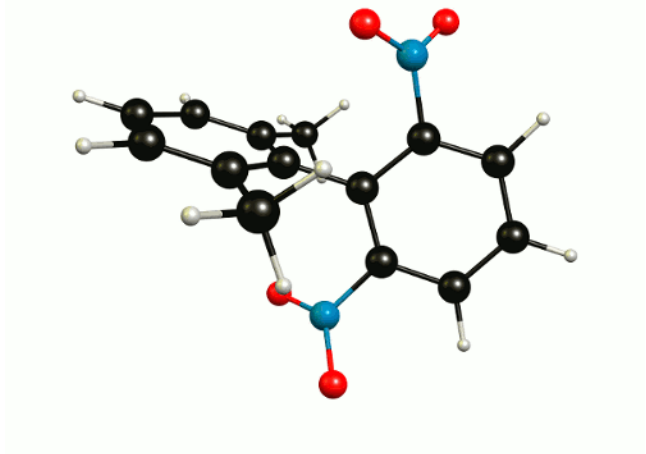
STEREOCHEMISTRY II B

PAPER-C-4 T



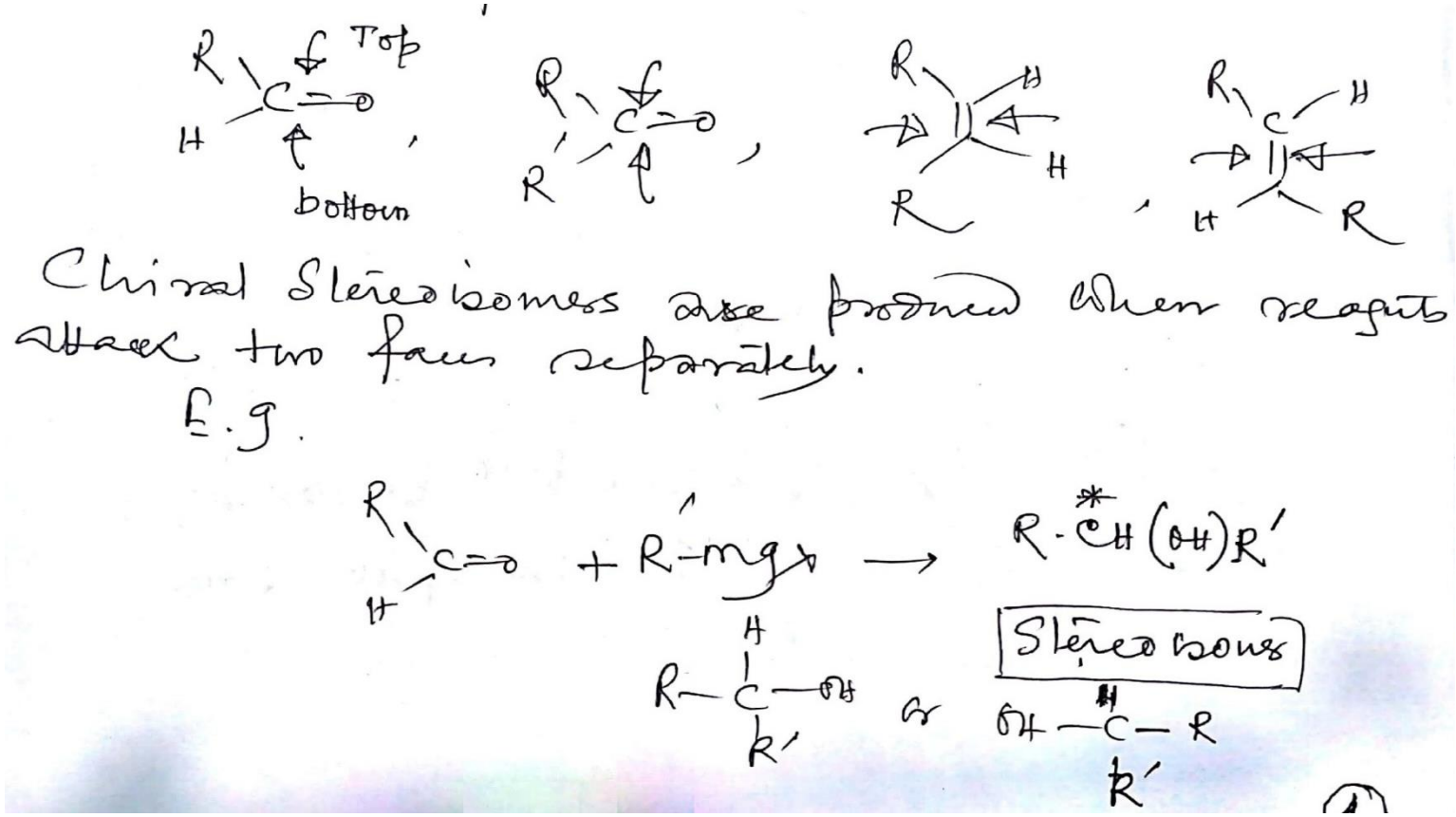
Indranil Chakraborty

ITEMS TO BE COVERED

- Topicity of faces
- Re /Si and re/si descriptors

Topicity of faces

Prochiral faces: **Chiral stereoisomers are produced when reagents attack two faces separately**

