Tutorial for Health Sciences and Pharmacy Students. Week 2-3

In these weeks we studied: the formation of chemical bonds using carbon, hybridisation of carbon, combining atomic orbitals, structures, electronegative atoms, polar covalent bonds, the formation of dipoles and dipole interactions, intermolecular bonding, formal charges, Lewis definition of acids and bases, reaction types, definition of nucleophiles and electrophiles, radicals, symmetrical and unsymmetrical bond breaking, halogenation, regiochemistry, isomers, structural isomers, conformational isomers, staggered *vs.* eclipsed conformers, Newman projection, cyclic compounds, cyclohexane, chiral molecules, stereogenic centres, plane of symmetry, handiness, diasteromers, meso compounds, enantiomers, 3D structures, optical activity, enantiomeric excess, stereoisomers *R* vs. *S*, determining absolute configuration, *cis vs. trans*, *E vs. Z*, Fischer projection. The questions below address some of these topics.

Question 1. An sp^3 hybrid orbital is formed by the combination of one *s* orbital and three *p* orbitals. The resulting sp^3 orbital is unsymmetrical about the molecules. Draw the resulting structure of the hybridisation of three sp^3 orbitals. These would give you a tetrahedral orbital.

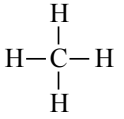
Question 2. When two sp^3 carbons come together a new C-C bond can be formed. Show this for the formation of ethane.

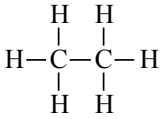
Question 3. Show the structure of an sp^2 carbon?

Question 4. How would you use two sp^2 hybridised carbons to form a new C=C bond?

Question 5. Formaldehyde (CH_2O) has a carbon-oxygen bond. Draw the Lewis and the line-bond structures of this compounds and indicate the hybridisation of the carbon atom.

Question 6. Draw the Lewis structure of the following molecules:


A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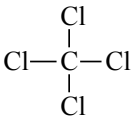
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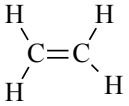
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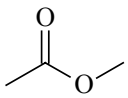
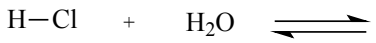
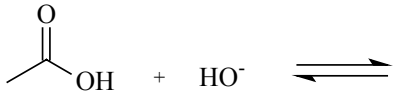
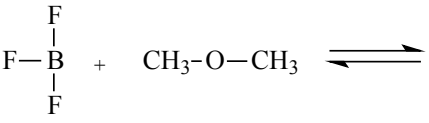
E

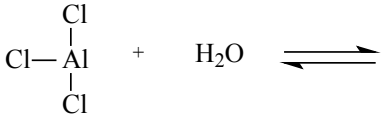

F

Question 7. Finish writing the equilibrium equations for the following acid-base reactions, and define which of these compounds are acids, and which are bases? It will help to draw the lone pairs (:).

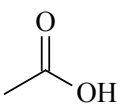
A 

B 

C 

D 

Question 8. Which of the following molecules have dipoles? Draw these and suggest how these molecules would interact with each other (e.*g.* how does one acetone molecule interact with another acetone molecule (intermolecular bonding) *etc.*).



A

B

H_2O C

H—Cl D

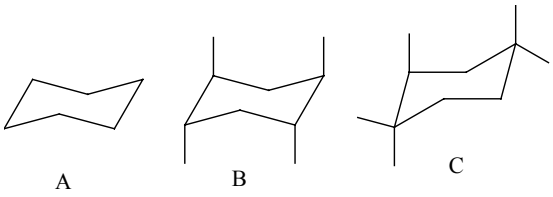
CH_4 E

CH_3Cl F

Question 9. Draw the 3D structure of:

a) Cyclopropane
b) Cyclobutane
c) The 'chair' form of cyclohexane
d) The 'boad' form of cyclohexane

Question 10. Identify the axial and the equatorial bonds in the following structures:



A B C

Question 11. Demonstrate the 'ring flip' in the chair form of cyclohexane.

Question 12. What is the 1,3-diaxial steric interactions in methyl cyclohexane?

Question 13. Draw the structure of 1,1-dimethylcyclohexane. Indicate whether each group is axial or equatorial. Do the same thing for 1,4-dimethylcyclohexane.

Question 14. Draw all the different conformers possible for ethane using Newman projections. Do the same thing for bromoethane and for 1,2-dibromoethane.

Question 15. Demonstrate a) homolytic (radical) bond breaking and b) heterolytic (polar) bond breaking for an A-B molecule. Then do the same thing for c) homolytic bond formation and d) heterolytic bond formation for an A-B molecule.

Question 16. Give one example of a) homolytic bond breaking and b) heterolytic bond breaking.

