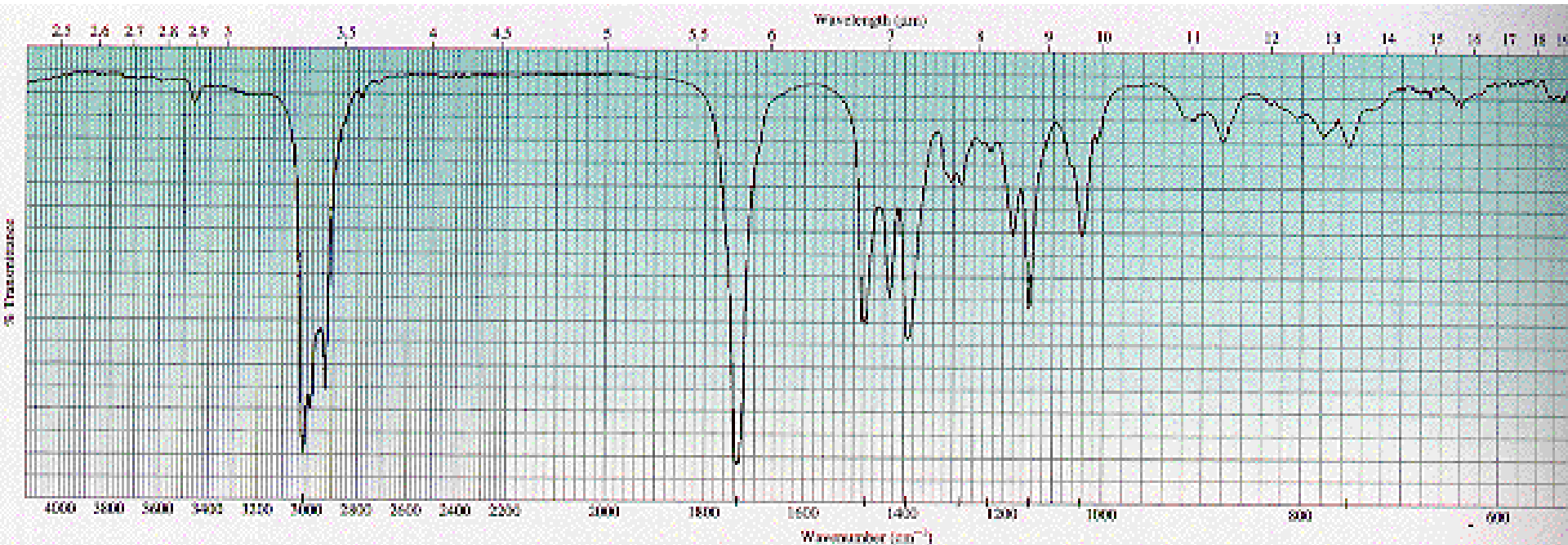
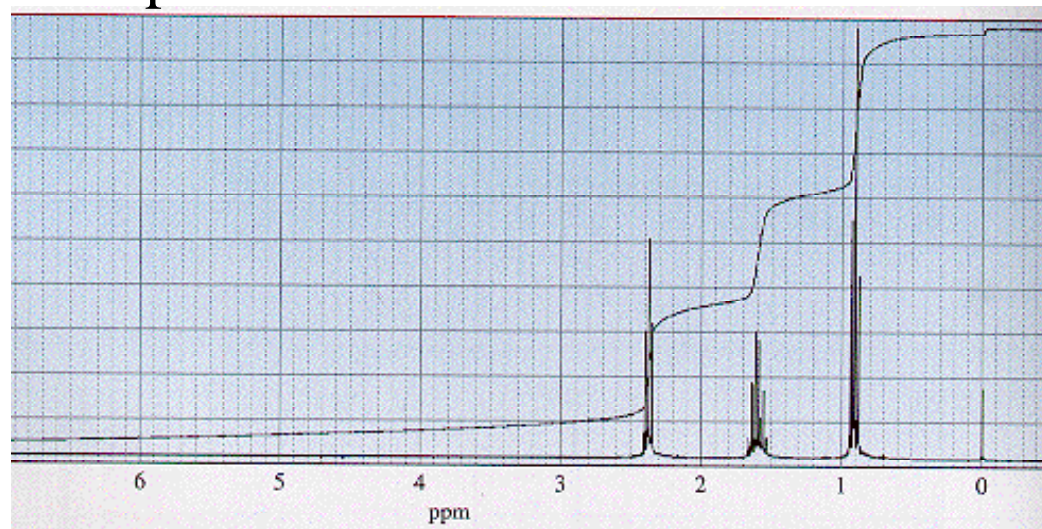
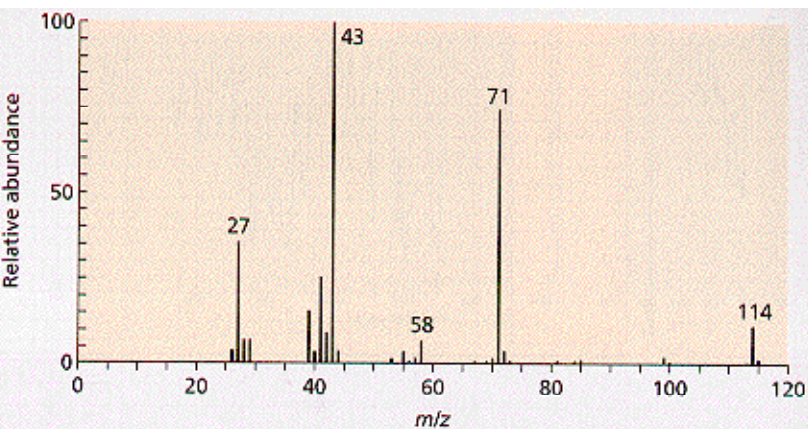