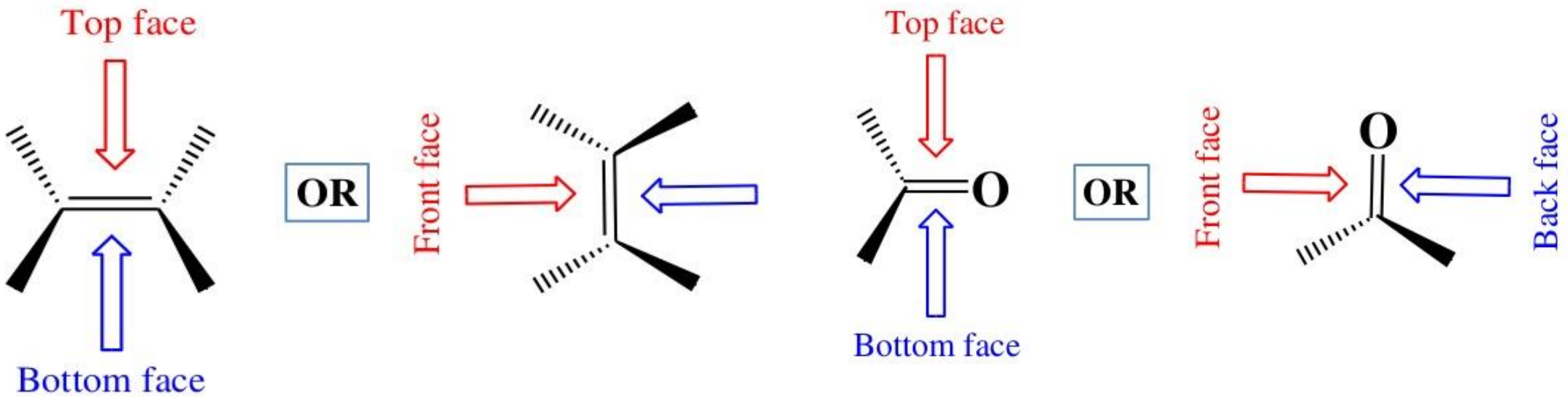


HOMOTOPIC FACES

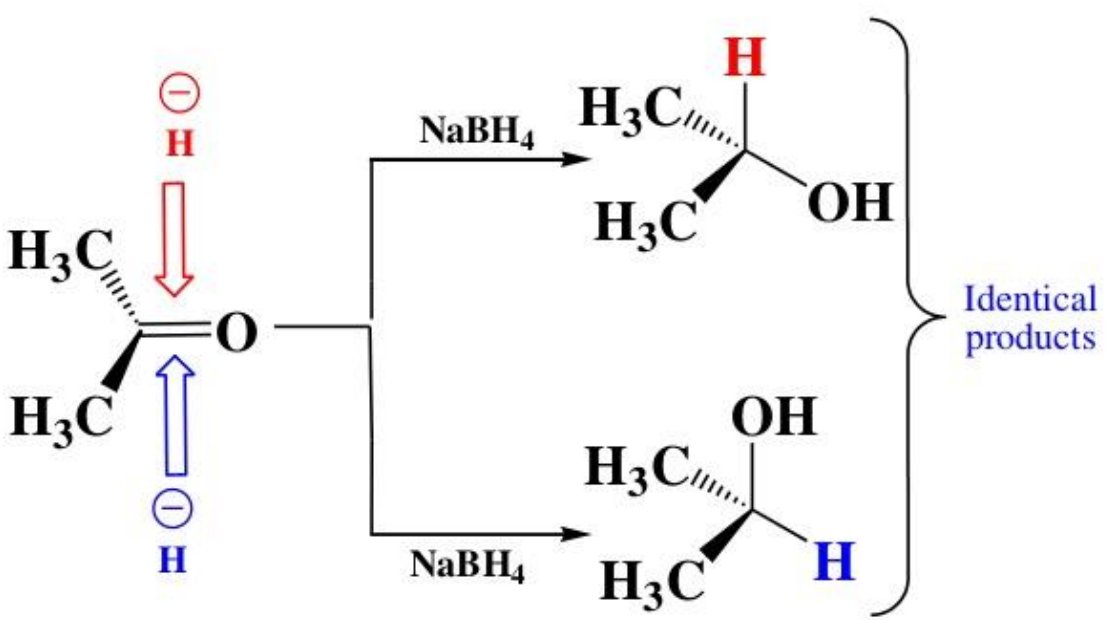
Criterion I: Addition of same reagents to either faces generate the same compound

