

INTRODUCTION TO CHEMISTRY

CML-101

Tutorial 3

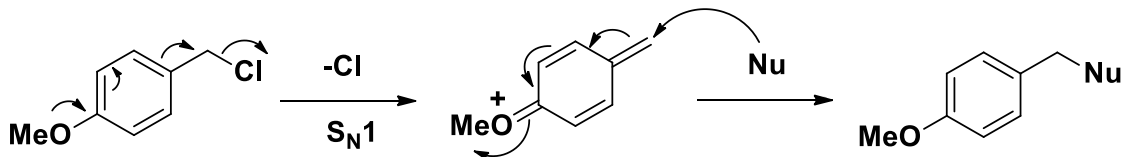


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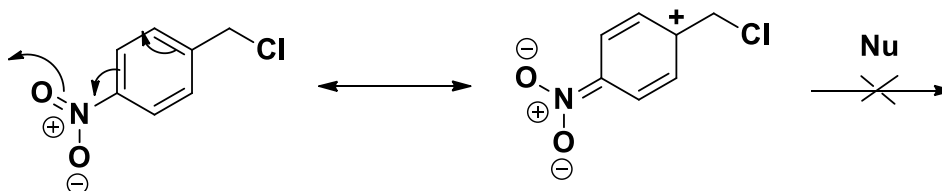
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Answer of Q1

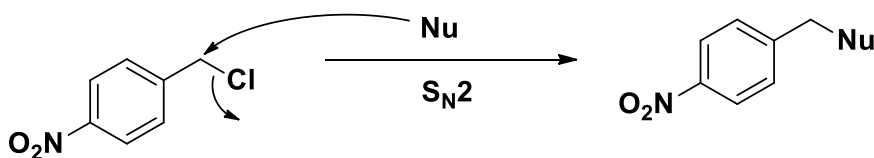
A benzylic chloride that favours the S_N1 mechanism