Unit I - Structure

Problems

Determine the structure from the spectra below.

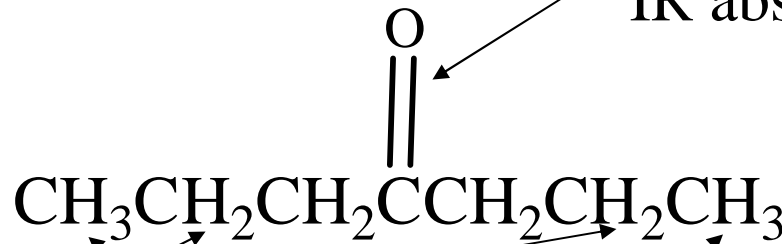


Problem 1 solution

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

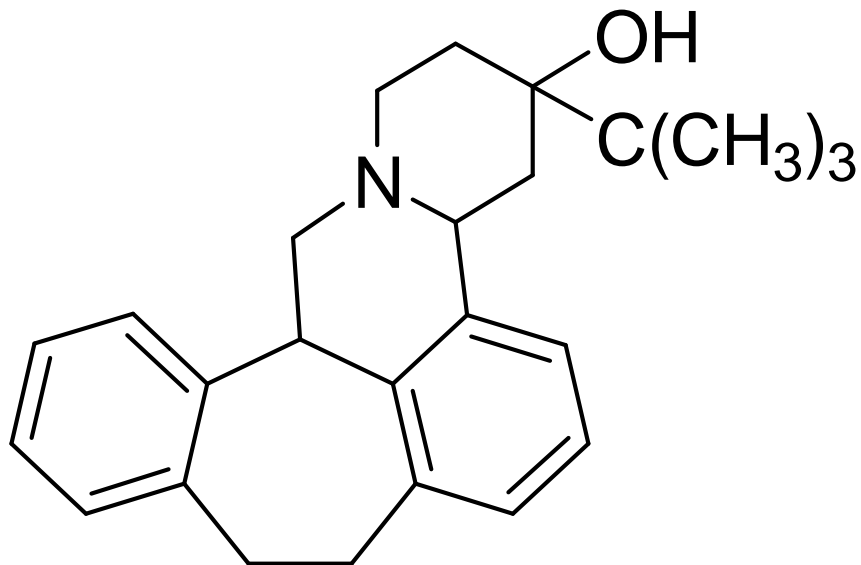


~1.6 ppm multiplet – lots of neighbors

~1 ppm triplet – terminal alkane w/2 neighbors