1. (b) Homo topic faces

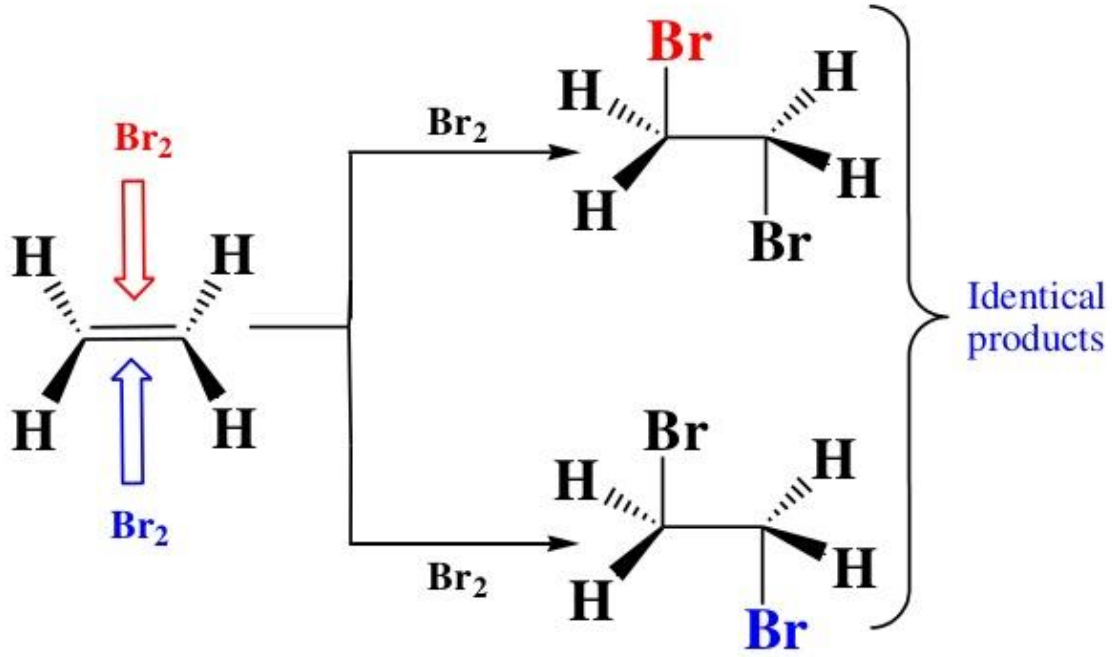
Two faces of a pi system or a double bond are homotopic if addition to either face gives same or identical product.



Same reagent attacking both faces separately



Two products are homomers. Hence, acetone has homotopic face

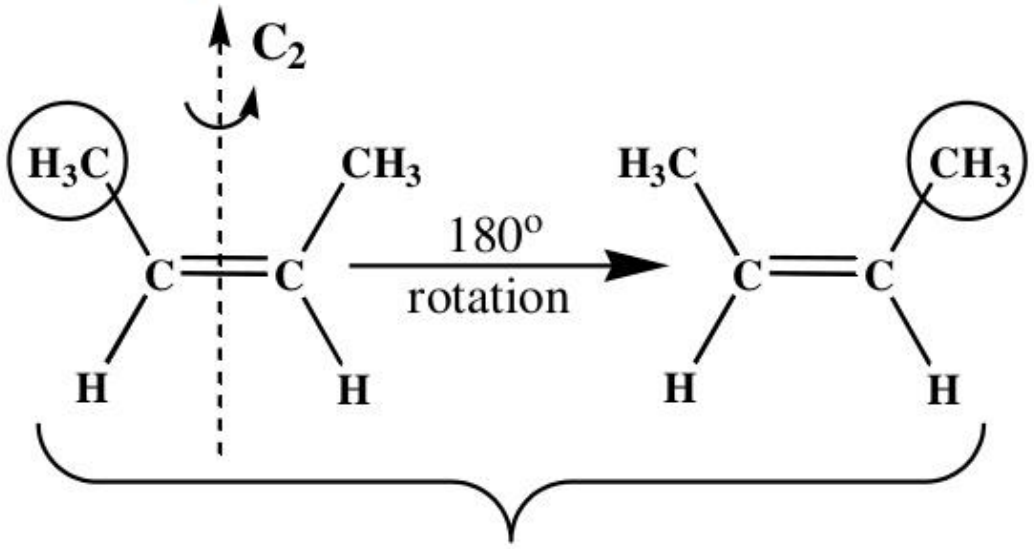


Hence, ethylene has homotopic face

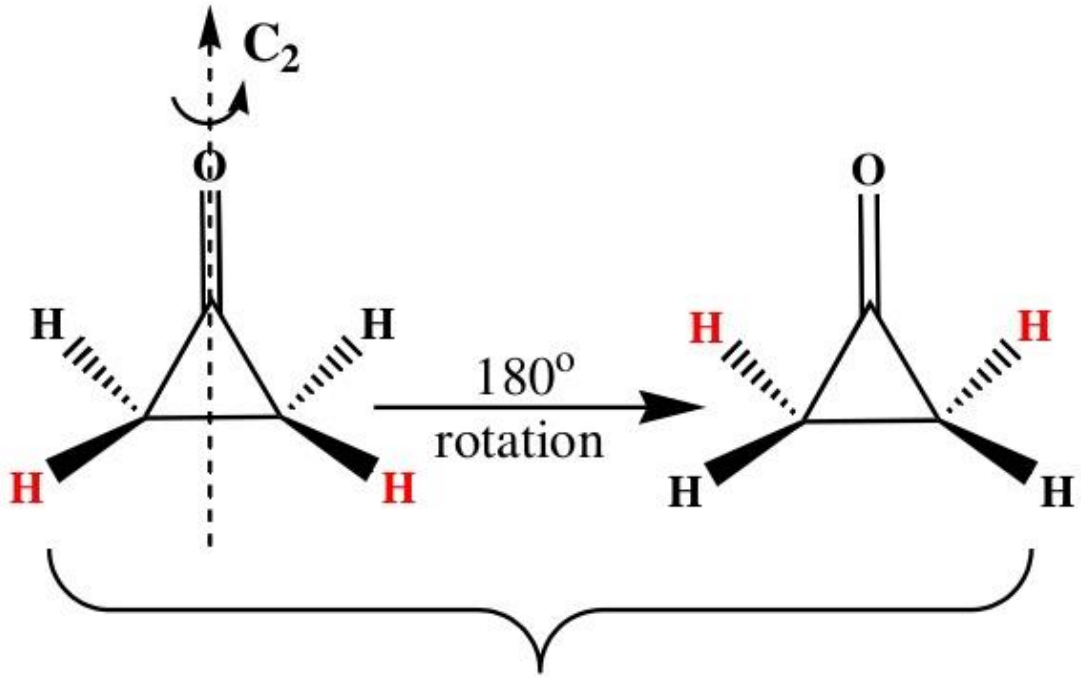
Criterion II: The two faces should be exchangeable by Cn (n = Even)

2. (b) Homo topic faces

Two faces of pi system are homotopic if they can interchange face result in same structure by rotation around C_2 axis.