But a benzylic chloride that disfavours the S_N1 mechanism

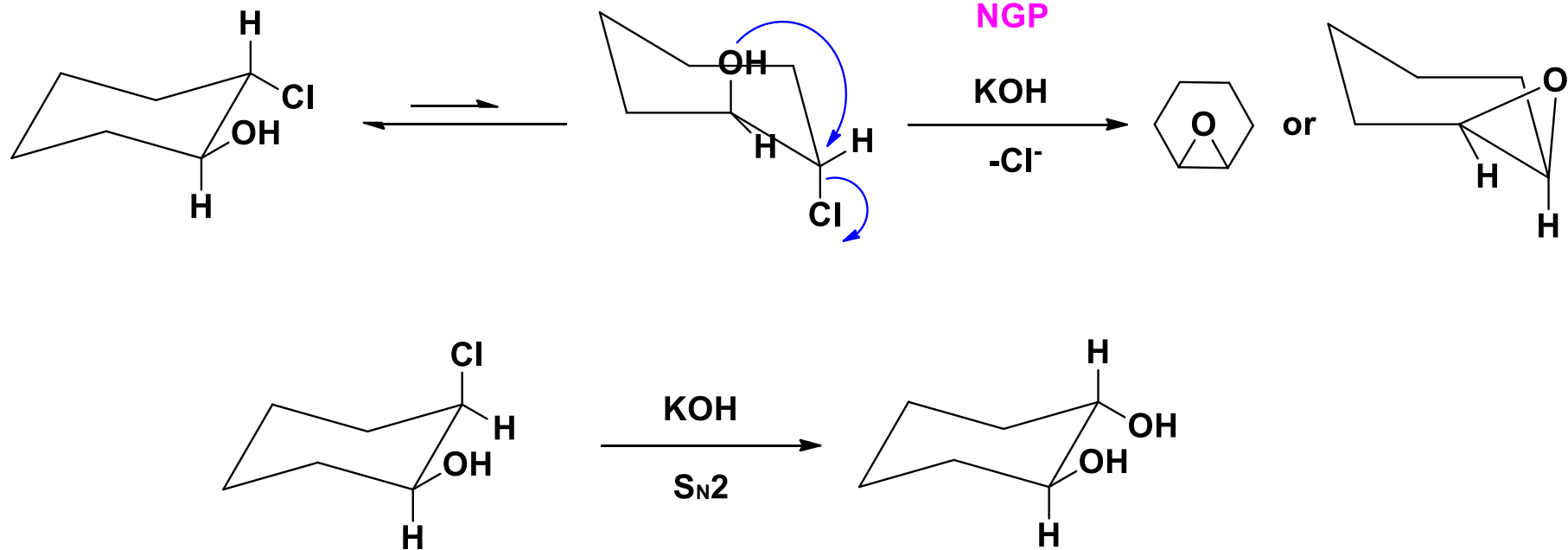


The same benzylic chloride that favours the S_N2 mechanism

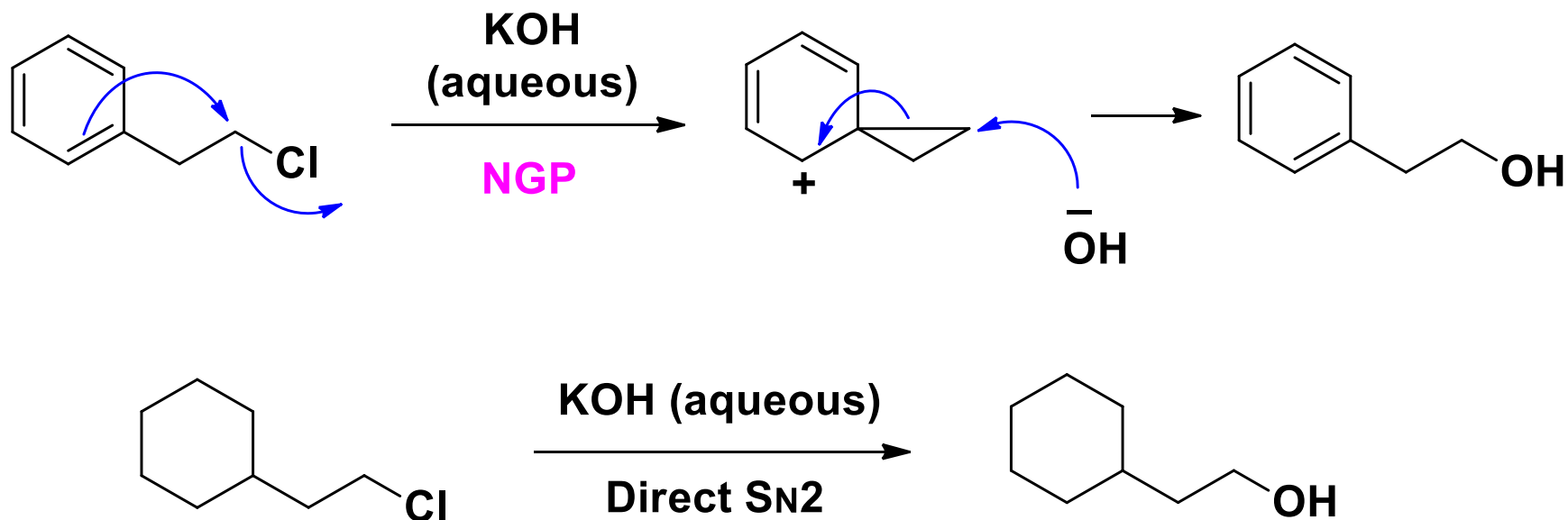


If we set the rate of substitution of the benzyl compound with methanol at 25 °C, then the 4-MeO benzyl compound reacts about 2500 times faster and the 4- NO_2 benzyl compound.