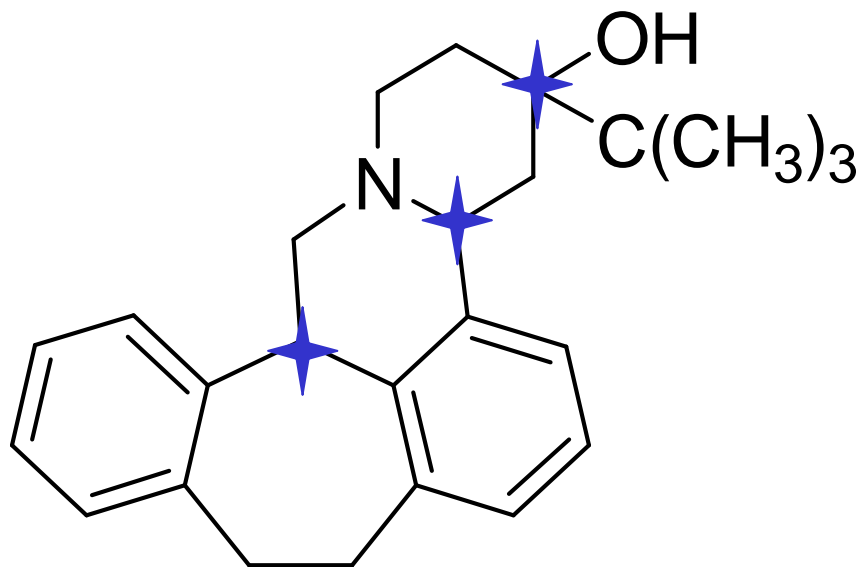
Problem 2

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



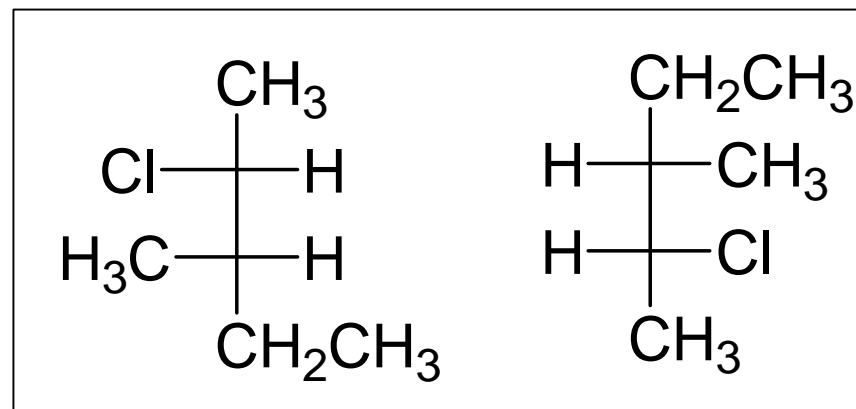
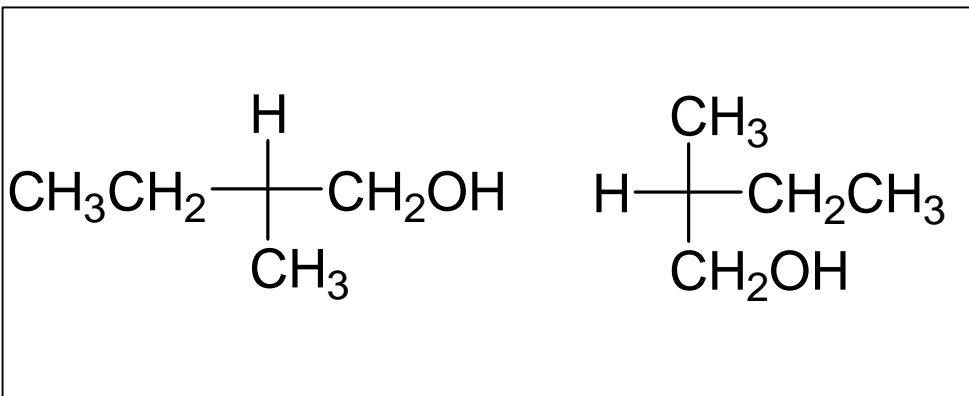
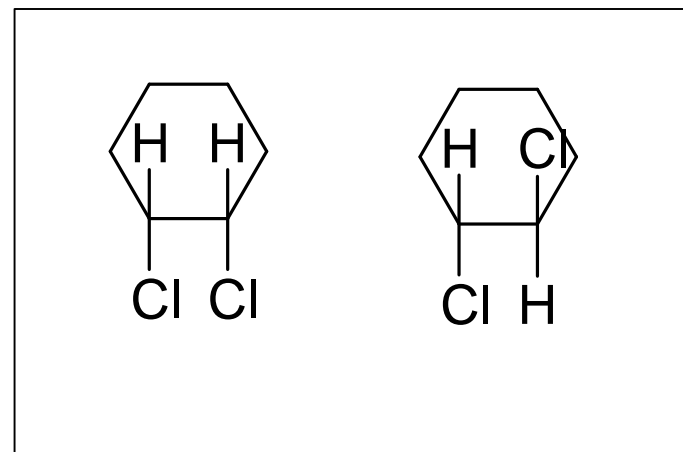
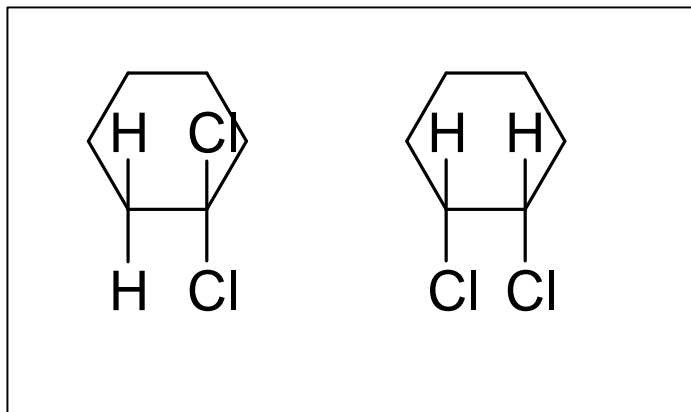
Problem 2 Solution

