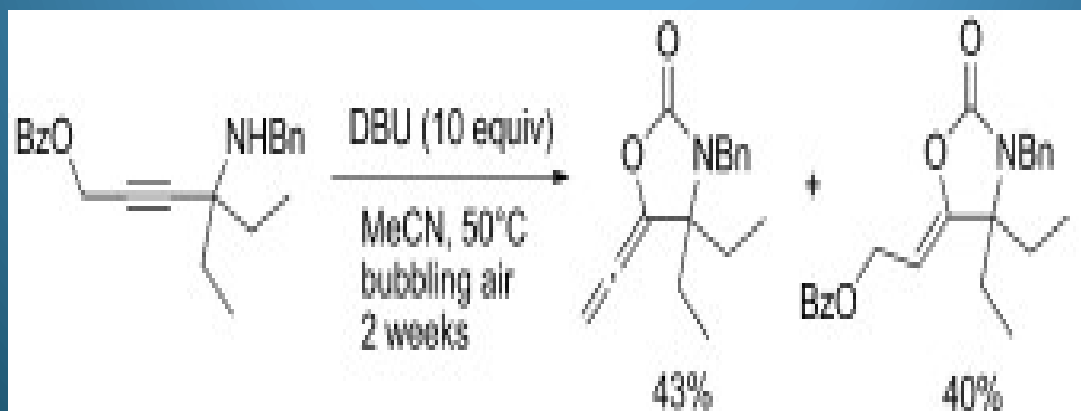


CO₂ fixation

In atmosphere CO₂ is abundant carbon source and it also has impact on global climate.

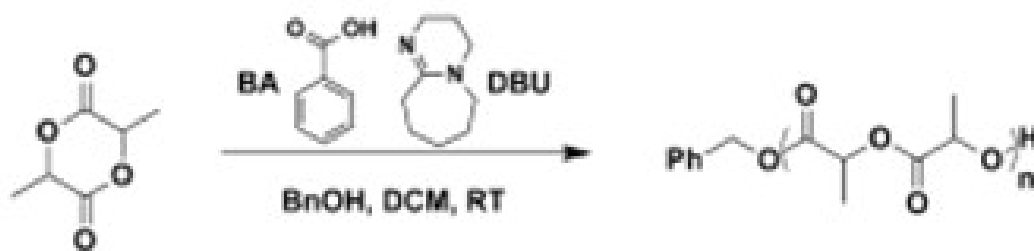
This represents attractive area of study in organic and green chemistry .

They have Recently reported synthesis of oxazolidinone by the DBU promoted reaction of propargylic amine by bubbling air through the reaction mixture it can fix excess amount of CO₂



Polymerization

the use of acid/base complexes for the ring opening polymerization of (L)-lactide. The salt formed from an equimolar reaction of benzoic acid and DBU produced a catalyst capable of controlled polymerizations allowing for targeted molecular weights and narrow polydispersities. The use of computational analysis suggests a bifunctional catalytic mechanism wherein both the monomer and propagating hydroxyl group are



(L)-Lactide polymerizations with varying amounts of BA relative to DBU

The background is a solid teal color with a gradient. At the top, there are several wavy, flowing lines in shades of blue and teal, creating a sense of movement and depth. The lines are smooth and organic, resembling liquid or fabric. The overall composition is clean and modern.

THANK YOU