STRUCTURE DETERMINATION OF TERPENOIDS
Part-1

Prerequisites

Knowledge of basic skeleton of organic compounds

Concept of organic reactions

Reaction mechanisms

RECAP

General Classification of terpenes

Structure of isoprene

Learning Outcomes

Determination of hydroxyl group

Determination of carbonyl group

Presence of unsaturation

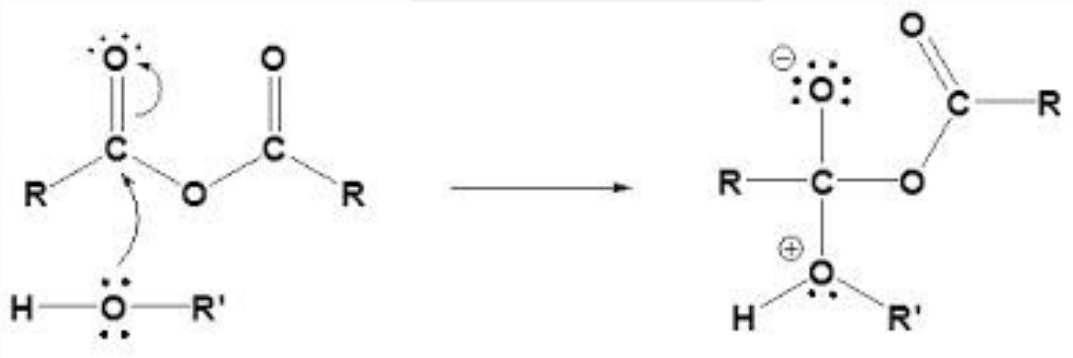
Determination of functional groups

Structure Determination of Terpenoids

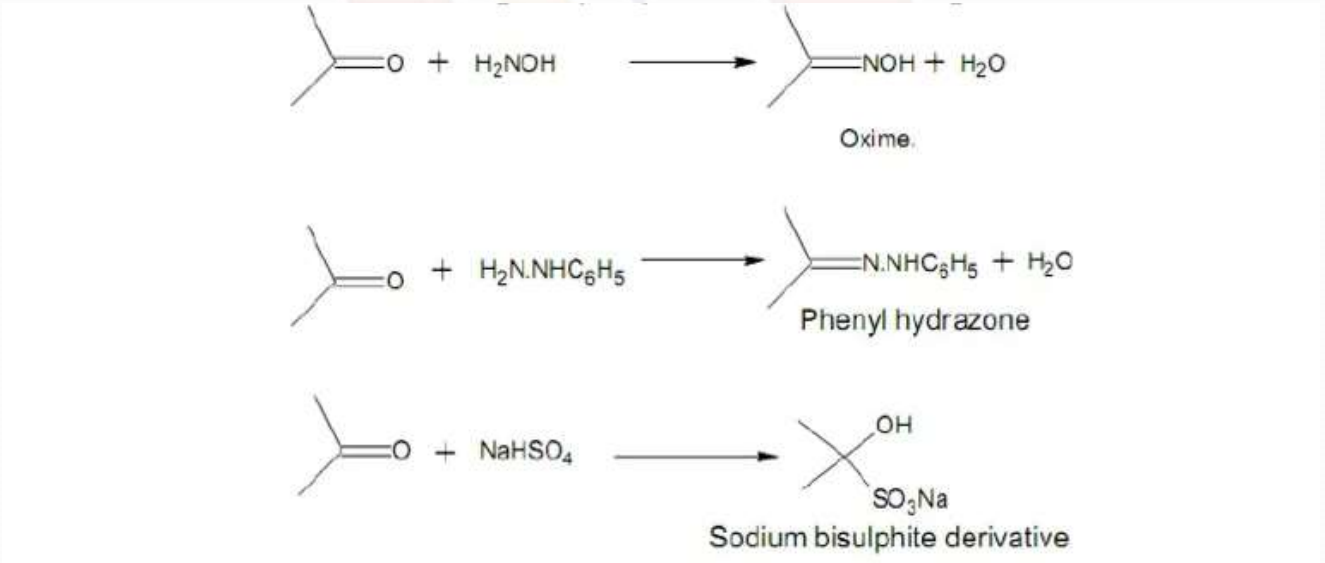
- i) **Molecular formula:** This is being done with the help of mass spectrometry. Specific rotation could be measured, if terpenoid is optically active.
- ii) **Nature of oxygen atom present:** If oxygen is present in terpenoids its functional nature is generally as alcohol aledhyde, ketone or carboxylic groups.
- a) **Presence of oxygen atom present:** presence of –OH group can be determined by the formation of acetates with acetic anhydride and benzoyate with 3.5-dinitirobenzoyl chloride.