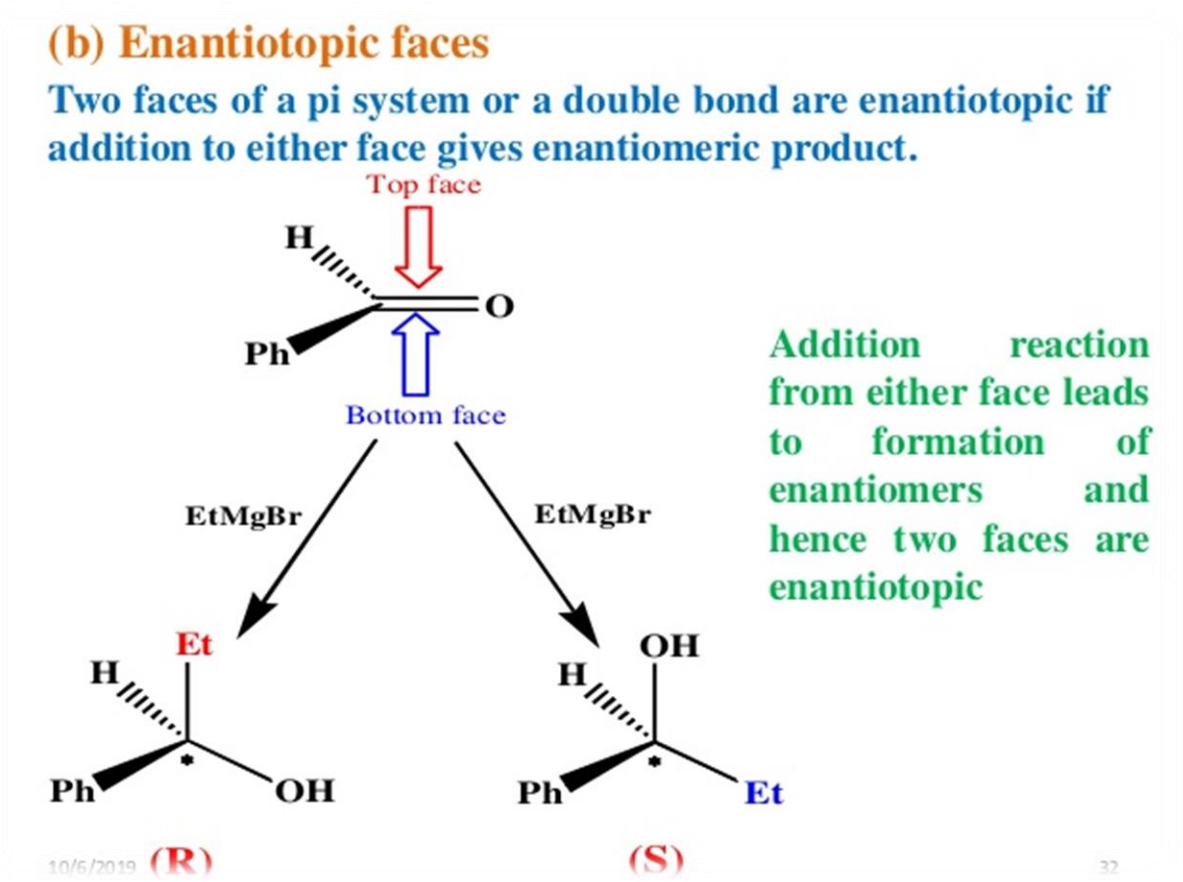
They are identical and hence it has homotopic face

