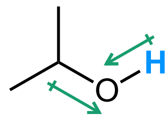
Solvents in Organic Chemistry

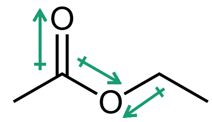
1. **Classify** the following **solvents** as **polar protic**, **polar aprotic**, or **nonpolar**. Justify your selection.

$CHCl_3$

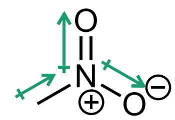
nonpolar
similar to CCl_4 and CH_2Cl_2



polar protic
O-H bond

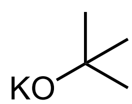
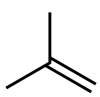


polar aprotic
C=O bond dipole, but only **C**-H bonds



polar aprotic
N-O bond dipoles, but only **C**-H bonds

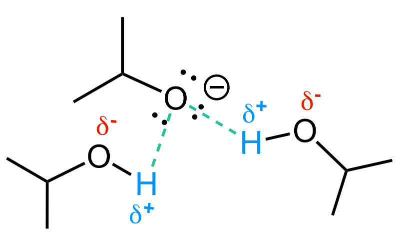
2. For the species on the left, select the most appropriate solvent from the choices on the right. Justify your selection.

	Solute(s)	Solvent choices	Explanation
A.		hexane or ***tert*-butanol**	In this case, the solute is an ionic compound, therefore a polar solvent (*t*BuOH) is required
B.	 + Br_2	$\mathbf{CH_2Cl_2}$ or water	In this case, the solutes are nonpolar, therefore a nonpolar solvent is required

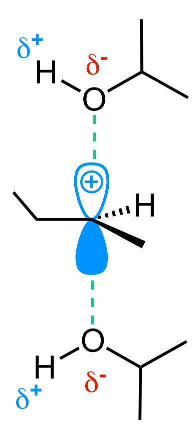
3. As described in the **Role of Solvents #4** in the **Solvent Core Concepts**, polar protic solvents can stabilize atoms with formal charges.

A. Show how two molecules of isopropyl alcohol solvent can orient and stabilize the alkoxide anion on the left.
B. Show how the same solvent can orient and stabilize the carbocation on the right.

Note: Be sure to draw the O-H bond when orienting the solvent molecules. Dotted lines are generally used to show attractive interactions that are not true covalent bonds.



To stabilize the negative charge of the anion, the solvent will orient itself such that the positive end of the O-H bond dipole will be closer to the anion.



To stabilize the cation (empty p-orbital in this case), the solvent will orient itself such that the negative end of the O-H bond dipole will be closer to the positively charged carbon.

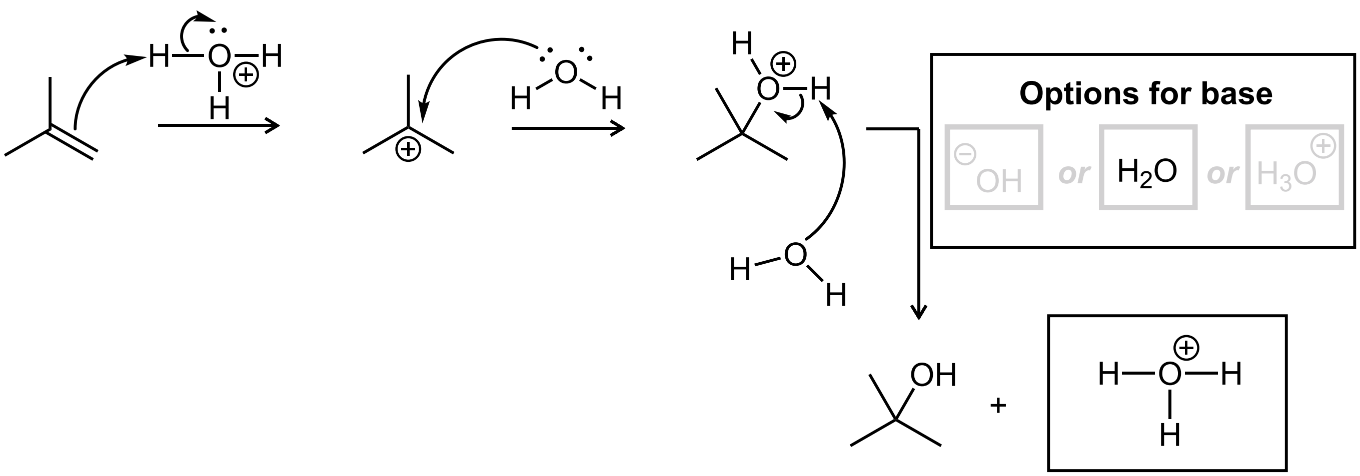
4. Shown below is a stepwise mechanism for the hydration of an alkene.

