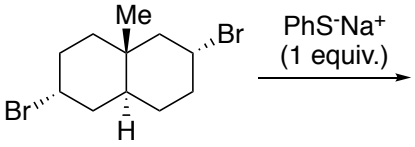
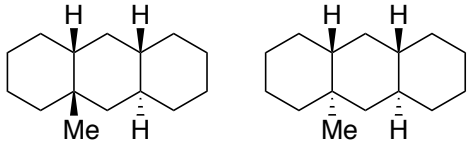
Tutorial 2

1. Predict the major product of the following reaction with correct stereochemistry and rationalize the outcome. Your explanation should contain appropriate conformational diagrams.



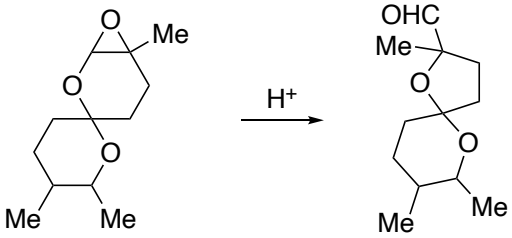
2. Write the most stable conformer of the following molecules **A** and **B**. Calculate the gauche interactions in each and find the difference in their energy.
(Eclipsing interactions: H/H = 1 kcal/mol and H/Me = 1.3 kcal/mol; Me/Me gauche interaction = 0.9 kcal/mol)



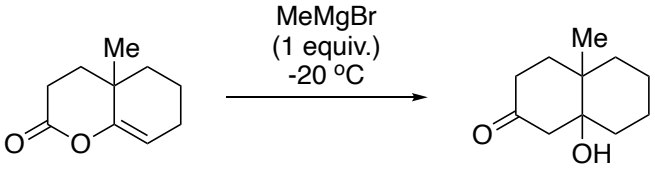
A **B**

3. Provide an arrow-pushing mechanism for the formation of the product in the following reactions.

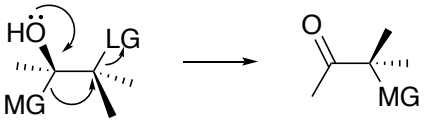
a.



b.

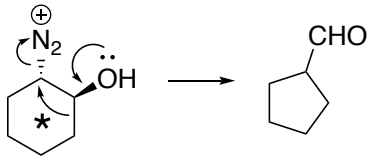


4. Given below is an example of a rearrangement reaction.

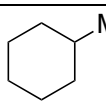
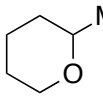
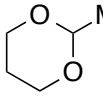
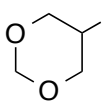


MG = migrating group
LG = leaving group

For the following reaction, identify the MO interactions involved for the arrow marked '*' in the migration step using appropriate conformational drawing.

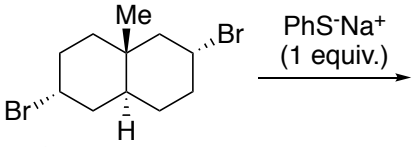


5. Draw the Newman projection of the most stable conformers of a. 2-methylpentane and b. 3-methylpentane and calculate the energy difference between them.
6. Match the structures in **Column P** with the 'A values' in **Column Q**. (*Take home problem)

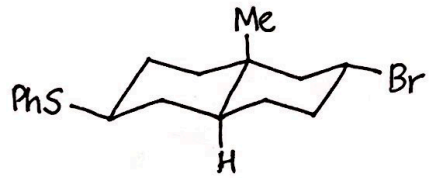
	Column P		**Column Q** (kcal/mol)
1.		a.	0.8
2.		b.	1.8
3.		c.	2.9
4.		d.	4.0

Tutorial 2 (Solution)

1. Predict the major product of the following reaction with correct stereochemistry and rationalize the outcome. Your explanation should contain appropriate conformational diagrams.

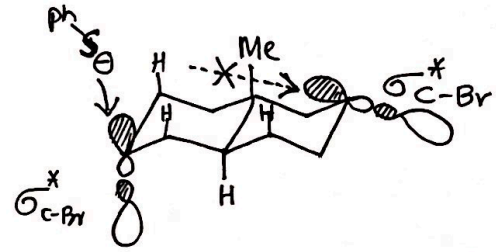


(2)



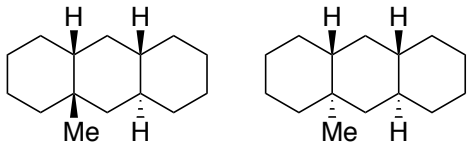
for showing the major product (1-mark)

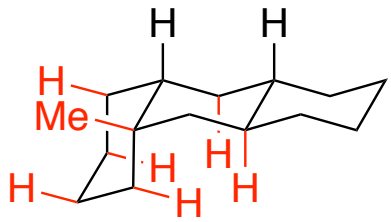
for reasoning (1 mark)



$(n_S)^2 \rightarrow \sigma^*_{C\text{-}Br}$ is a better interaction as the approach of $PhS^{\ominus}$ to other site will be hindered due to repulsion with axial C–CH_3 bond.