- ✦ Nitrogen has potential to be stereogenic, but converts rapidly at room temperature as sp^3 and sp^2 are close in energy



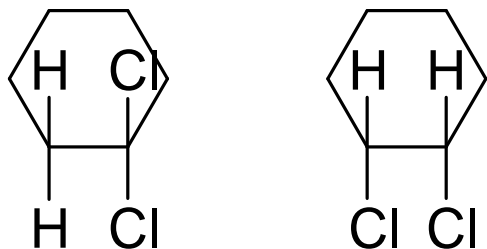
Problem 3

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

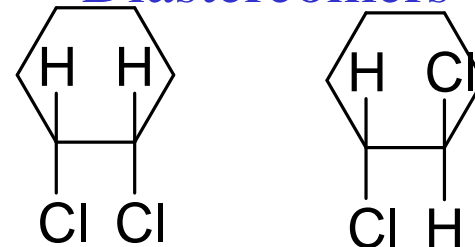


Problem 3 Solution

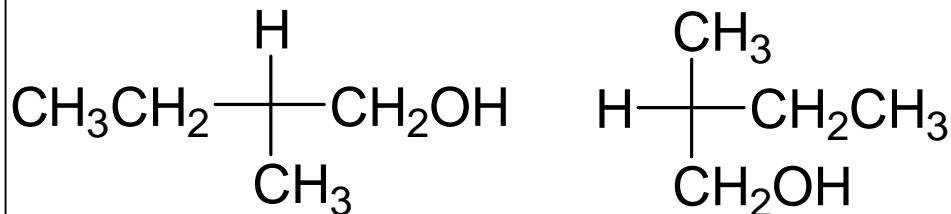
Constitutional



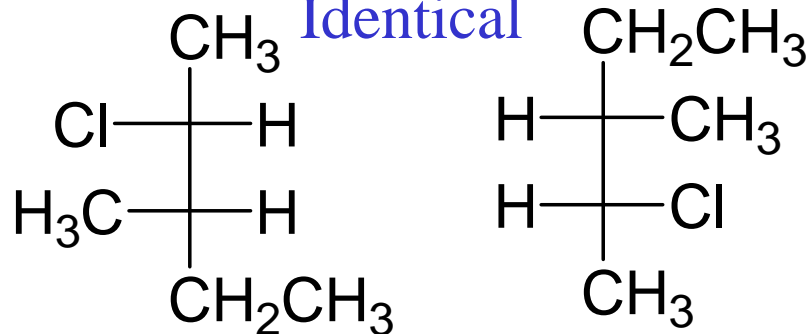
Diastereomers



Enantiomers

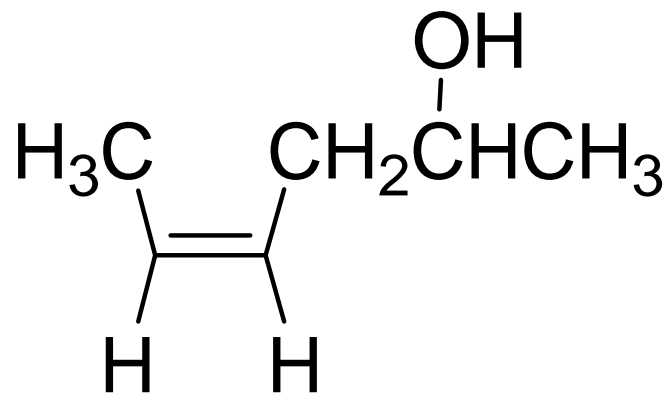
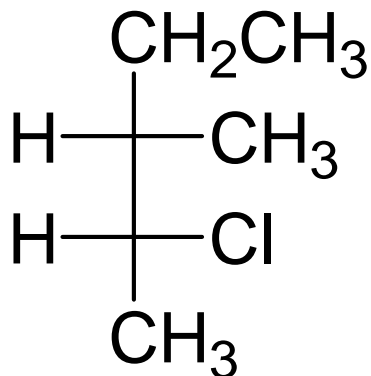


Identical