Answer of Q2

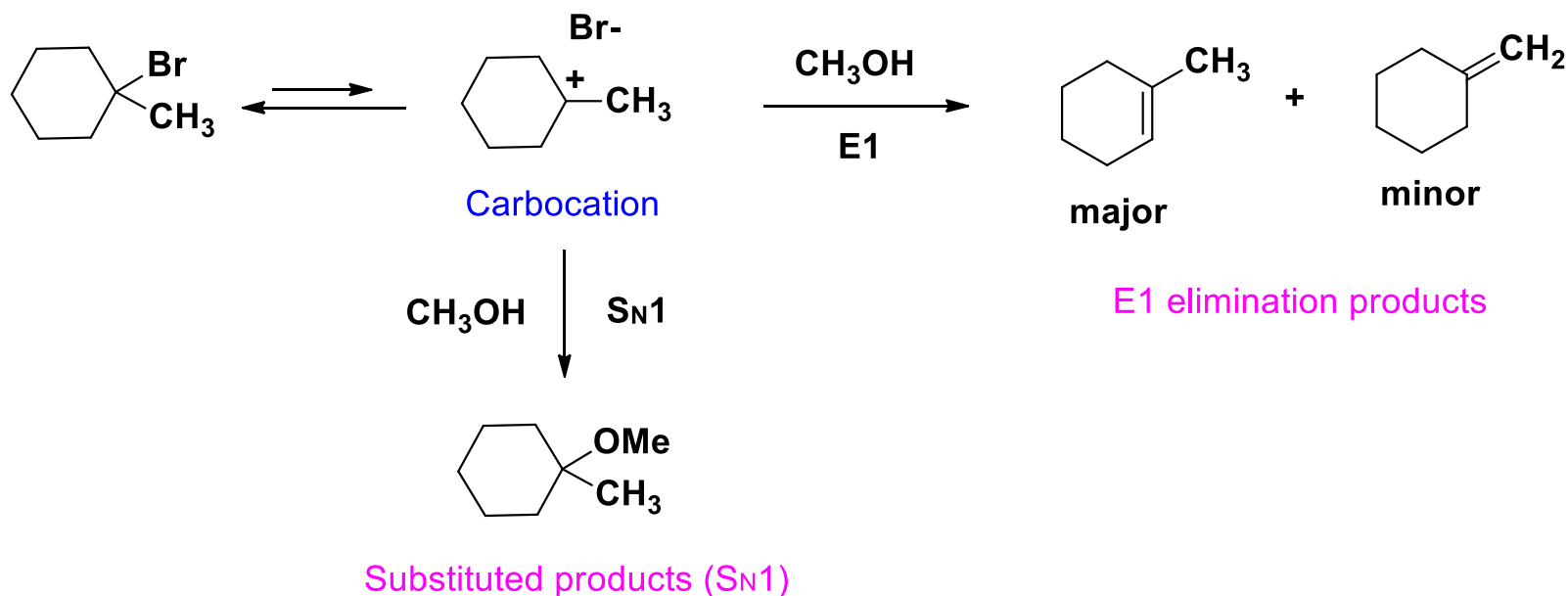


Answer of Q3



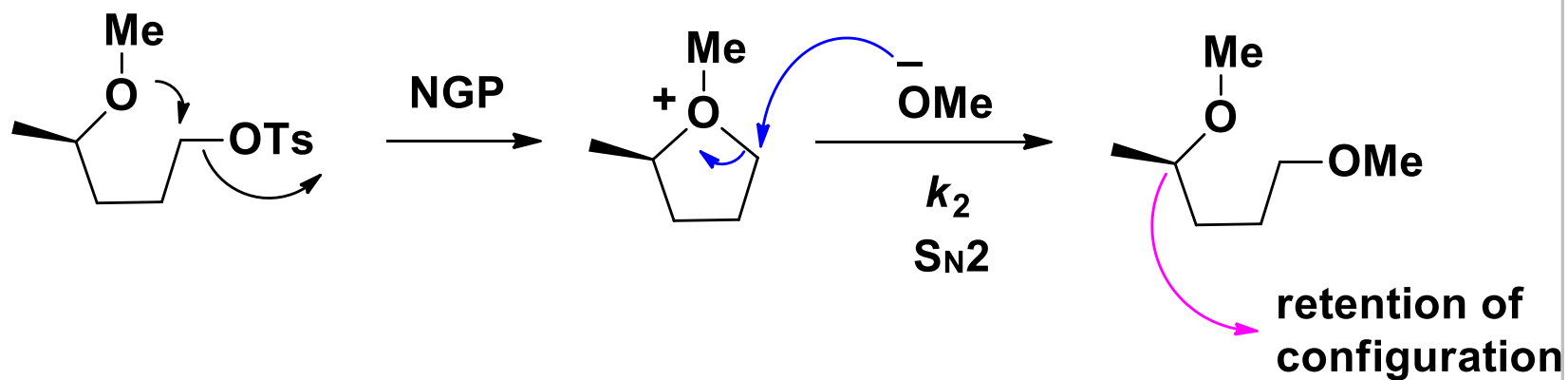
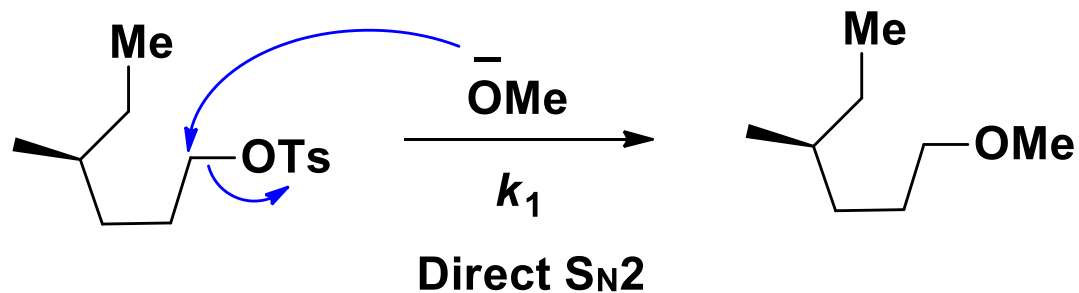
The rate of the substitution reaction will be much faster in the first case as because of NGP of the Phenyl ring.