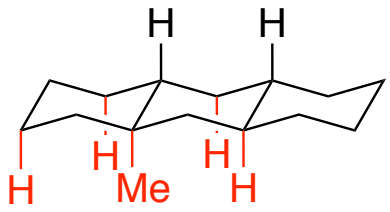
2. Write the most stable conformer of the following molecules **A** and **B**. Calculate the gauche interactions in each and find the difference in their energy.
(Eclipsing interactions: H/H = 1 kcal/mol and H/Me = 1.3 kcal/mol; Me/Me gauche interaction = 0.9 kcal/mol)





5 x 0.9 = 4.5 kcal/mol

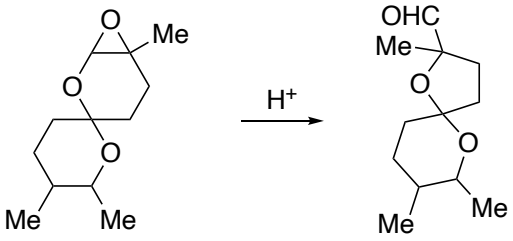
Difference = 4.5 – 3.6 = 0.9 kcal/mol



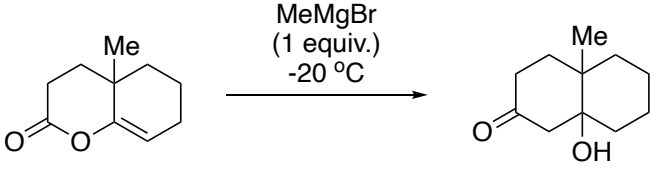
4 x 0.9 = 3.6 kcal/mol

3. Provide an arrow-pushing mechanism for the formation of the product in the following reactions.

a.

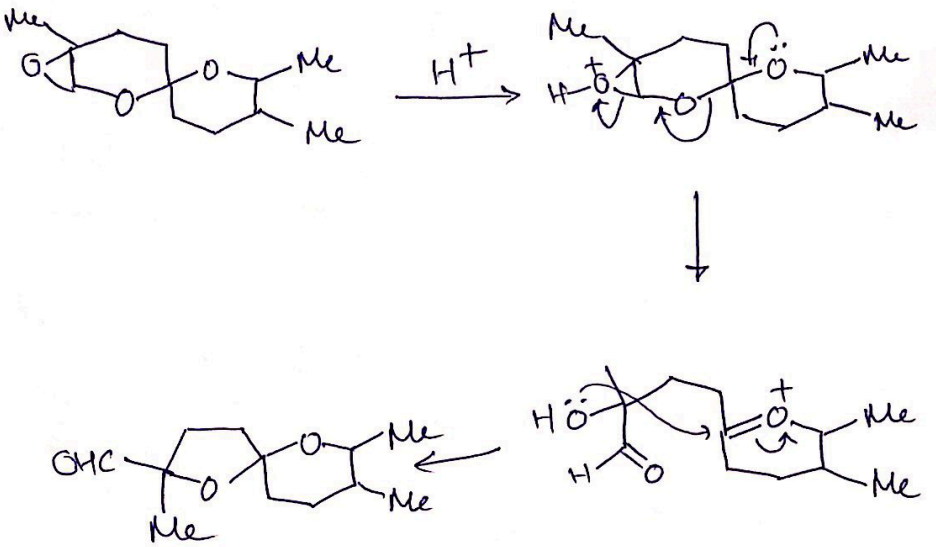


b.