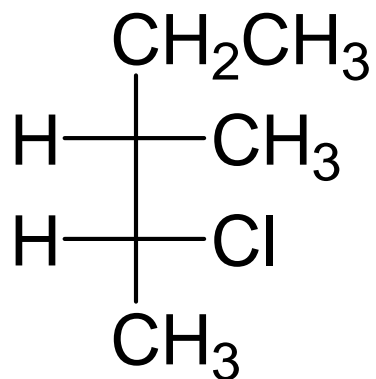
Problem 4

- Provide systematic (IUPAC) names for the following structures

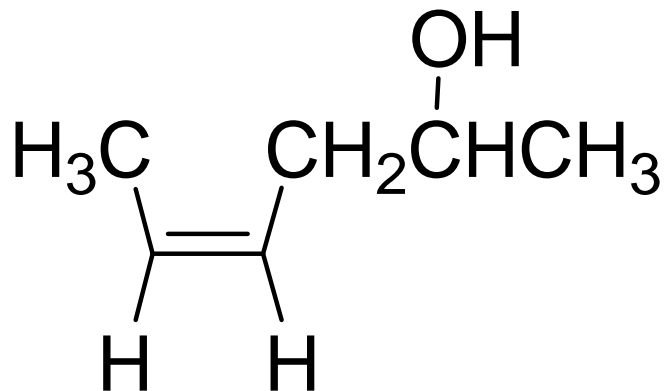


Problem 4 Solution

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



- Z-4-hexen-2-ol

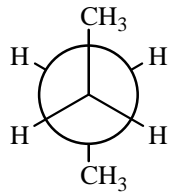


Problem 5

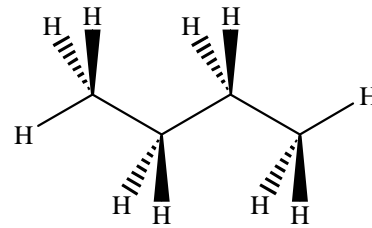
- Draw the most stable conformation of:
 - Butane
 - Cis-1,2-dimethylcyclohexane

Problem 5 Solution

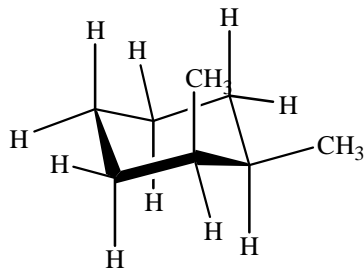
- Butane



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

