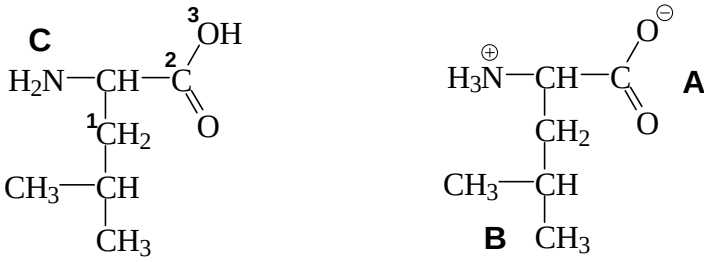
Marks 8

- Shown here are the classical and the zwitterionic forms of the amino acid leucine.



List the types of intermolecular interactions in which each of the indicated sites (**A**, **B** and **C**) in leucine could be involved.

A	**ion-ion, ion-dipole, ion-induced dipole**
B	**dispersion**
C	**hydrogen bonding, dipole-dipole, dipole-induced dipole**

Provide the requested information for each of the indicated atoms in leucine.

Atom	Geometric arrangement of the electron pairs around the atom	Hybridisation of the atom	Geometry/shape of σ-bonding electron pairs around the atom
^{1}C	**tetrahedral**	sp^3	**tetrahedral**
^{2}C	**trigonal planar**	sp^2	**trigonal planar**
^{3}O	**tetrahedral**	sp^3	**bent**

Given that the pK_a of the carboxylic acid group of leucine is 2.32 and the pK_b of the amine group is 4.24, do you expect the classical or the zwitterionic form to predominate when leucine is dissolved in water? In other words, does the following equilibrium lie to the right or left? Show your reasoning.

$$H_2N{-}CH(CH_2CH(CH_3)_2){-}COOH \rightleftharpoons H_3\overset{\oplus}{N}{-}CH(CH_2CH(CH_3)_2){-}CO_2^{\ominus}$$

The equilibrium for the K_a of the acid group is:

$$\mathbf{H_2N\text{-}CHR\text{-}COOH \rightleftharpoons H_2N\text{-}CHR\text{-}COO^- + H^+}$$

for which:

$$\mathbf{K_{a(COOH)} = \frac{[H^+][H_2NCHR-COO^-]}{[H_2NCHR-COOH]} = 10^{-2.32}}$$

The equilibrium for protonation of the amine group is:

$$\mathbf{H_2N\text{-}CHR\text{-}COO^- + H^+ \rightleftharpoons H_3N^+\text{-}CHR\text{-}COO^-}$$

ANSWER CONTINUES ON THE NEXT PAGE

for which:

$$K = \frac{[H_3N^+ - CHR - COO^-]}{[H_2NCHR - COO^-][H^+]} = \frac{1}{K_{a(NH_3^+)}} = \frac{1}{10^{-9.76}} = 10^{+9.76}$$

in which pK_a + pK_b = 14 has been used.

The equilibrium for formation of the zwitterionic form in the question is:

$$H_2N\text{-}CHR\text{-}COOH \rightleftharpoons H_3N^+\text{-}CHR\text{-}COO^-$$

for which:

$$K' = \frac{[H_3N^+ - CHR - COO^-]}{[H_2NCHR - COOH]} = \frac{K_{a(COOH)}}{K_{a(NH_3^+)}} = 10^{-2.32} \times 10^{+9.76} = 10^{7.44}$$

$$>> 1$$

As the equilibrium constant >> 1, the equilibrium lies far to the right and so the zwitterionic form dominates.