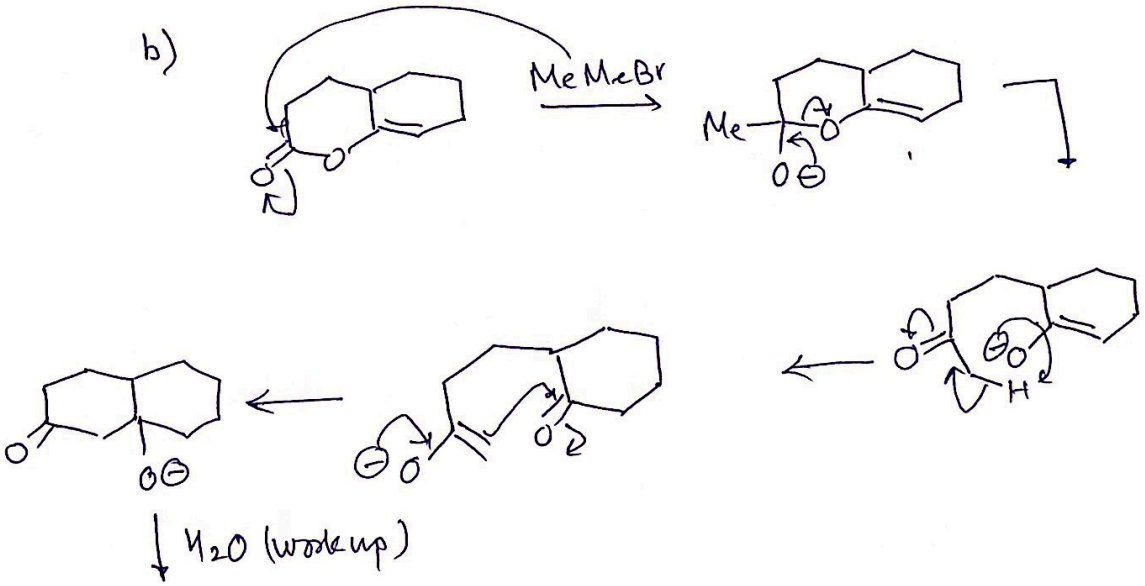


Q. 6

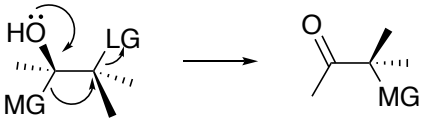
a)



b)

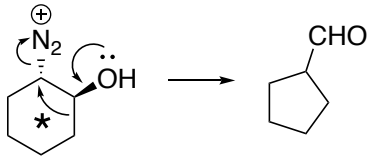


4. Given below is an example of a rearrangement reaction.



MG = migrating group
LG = leaving group

For the following reaction, identify the MO interactions involved for the arrow marked '*' in the migration step using appropriate conformational drawing.



(11) For showing the geometry of orbital interactions in its appropriate conformer (1-mark)

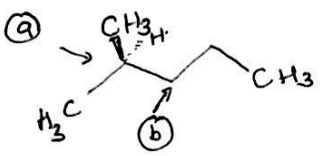
$(\sigma_{C-C})^2 \rightarrow (\sigma^*_{C-N})^0$

For conformational diagram with 1,2-diequatorial arrangement of N_2 and OH (1 mark)

5. Draw the Newman projection of the most stable conformers of a. 2-methylpentane and b. 3-methylpentane and calculate the energy difference between them.

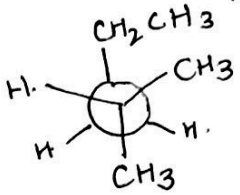
5) Most stable conformation.

a) 2- methyl pentane.



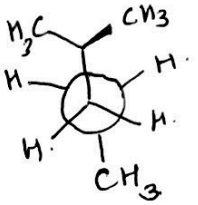
Can be represented as a combination of view (a) and (b)

View (a)



0.9 K cal/mol

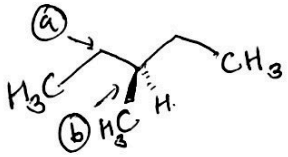
View (b)



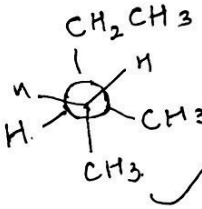
No gauche butane. visible

∴ Total Energy = 0.9 K Cal / mol

b) 3- methye pentane.

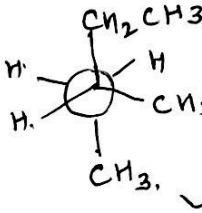


View (a)



0.9 K cal/mol.

View (b).

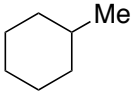
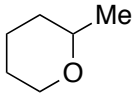
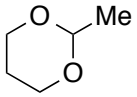
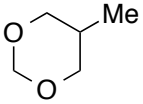


0.9 K cal /mol.

∴ Total Energy = 0.9 + 0.9 = 1.8 K Cal/mol.

∴ Energy difference = 0.9 K Cal / mol

6. Match the structures in **Column P** with the 'A values' in **Column Q**. (*Take home problem)

	Column P		**Column Q** (kcal/mol)
1.		a.	0.8
2.		b.	1.8
3.		c.	2.9
4.		d.	4.0

1 – b
2 – c
3 – d
4 – a