Answer of Q4



There is no such strong base or nucleophile present, so this reaction must be first order, with an ionization of the alkyl halide as the slow step. Deprotonation of the carbocation gives either of two elimination products, and nucleophile attack gives a substitution product.

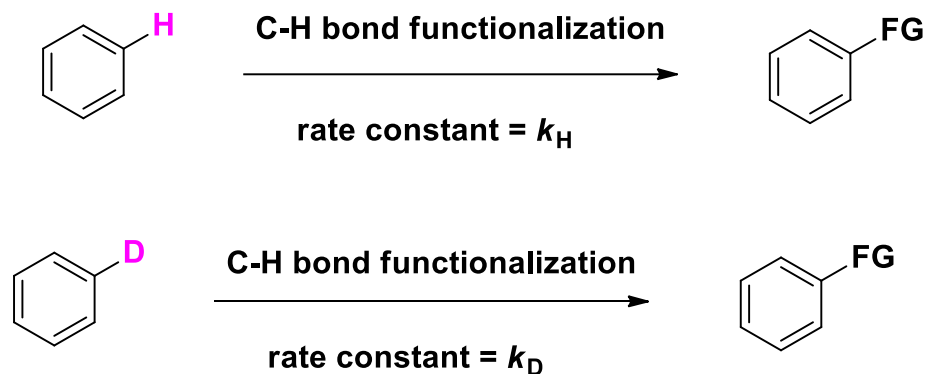
Answer of Q5



Therefore, $k_2 \gg k_1$

Answer of Q6

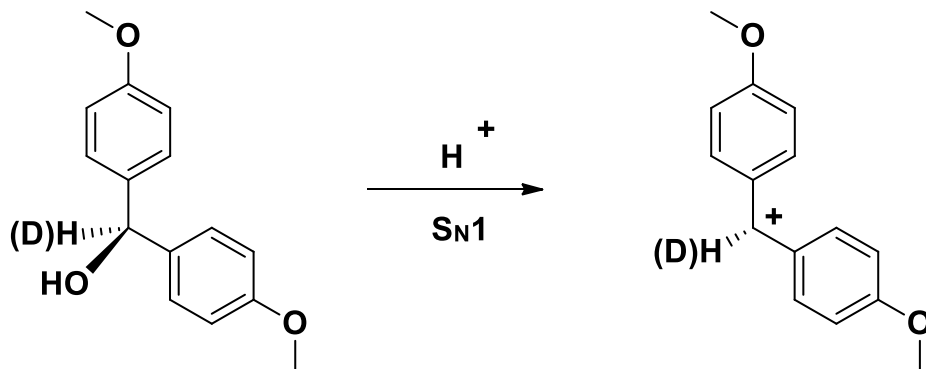
Two parallel reactions are taken here



Case 1

Primary kinetic isotope effects as C-H and C-D bond directly broken in the rate determining step

Generally $k_H / k_D \sim 1.5$ to 8 (approx value only)



Case 2

Secondary kinetic isotope effects as C-H and C-D bonds are not broken in the rate determining step.

