

IR SPECTROSCOPY – TEST 2

QUESTION 1

Which one of the following pieces of information cannot be obtained from an infra-red spectrum?

- A The molecular mass
- B The presence of C=O bonds
- C The presence of O-H bonds
- D The identity of a compound through comparison with other spectra

QUESTION 2

Infrared spectroscopy provides valuable information about

- A molecular weight.
- B melting point.
- C arrangement of H atoms.
- D functional groups.

QUESTION 3

For a molecule to absorb IR, why must the molecule's vibrations cause fluctuations in the dipole moment of the molecule?

- A Because a change in dipole moment lowers the energy required for electronic transitions
- B Because for absorption to occur, the radiation must interact with the electric field caused by changing dipole moment
- C Because fluctuations in the dipole moment allow the molecule to deform by bending and stretching
- D None of the above

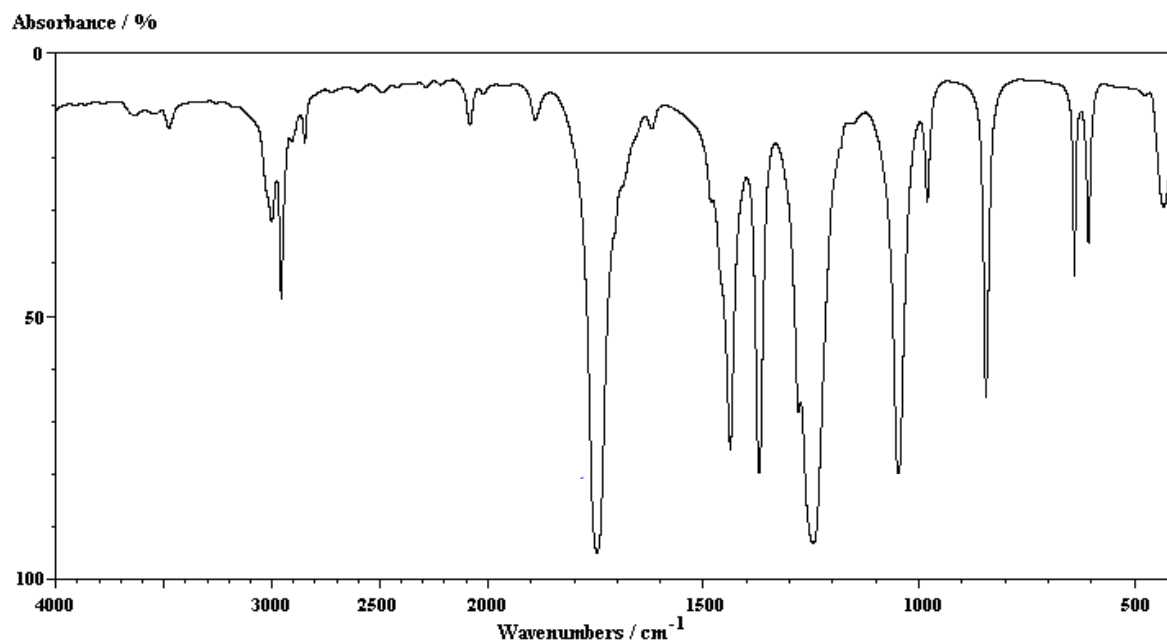
QUESTION 4

Which of the following statements regarding IR spectroscopy is incorrect?

- A Infrared radiation is higher in energy than UV radiation.
- B Infrared spectra record the transmission of IR radiation.
- C Molecular vibrations are due to periodic motions of atoms in molecules, and include bond stretching, rocking and twisting.
- D Infrared spectra give information about bonding features and functional groups in molecules.

QUESTION 5

The Infrared spectrum of an organic compound is given below.



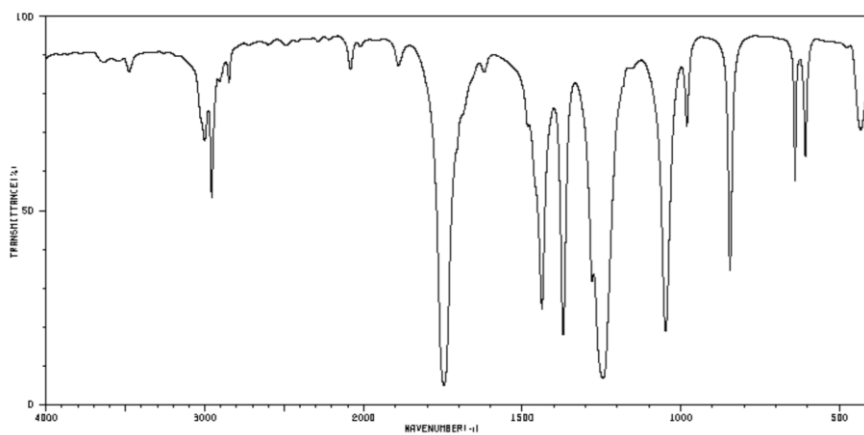
The molecule that produced this spectrum is most likely to be