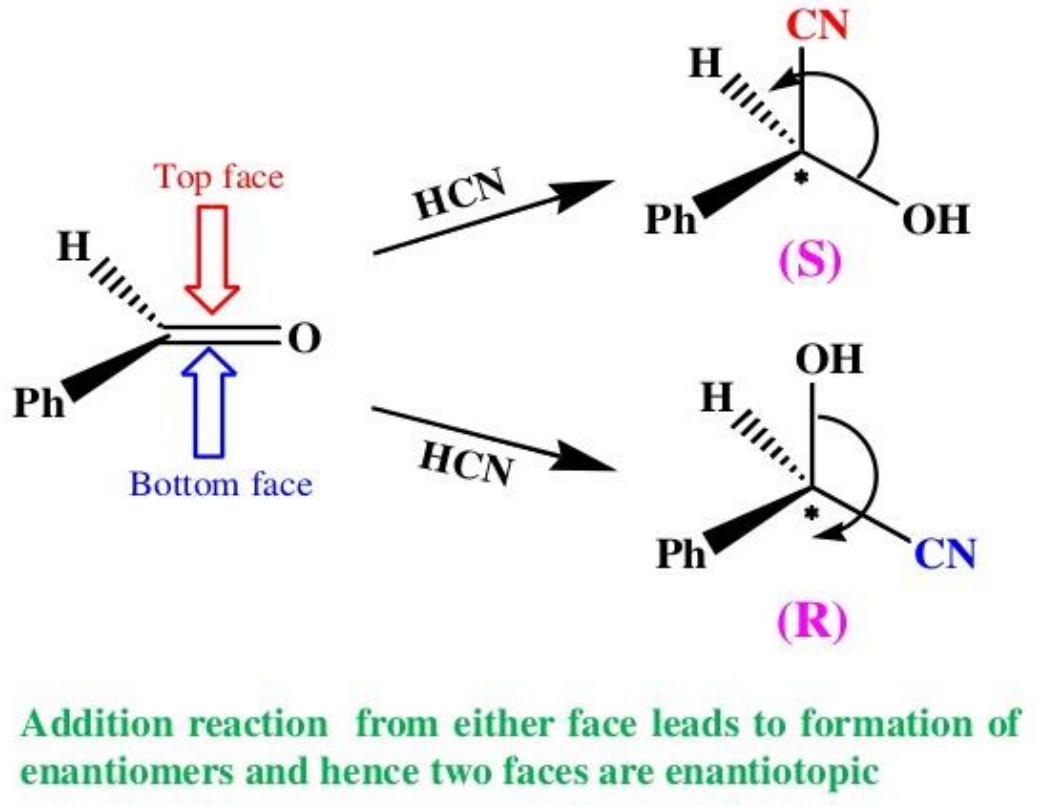


They are identical and hence it has homotopic face

Enantiotopic faces

Criterion I: Addition of same reagents to either faces generate a pair of enantiomers

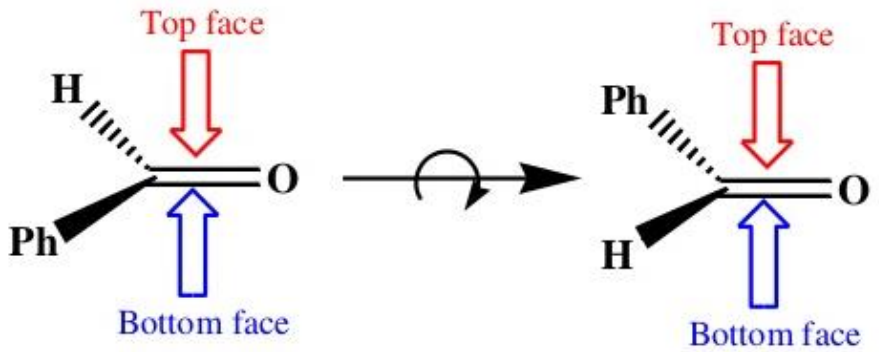




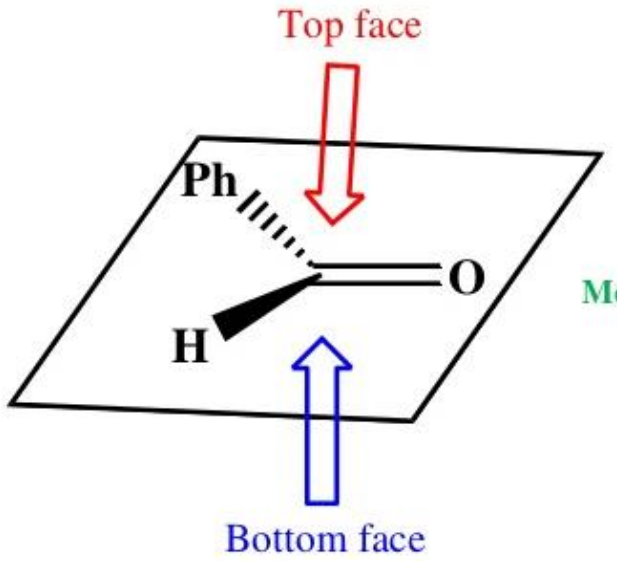
Criterion II: The two faces should be exchangeable by Sigma, Sn or i