$k_H / k_D \sim 1.18$

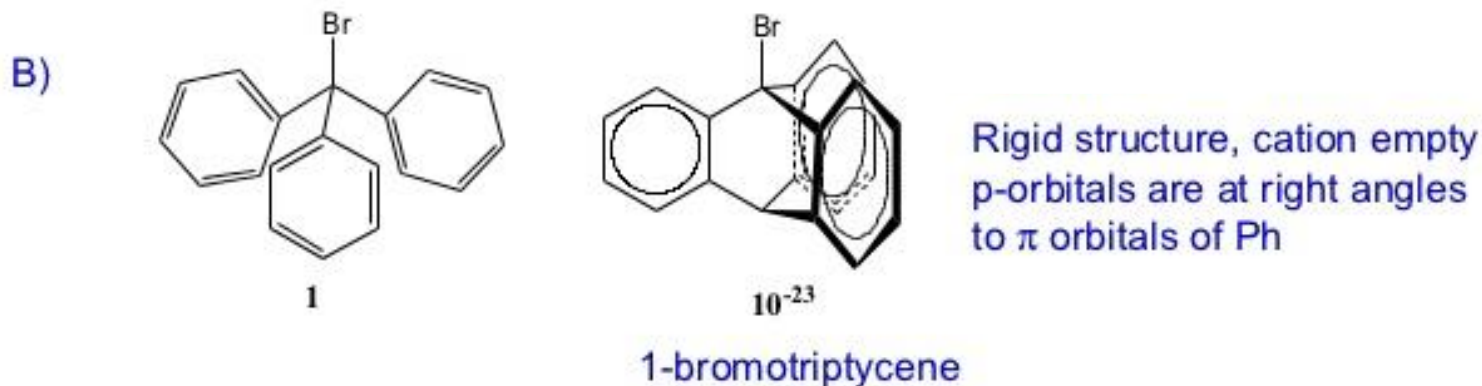
Answer of Q7

1) S_N2 reaction by EtO⁻ in EtOH:

You can give the explanation based on the steric hindrance of the reacting center

	<chem>CH3CH2-Br</chem>	<chem>CH3CH2CH2-Br</chem>	<chem>Me2HCCH2-Br</chem>	<chem>Me3CCH2-Br</chem>
relative rate	1	2.8×10^{-1}	3.0×10^{-2}	24.2×10^{-6}

2) Rate of solvolysis in EtOH :

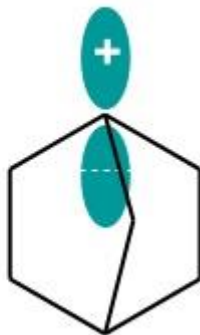
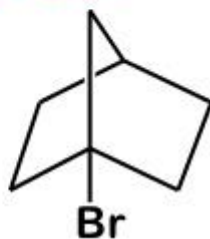


Answer of Q7 continue.....

rigid bicyclic molecule.

You can't have p orbitals on a bridgehead position

-- You cannot form a carbocation at a bridgehead position.



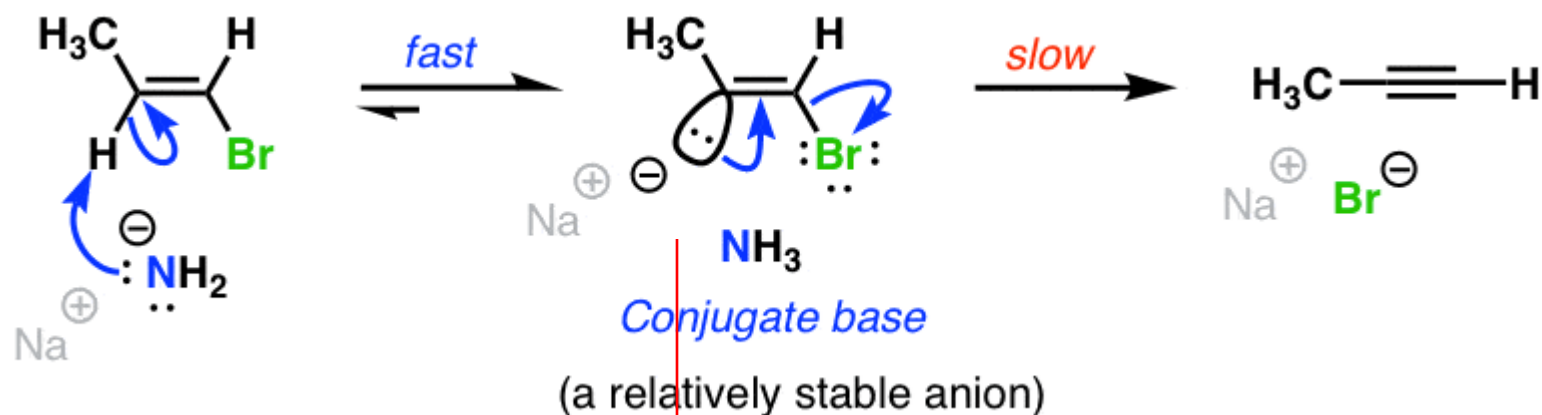
"steric rigidity"



Answer of Q8

Step 1: Deprotonation of alkenyl halide

Step 2: Elimination to give alkyne



Example of an E1cB process: Elimination Of Alkenyl Halides To Alkynes

Here, one interesting point is that elimination of the trans alkenyl halides is much faster than the elimination of the cis alkenyl halides.