CH1010 Tutorial 3 Answers

1. Provide **IUPAC** names for the following compounds:

OHCCH₂CH₂CH₂CHO

pentanedial

ANS:

3,5-dimethylphenol

ANS:

N-cyclopentyl-3-methylbutanamide

- 2. Draw **line-angle structures** corresponding to the following IUPAC names:
 - *N*-ethyl-*N*-methylcyclohexylamine

• 2,2-dimethyl-propanoic acid

3. **Classify** each of the following **nitrogen atoms** in the following compounds as primary, secondary, tertiary, or quaternary.

4. At what approximate positions might this compound show **infrared** absorptions?

$$\begin{array}{c}
O \\
|| \\
N \equiv C - CH_2 - C - CCH_2CH_3
\end{array}$$

ANS:

This compound should show a medium absorption at 2210-2260 cm⁻¹ for the nitrile, a strong absorption at about 1735 cm⁻¹ for the ester carbonyl. There would also be a strong absorption at about 1100 cm⁻¹ for the C-O bond of the ester in the fingerprint region.

5. Circle any **conjugated portions** in the molecules below.

$$H_2C=CH-C\equiv N$$

ANS:
$$H_2C = CH - C \equiv N$$

ANS: not conjugated

6. An impure organic liquid was obtained from the wood of the sandalwood tree *Santalum austrocaledonian* using standard laboratory techniques.

• How could **purification** of the liquid be carried out?

A minor component of the organic liquid was obtained in a pure form and gave the following microanalytical results:

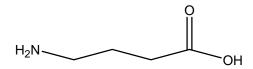
C: 46.59 % H: 8.80 % N: 13.58 %

Infrared spectroscopy of a sample of the liquid gave several strong bands at 3390, 2900 and 1705 cm⁻¹. In a mass spectrum of the compound a molecular ion was obtained at m/z 103.

- Determine the **empirical** and **molecular formulae** for this compound.
- Draw a **line-angle structure** for a possible molecule that obeys this molecular formula, and indicate how this could be verified using **infrared spectroscopy**.

The compound would be purified by fractional distillation and the purity verified by boiling point, TLC or further microanalysis.

NH₂CH₂CH₂CH₂COOH 4-aminobutanoic acid



Working:

empirical + molecular formulae $C_4H_9O_2N$ IR Bands: NH 3390, OH(COOH) 2900, CO(COOH) 1705, CH 2900