- A CH_3COOCH_3
- B CH_3CH_2COOH
- C CH_3CH_2OH
- D $CH_3CH_2NH_2$

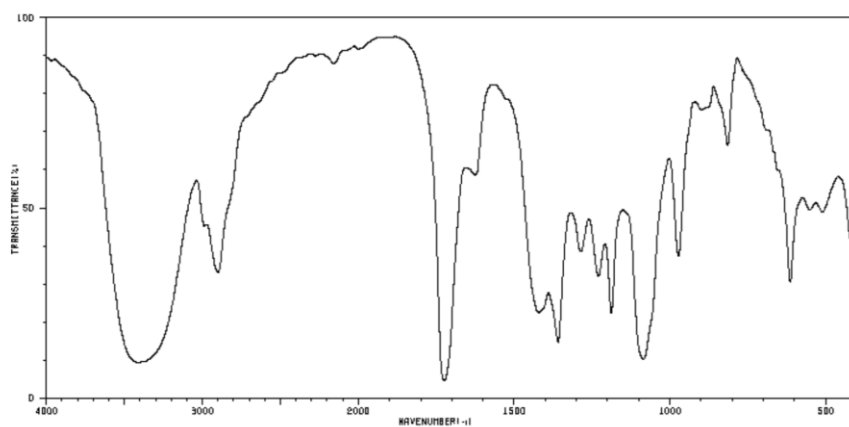
QUESTION 6

The IR spectra of three isomeric compounds are given below.

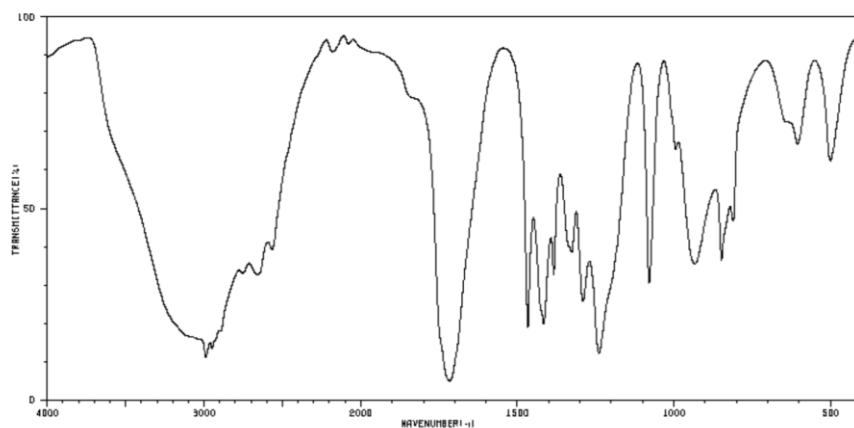
Spectrum 1



Spectrum 2



Spectrum 3



Match each of the following compounds to their correct spectrum. In each case, give a reason for your answer.

