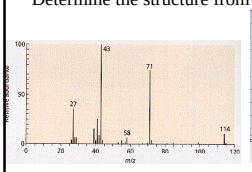
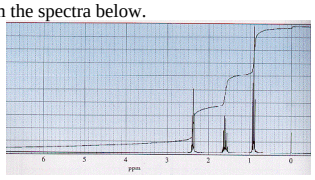
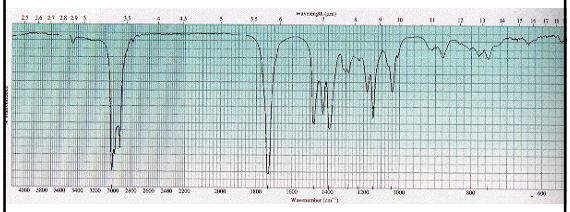
Unit I - Structure

Problems

Determine the structure from the spectra below.





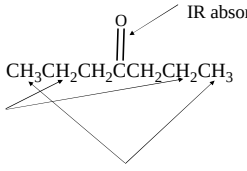


Problem 1 solution

Molecular ion: 114 indicates need to double the propyl group

Other hydrogens ~2.5 ppm triplet – 2 neighbors

indicated by IR absorbance ~1750 cm^{-1}

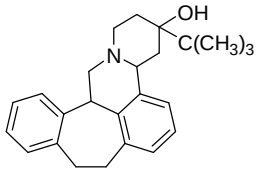


~1.6 ppm multiplet – lots of neighbors

~1ppm triplet – terminal alkane w/2 neighbors

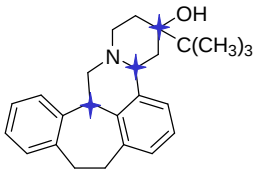
Problem 2

- Butaclamol is an antipsychotic used in the treatment of schizophrenia. How many stereocenters does it have?



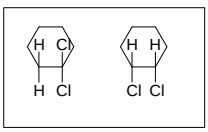
Problem 2 Solution

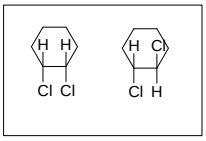
- Nitrogen has potential to be stereogenic, but converts rapidly at room temperature as sp3 and sp2 are close in energy

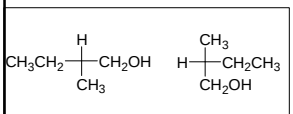


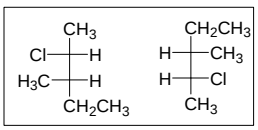
Problem 3

- Are the structures in the following pairs identical, constitutional isomers, enantiomers, or diastereomers?

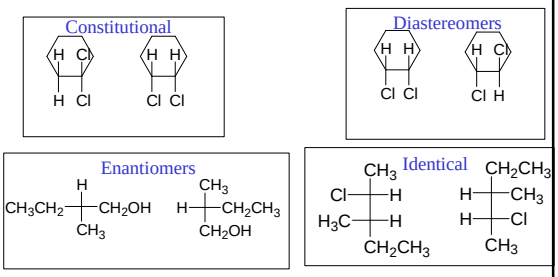






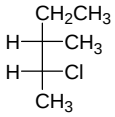


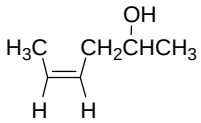
Problem 3 Solution



Problem 4

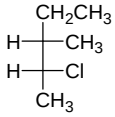
- Provide systematic (IUPAC) names for the following structures



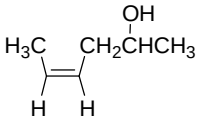


Problem 4 Solution

- (2R, 3S)-2-chloro-3-methylpentane



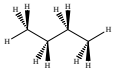
- Z-4-hexen-2-ol

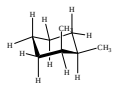


Problem 5

- Draw the most stable conformation of:
  - Butane
  - Cis-1,2-dimethylcyclohexane

Problem 5 Solution

- Butane  OR 
- Cis-1,2-dimethylcyclohexane



If you draw both methyl groups equatorial, it will be trans, so this is the best you can do for this structure

Problem 6

- (2R)-2-pentanol is a colorless liquid that has a melting point of -50 C and a boiling point of 118 C.
  - Draw its structure.
- An unknown colorless liquid has a melting point of -50 C and a boiling point of 118 C.
  - Is the unknown colorless liquid (2R)-2-pentanol?
  - Why or why not?
  - If not, what else could it be and how could you distinguish the two?

Problem 6 Solution

- Is the unknown colorless liquid (2R)-2-pentanol?
  - Not necessarily
- Why or why not? – Both enantiomers have identical physical properties
- If not, what else could it be and how could you distinguish the two? – it could be (2S)-2-pentanol, and optical rotation (or odor possibly) could distinguish the two