(b) Enantiotopic faces

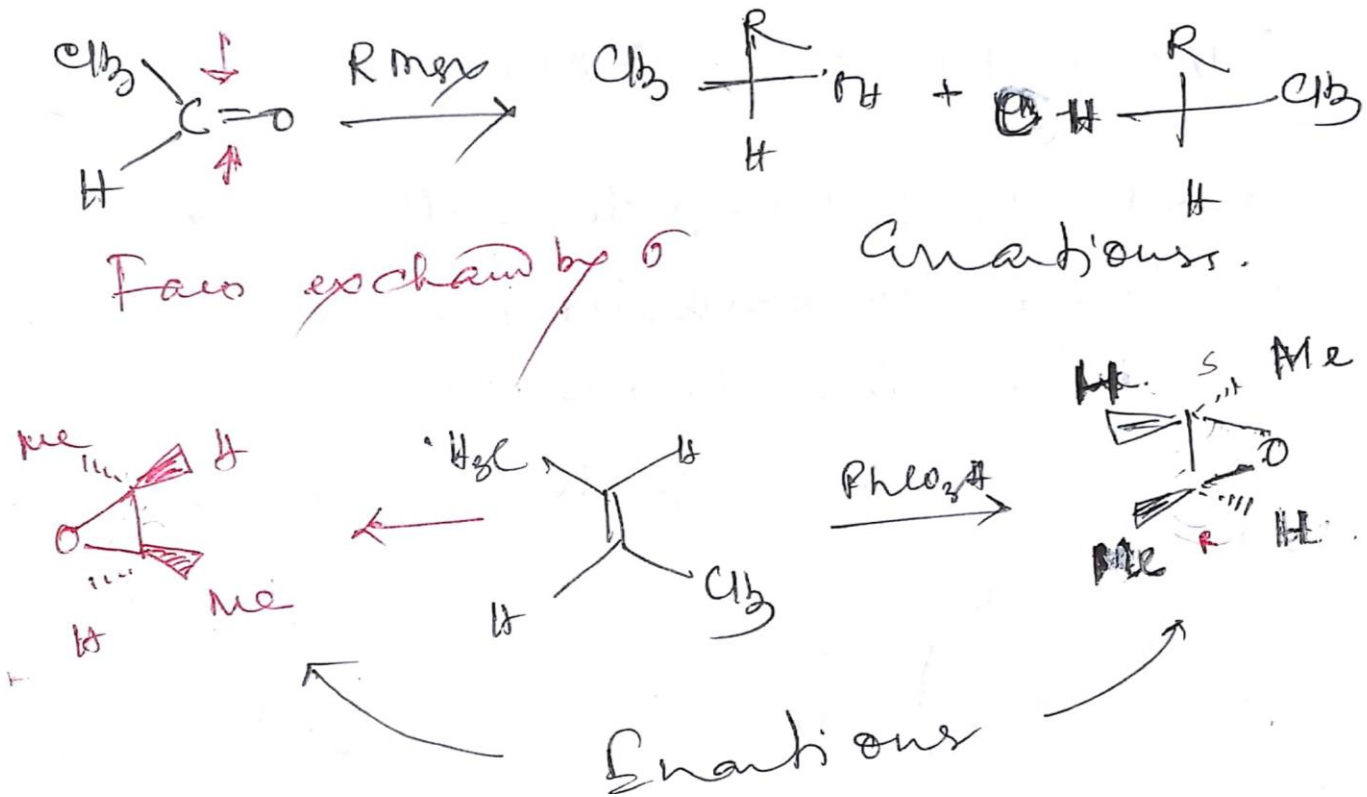
Two faces are enantiotopic if they can interchangeable through plane of symmetry or center of inversion or S_n axis.



Structure is not same upon rotation hence mirror plane exists.



Molecular mirror plane exists


R Mgx
Face exchange by σ
Enantiomers.
Me
H
Me
H
PhCO3H
Me
R
Enantiomers

Behaviour of ligands towards NMR

NMR Spectroscopy of Homotopic Hydrogen

If the hydrogen atoms in the molecule are homotopic, then they are chemically equivalent. Hence they will resonate at same chemical shift values.

NMR Spectroscopy of Enantiotopic Hydrogen

If the hydrogen atoms in the molecule are enantiotopic, then they are chemically equivalent. Hence they will resonate at same chemical shift values.

NMR Spectroscopy of Diastereotopic Hydrogen

If the hydrogen atoms in the molecule are diastereotopic, then they are chemically and magnetically non equivalent. Hence they will resonate at different chemical shift values.

SUMMARY of the Faces

Between homotopic groups and faces no differentiation is possible either by enzyme or by NMR or by human being because they are homomers or identical.

Topicity	Substitution-addition criteria	Symmetry criteria	Reactivity
Homotopic groups and faces	Homomers / Identical	C_n or C_2	No differentiation possible

Between enantiotopic groups and faces differentiation is possible either by enzyme or by NMR in chiral reagent or catalyst.

Topicity	Substitution-addition criteria	Symmetry criteria	Reactivity
Enantiotopic groups and faces	Enantiomers	σ_h or S_n	Differentiation possible

Between diastereotopic groups and faces differentiation is possible either by enzyme or by reagent or by NMR.

Topicity	Substitution-addition criteria	Symmetry criteria	Reactivity
Diastereotopic groups and faces	Diastereomers	Not applicable	Differentiation possible