Propanoic acid: CH_3CH_2COOH

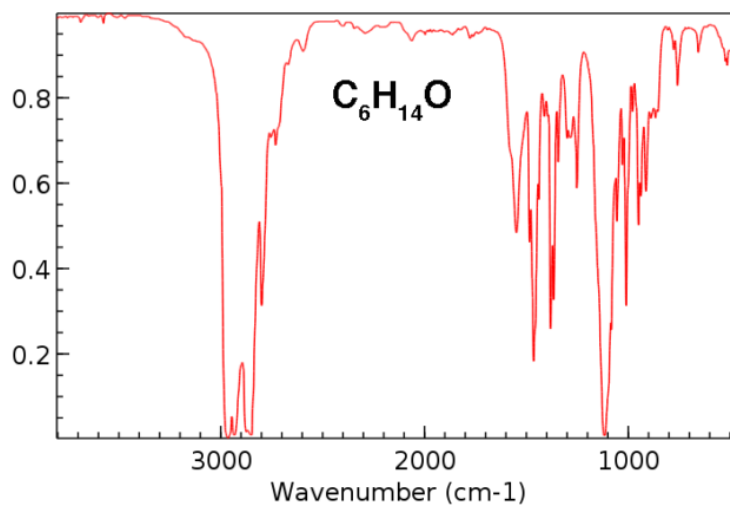
Methyl ethanoate: CH_3COOCH_3

Hydroxypropanone: CH_3COCH_2OH

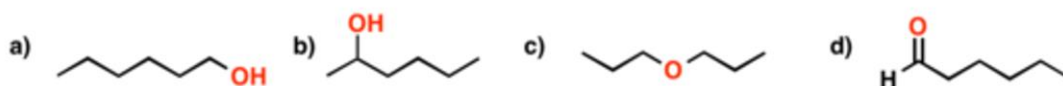
Solution

QUESTION 7

The following IR spectrum was produced by a molecule with formula $C_6H_{14}O$.



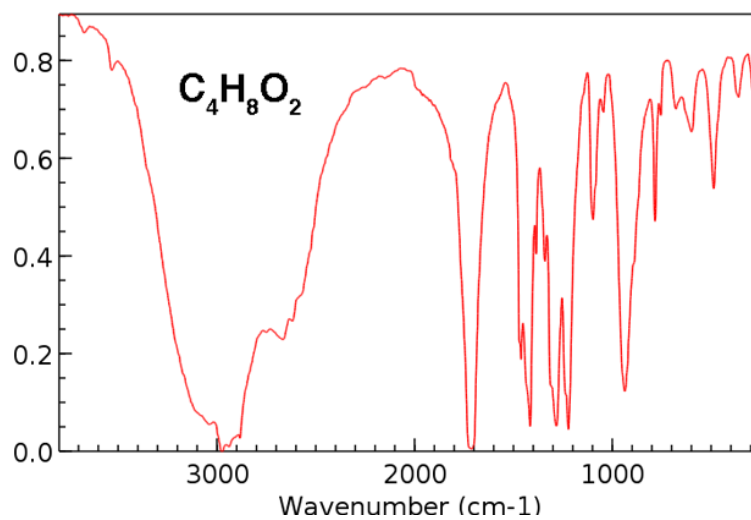
Which of the following molecules produced this spectrum?



