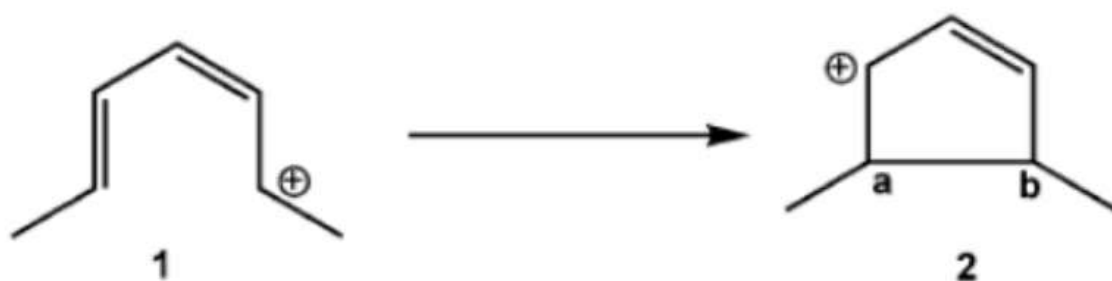


Based on the MO symmetry/phase considerations through the analysis of HOMO (show orbital picture) provide the relative stereochemistry (cis/trans) of the Me carbons at position a and b of compound **2**.



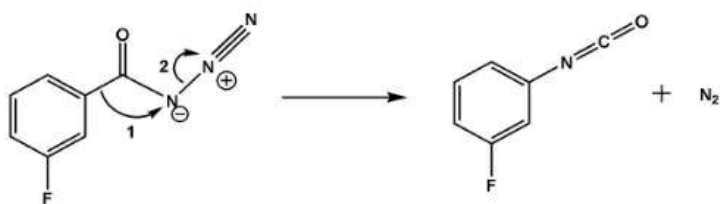
The orbital coefficients of two MOs of a cation are given below.

$$\Psi_N = 0.5\phi_1 + 0.5\phi_2 - 0.5\phi_4 - 0.5\phi_5$$

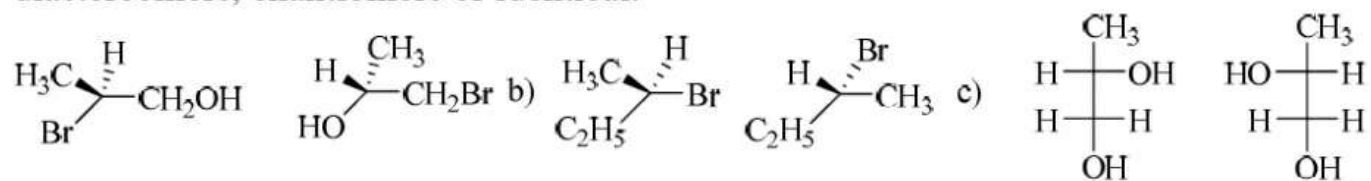
$$\Psi_N = 0.58\phi_1 - 0.58\phi_3 + 0.58\phi_5$$

- a) Show the orbital pictures and specify which orbital is of lower energy.
- b) Identify cation 1.

4. Mechanism of a molecular rearrangement reaction (reaction in which bonds migrate) is shown below. Identify the **frontier orbitals** involved in the **first step (arrow 1)** of this rearrangement. Also identify the **type of frontier orbital interactions (σ/π)** involved in **first step** by **sketching** the orbital interaction.

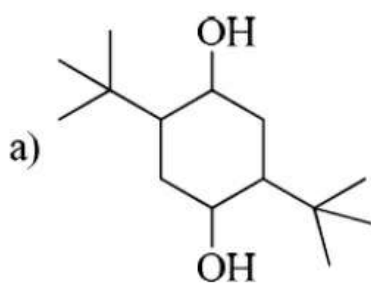


Identify the relationship in each of the following pairs as constitutional isomers, diastereomers, enantiomers or identical.

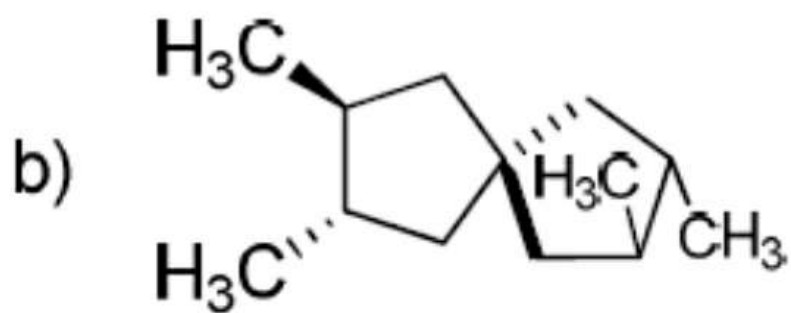
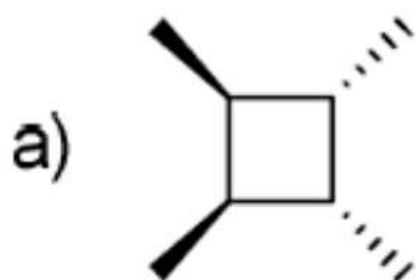


- (a) Calculate the rotational energy barrier along the C-C bond of 2,2-dimethylpropane, which would have maximum barrier for rotation?
- (b) Sketch the energy versus torsional angle profile for 2,2-dimethylpropane

Draw the preferred conformations of the following compounds.



Identify the elements of symmetry in the given molecules and determine if they are chiral.



In each of the given cases, identify (i) the nucleophile and the electrophile (ii) show using 'electron-pushing' arrows how the following reaction happens (iii) what kind orbitals (such as n, σ , σ^* , π , π^* or AO) of the nucleophile and the electrophile are involved in these reactions.