A. **Why is H_3O^+ being shown as the acid** and not H_2SO_4?

$$H_2SO_4 + H_2O \longrightarrow HSO_4^{-} + H_3O^{+}$$

Strong acids in water completely dissociate and generate H_3O^+

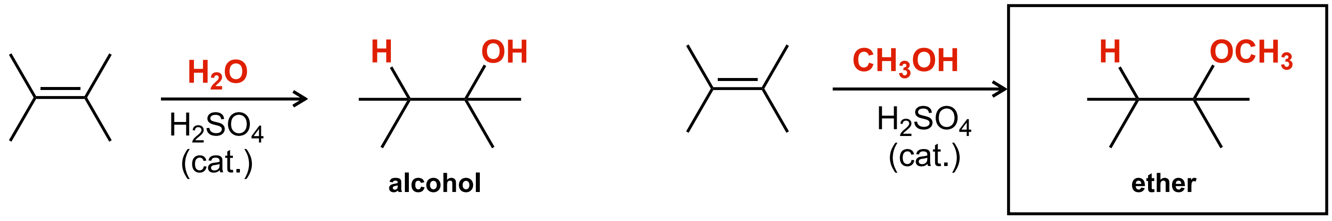
B. For the final mechanistic step, **select the appropriate base** from the three shown. Then **draw the mechanism for the last step of the reaction** and **provide the missing by-product**.



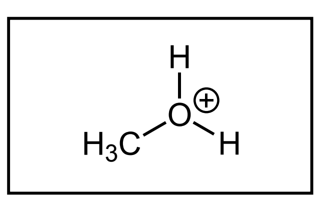
C. **Why is H_3O^+ (or rather H_2SO_4) referred to as a catalyst** in this reaction?
One way to identify a catalyst in a reaction is if it is regenerated at some point in the reaction mechanism. Notice that H_3O^+ is used in the first step of this reaction (becoming H_2O), but is regenerated in the final step. This suggests that the H_3O^+ produced in the final step can be used again to protonate another alkene substrate.

5. Water is not the only molecule that can act as a solvent ***and*** a reactant in a reaction. The hydration reaction from the Solvent Core Concepts is shown below.

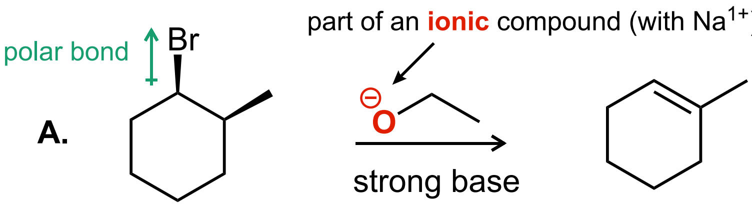
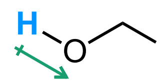
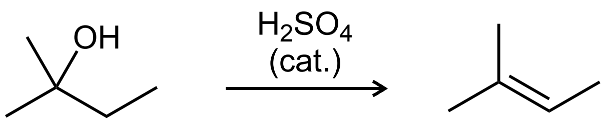
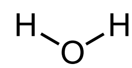
A. Use this reaction as a guide to **draw the structure of the product for the reaction on the right**.
B. What **functional group** is generated?
Hint: the product ***is not*** an alcohol.



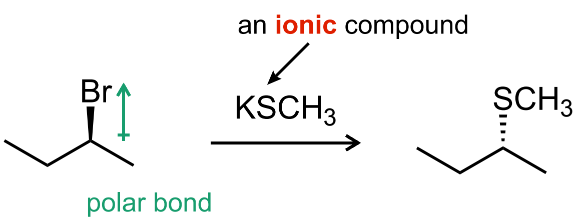
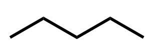
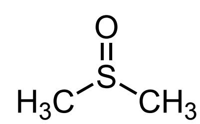
C. In the reaction on the left, *water* reacts with H_2SO_4 in solution to create H_3O^+, which acts as the acid in solution. In the box provided below, **draw the structure of the acid for the reaction on the right**, considering that *methanol* reacts with H_2SO_4?



6. In some situations, the solvent is not explicitly written, but is implied based on the reactants involved in the reaction. **Use context clues to identify the solvent (or a likely solvent choice) for the reactions shown below.**

Reaction	Solvent
A. 	 The structural similarities that make EtOH an appropriate solvent are shown in blue. Additionally, any potential reaction between the solvent (EtOH) and the base (EtO^-), creates the same species in solution (EtOH & EtO^-) forcing EtO^- to carry out the intended E2 reaction.
B. 	 Both reactants in this reaction contain OH bonds, making both structurally similar to and therefore soluble in H_2O. Additionally, the use of water allows for the formation of H_3O^+ to catalyze this dehydration reaction.

7. An example of an S_N2 reaction is shown below. **Answer the questions below** giiven the options of the solvents below.

Reaction	Solvent choices				
	 **nonpolar** **not suitable**	***or***	CH_3OH **polar protic**	***or***	 **polar aprotic** **fastest**

a) Which solvent results in the fastest rate of reaction? Why? Describe the class of solvent in your answer.
DMSO should have the fastest rate as it is a polar aprotic solvent. Its polar nature allows it to dissolve the reactants but its aprotic nature (lacking H-bonding) prevents it from solvating the nucleophile ($^-SCH_3$) too effectively, allowing the S_N2 reaction to proceed.

b)Which solvent is not suitable for this reaction? Why? Describe the class of solvent in your answer.
Pentane is not suitable as it is nonpolar and therefore unlikely to solvate $KSCH_3$, an inonic compound.