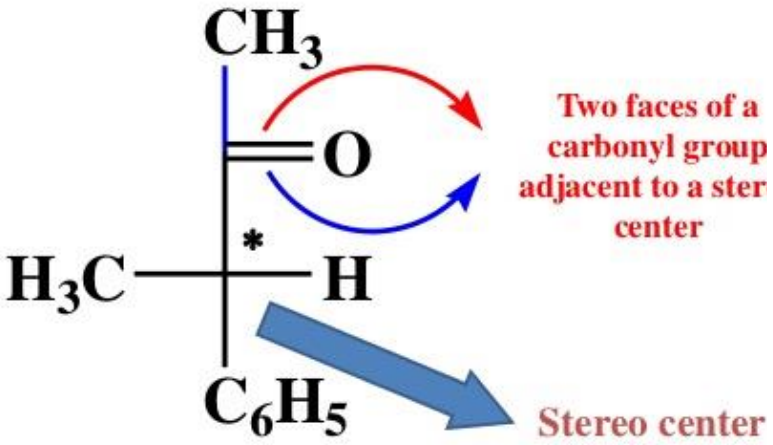
Diastereotopic faces

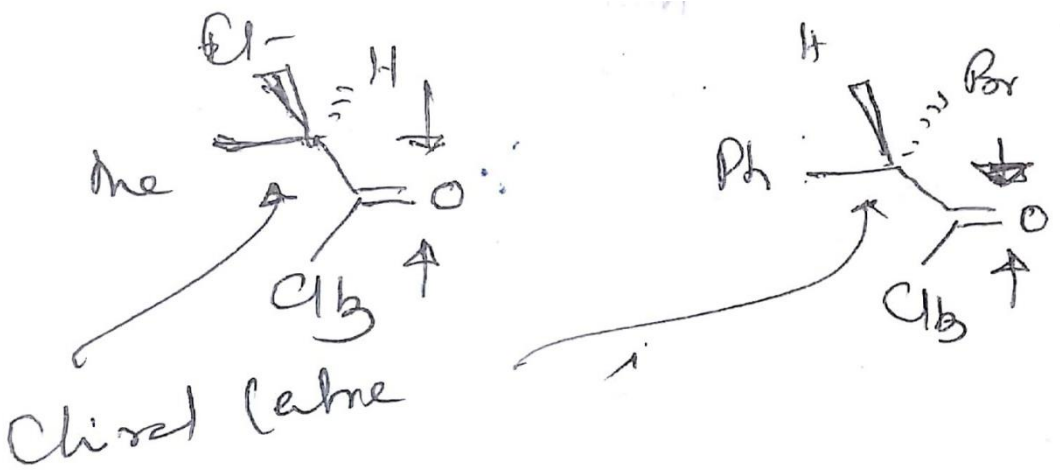
Criterion I: Reagents added to either sides of the faces lead to diastereomers

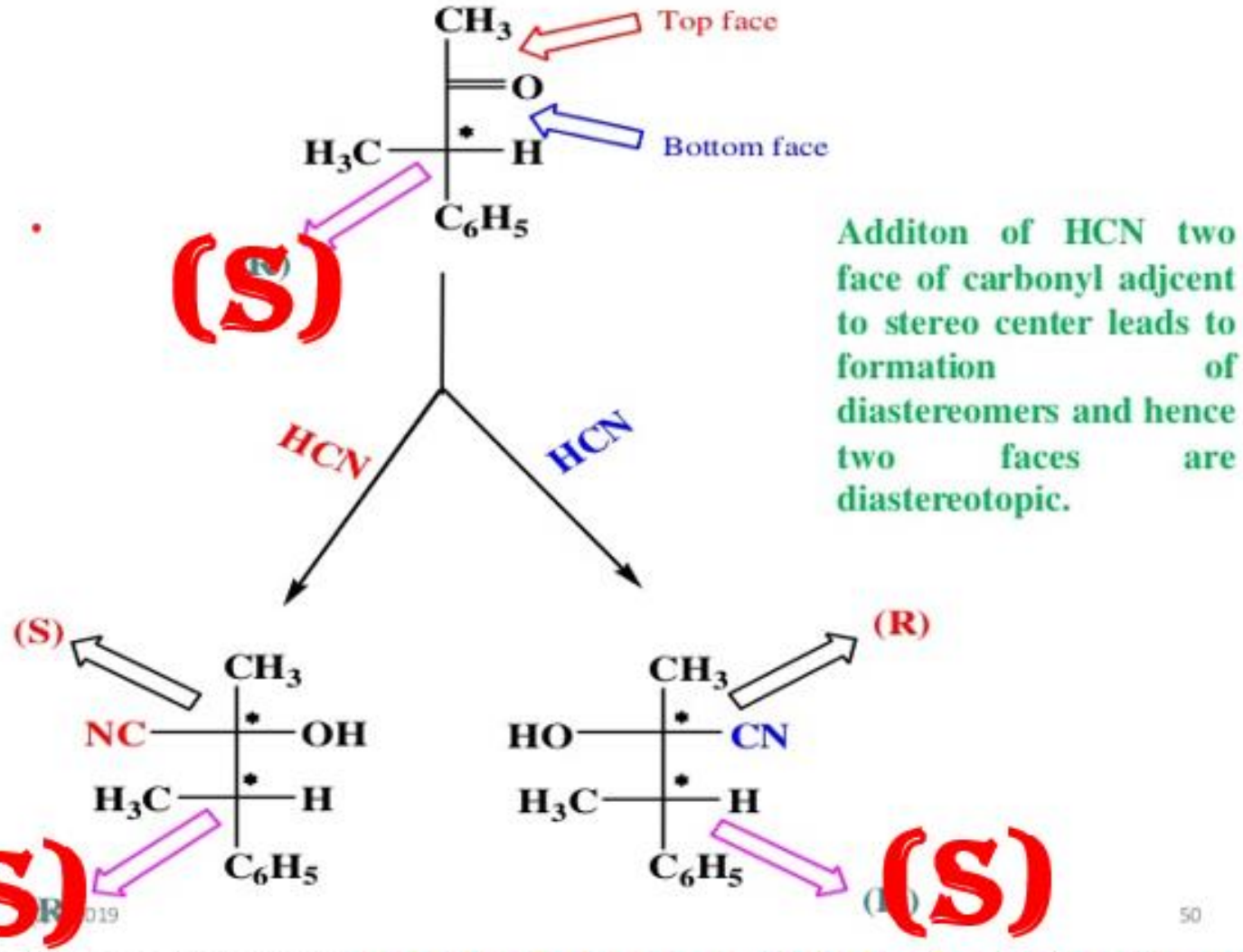
Crite[illegible] by any symmetry elements

(b) Diastereotopic faces

Two faces of a carbonyl group adjacent to a stereo center on addition reaction leads to diastereomers and possess diastereotopic face.





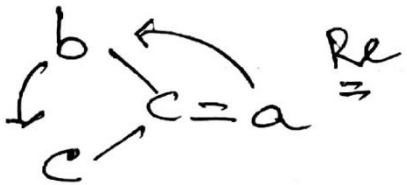


Additon of HCN two face of carbonyl adjcent to stereo center leads to formation of diastereomers and hence two faces are diastereotopic.