Structure Determination of Terpenoids

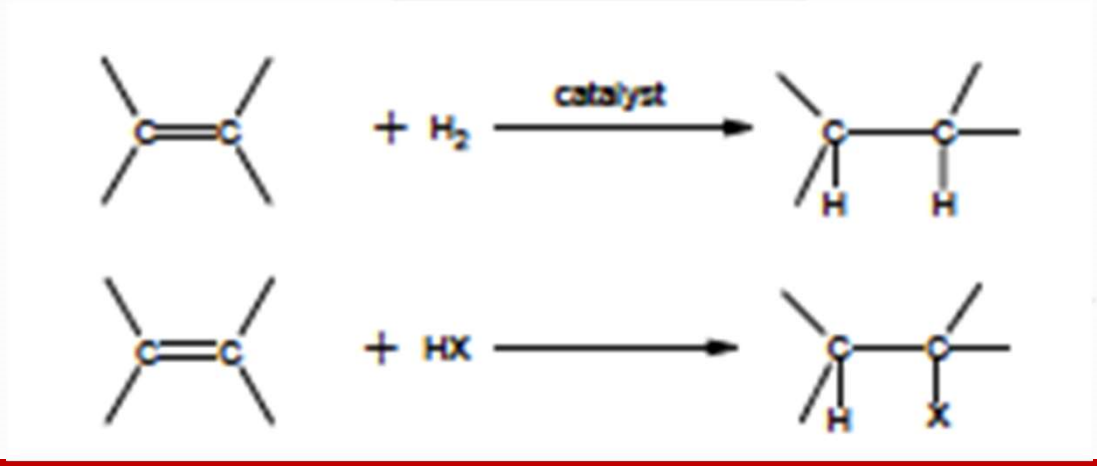
- Primary alcoholic group undergo esterification more readily than secondary and tertiary alcohols.



- b) **Presence of >C=O group:** Terpenoids containing carbonyl function form crystalline addition products like oxime, phenyl hydrazone and bisulphite etc.

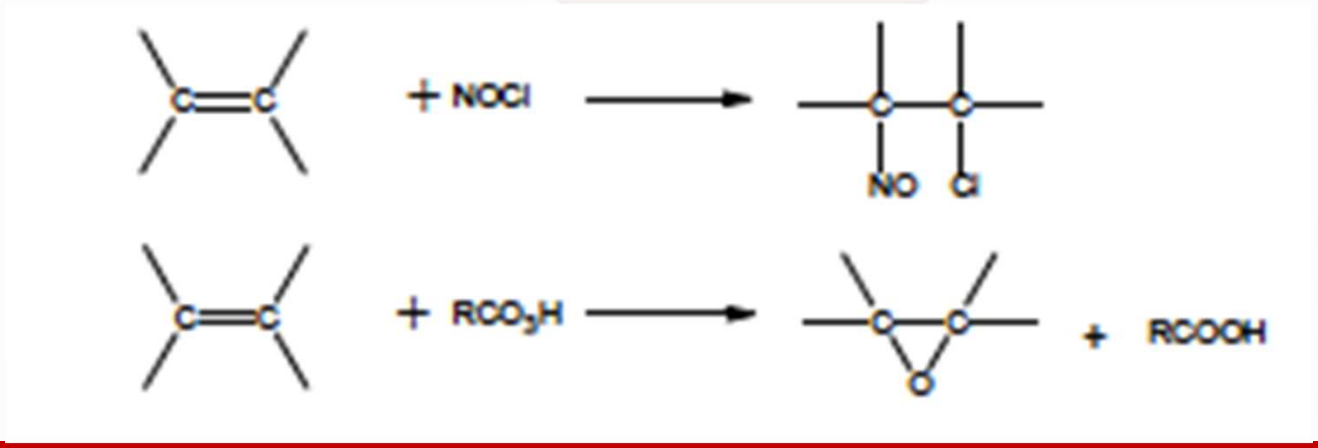


- iii) **Unsaturation:** The presence of olefinic double bond is confirmed by means of bromine, and number of double bond determination by analysis of the bromide or by quantitative hydrogenation or by titration with monoperpthalic acid. Presence of double bond also confirmed by means of catalytic hydrogenation or addition of halogen acids. Number of moles of HX absorbed by one molecule is equal to number of double bonds present.



Structure Determination of Terpenoids

- Addition of nitrosyl chloride(NOCl) (**Tilden's reagent**) and epoxide formation with peracid also gives idea about double bonds present in terpenoid molecule.



References

1. Christianson, D. W. (2006). Structural biology and chemistry of the terpenoid cyclases. *Chemical reviews*, *106*(8), 3412-3442..

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3. Hanson, J. R. (2001). The development of strategies for terpenoid structure determination. *Natural product reports*, *18*(6), 607-617.

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THANKYOU