(a) Chloroprene (or 2-chloro-1,3-butadiene in proper IUPAC nomenclature), CH₂=CCl–CH=CH₂, can be reacted by addition polymerization to form polychloroprene (CR), also known as Neoprene™ (the name given to it by DuPont). The mer unit of CR is (−CH₂−CCl=CH−CH₂−)_n. The process is initiated with the radical, I⁻. Draw a segment of isotactic CR showing two repeat units. Place the radical initiator at the left end of the dimer and indicate the location of the unpaired electron.

(b) Calculate the degree of polymerization, n, of CR with a molecular weight of 3.091 × 10⁵ g mol⁻¹?

\[
\text{MW of mer unit:} \\
4 \times 12 = 48 \\
5 \times 1 = 5 \\
1 \times 35.5 = 35.5 \\
\frac{3.091 \times 10^5}{88.5} = 3493
\]

(c) CR has been dubbed the world’s first synthetic rubber, which in polymer circles is termed an elastomer. What structural feature of CR enables it to be made into an elastomer? Explain with the aid of a sketch that shows the molecular origin of the rubbery nature of the polymer.

When chlorobutadiene polymerizes it retains a C=C double bond in the backbone of the macromolecule. This gives the polymer the capability to form disulfide linkages between chains, thereby forming a network solid that can flex.

(d) Classify CR as either a thermoset or a thermoplastic, and with reference to its molecular structure assess its recyclability.
(a) For an aqueous solution of glycine (Gly) alone, calculate the value of $pH$ at which the ratio of the concentration of neutral glycine zwitterion to the concentration of deprotonated anion is $10^{-4}$.

\[
HA = H^+ + A^- \\
\therefore K_a = \frac{[H^+][A^-]}{[HA]} \\
\therefore pK_a = pH - \log \frac{[A^-]}{[HA]}
\]

\[
\begin{align*}
pK_a &= 9.78 \\
pH &= pK_a + \log_{10} \frac{[HA]}{[A^-]} \\
 &= 9.78 + \log_{10} (10^{-4}) \\
 &= 9.78 + 4 \\
&= 13.78
\end{align*}
\]

(b) Draw the skeletal structure of glutamic acid (Glu) when it is solvated in an aqueous solution under each of the following conditions.

(i) $pH = 1.5$  
(ii) $pH = 14$  
(iii) $pH = pI$, the isoelectric point
2008 Final Exam, Problem #4 (continued)

(c) Calculate the value of pH at which glutamic acid (Glu) exists as the neutral zwitterion.

\[ pI = \frac{pK_a + pK_a}{2} = \frac{4.07 + 2.19}{2} = 3.11 \]

(d) Draw the skeletal structure of the dipeptide, Glu-Gly, when it is solvated in an aqueous solution of extreme acidity, i.e., pH < 1.

![Skeletal structure of Glu-Gly dipeptide](image)

(e) The figure below shows various features of the tertiary structure along a length of protein in aqueous solution.

![Tertiary structure of protein](image)

For each of the following changes from the conditions that sustain the structure shown above, (1) identify the numbered site or sites at which the tertiary structure is affected and (2) explain the potential impact on the conformation of the protein.

1. Increase in pH
   - inc. in pH will cause $H_3N^+$ to deprotonate and become neutral; $\equiv$ electrostatic attraction will be neutralized and bond will be broken; chain will not be constrained.

2. Increase in concentration of detergent
   - inc. in detergent will pull on the hydrophobic pocket and open up the loop.