Point to note(Printing mistake): In the lowermost chiral centre the configuration will be "S" instead of R

Re/Si notations for stereo heterotopic faces

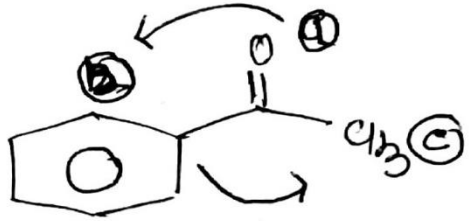
a-b-c Clockwise- Re :: **a-b-c Anticlockwise-** Si



If $a \rightarrow b \rightarrow c$ is clockwise specification is Re

$a \rightarrow b \rightarrow c$ " anti " " " Si

* Re and Si faces are reflection variant.

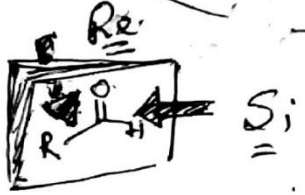


Invert-to-get-bottom face

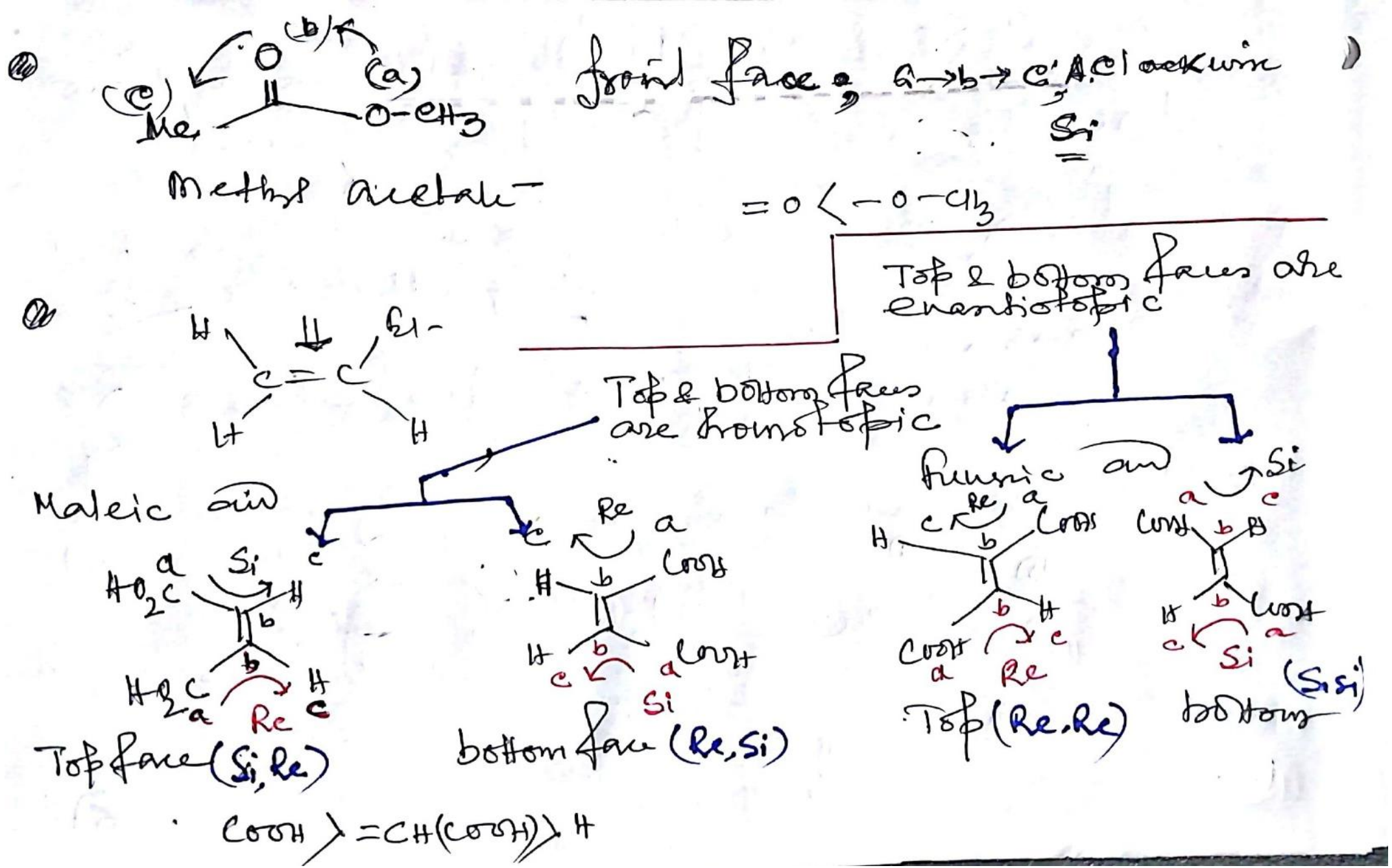
bottom face

Top face

Si



Re


front face; a→b→c, Anticlockwise
Si
Methyl acetate
=O<—O—CH3
Top & bottom faces are enantiotopic
Top & bottom faces are homotopic
Maleic acid
Fumaric acid
Top face (Si, Re)
bottom face (Re, Si)
Top (Re, Re)
bottom (Si, Si)
COOH>=CH(COOH)>H