Solution

QUESTION 8

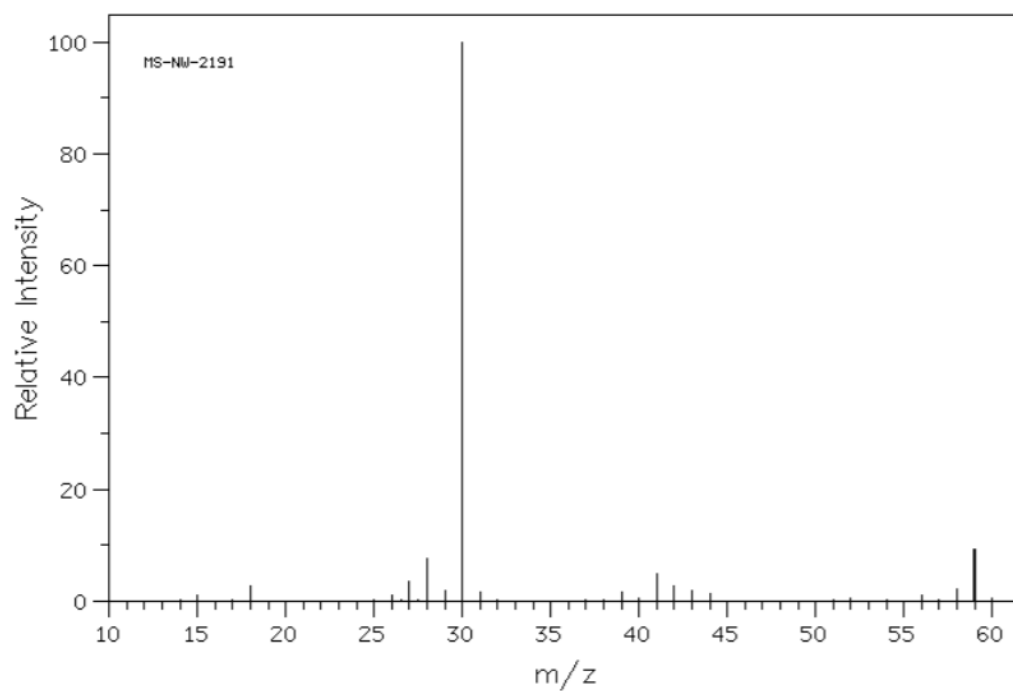
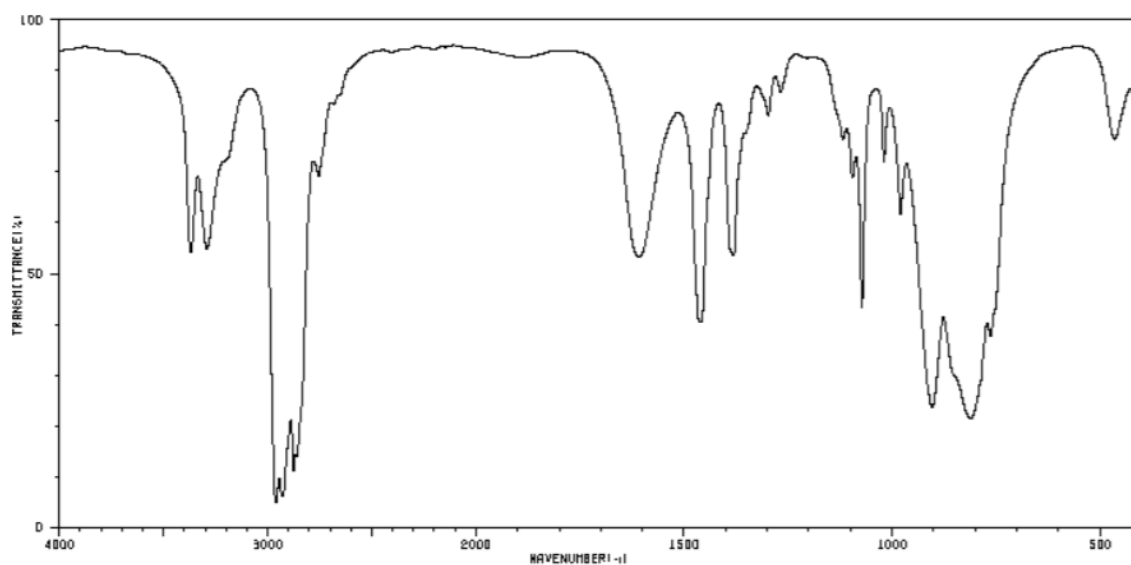
An unknown molecule with formula $C_4H_8O_2$ produced the following IR spectrum. Draw a possible structure for this molecule.



Solution

QUESTION 9

A three carbon compound produced the following mass and infrared spectra. Sketch a possible structure for this compound.



Solution

SOLUTIONS

QUESTION 1 Answer is A

QUESTION 2 Answer is D

QUESTION 3 Answer is B

QUESTION 4 Answer is A

QUESTION 5 Answer is A

Molecule is an ester with characteristic absorptions at 1735 cm^{-1} (C=O) and 1250 cm^{-1} (C-O).

Note: Look for the presence and absence of bands characteristic to the common functional groups.

QUESTION 6

Spectrum 1:

Present: C=O peak

Absent: O-H peak

Therefore, the molecule cannot be an alcohol or carboxylic acid. It is an ester.
i.e. Methyl ethanoate ($\text{CH}_3\text{COOCH}_3$)

Spectrum 2:

Present: C=O peak and O-H peak

The molecule could be a carboxylic acid or ketone or aldehyde. As the peak above 3000cm^{-1} is not as broad as that in spectrum 3, the spectrum will most likely have been produced by an alcohol with a C=O group. This is hydroxypropanone.

Spectrum 3:

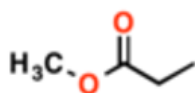
Present: C=O peak and O-H peak

Due to the very broad peak above 3000cm^{-1} this molecule is most likely a carboxylic acid. i.e. Propanoic acid.

QUESTION 7

The infrared spectrum does not include an O-H stretch or C=O stretch, therefore, C is the only possible answer.

QUESTION 8



QUESTION 9

The IR spectrum indicates that the compound has an amino group, but no OH or CO functional groups. The molecular weight of the compound is 59 amu. A possible molecular formula could therefore be C_3H_9N .