Question 17. When a carbon atom bonds to an electronegative atom the bond is polarised. This gives rise to the formation of a partial positive charge (δ^+) and a partial negative charge (δ^-) in the molecule. Conversely, when a carbon bonds to an atom that is less electronegative than itself, the opposite polarity results. Give six examples of such interactions, three for each, where the carbon has either got a δ^+ or a δ^- on it.

Question 18. What is the definition of: a) electrophile, and b) nucleophile?

Question 19. Show the flow of 'electron' in a reaction between $:B^-$ and A^+ , to give the new molecule A-B? Which one of these is the electrophile and which one is the nucleophile?

Question 20. Which one of the following are most likely to behave as electrophiles and which as nucleophiles?

a)H^+ b)Cl^- c)Br^- d)NH_3 e)$H_2C{=}CH_2$ f)HO^- g)Cl_2 h)CH_3SH i)CH_3OH, j)CH_3HO

Question 21. What is/are the product(s) of the following reactions?

A $CH_4 + Cl_2 \xrightarrow{\text{light}}$

B  $+ Cl_2 \xrightarrow{\text{light}}$

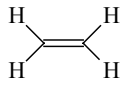
C $CH_3Cl + Br_2 \xrightarrow{\text{light}}$

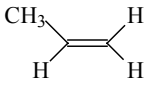
Question 22. What is the meaning of "reaction rates" and "equilibrium" when describing reactions between molecules such as A and B to give A-B?

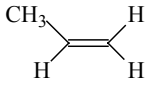
Question 23. Draw a 'typical' reaction energy diagram for the above reaction. Then draw a reaction that is in one-step and what is both fast and highly 'exothermic'!

Question 24. Draw the mechanism for the reaction between ethylene and HCl. Identify the nucleophiles(s) and the electrophiles(s) in this reaction!

Question 25. Which isomers are formed in the following reactions?

A  + HBr ⟶

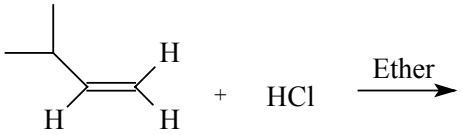
B  + H_2O ⟶

C  + Br_2 ⟶

Question 26. Name the products of the above reactions.

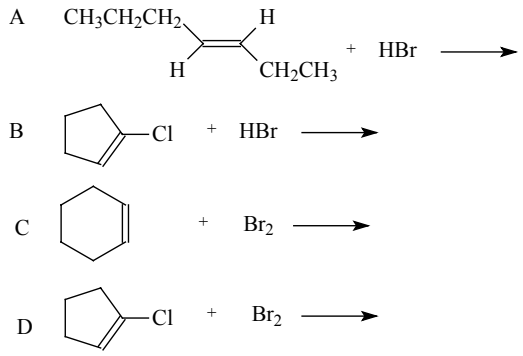
Question 27. Describe what gives rise to the stability of carbocations?

Question 28. Investigate the following reaction:



a) What is/are the product(s)?
b) Why is this reaction 'regiospecific'?
c) What are the names of all the possible products?
d) What is the role of 'Ether' in this reaction?
e) The reaction is carried out at 25° C. What does that tell you?

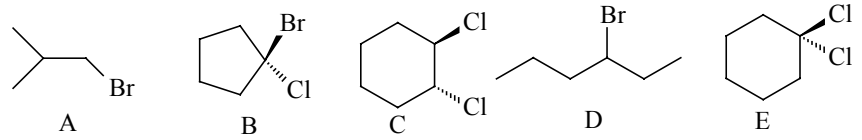
Question 29. What is the mechanism for the following reactions and what are the products? What rule can you apply to predict the structure of the product prior to the reaction?



Question 30. Name the products of the above reactions.

Question 31. Draw the Newman-projection for the product of c) in **Q. 29**, when looking through the C-C bond of the *–CHBr-CHBr-* fragment. How many possible Newman-Projections can you draw?

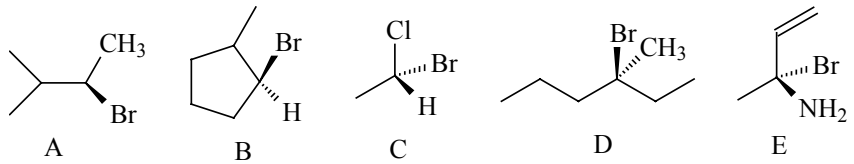
Question 32. What are the starting materials of the following alkyl halides?



Question 33. a) The product D in Q. 32, is chiral, why? Draw the 3D structure of this product; what would you expect to see? **b**) Is compound C chiral as well? **c)** what about B?

Question 34. What rules do you need to apply when assigning the absolute configuration of a chiral compound?

Question 35. Apply these rules when assigning the following compounds as either *R* or *S*.



Question 36. a) Assign the compounds below as either *cis* or *trans*. b) Do the same thing using either *E* or *Z*.