16 points

own to exist in three conformational states that are denoted by the symbols:
further known that:

(1) The states B and C have the same energy i.e. $E_B = E_C$, and (2) The state A has the lowest energy such that $E_A = \frac{1}{2}E_B$.

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(a) State (with reasoning) the ratio of the probabilities that the molecule will exist in conformation B vs. in conformation C at a temperature T_1 (i.e. ratio $\frac{P_B}{P_C}$).

For same energy, they are equally probable

$$P_B = \frac{e^{-\beta E_B}}{\cancel{\Sigma}\, e^{-\beta(E_A+E_B+E_C)}}$$

$$P_C = \frac{e^{-\beta E_C}}{e^{-\beta(E_A+E_B+E_C)}}$$

$$\frac{P_B}{P_C} = \frac{e^{-\beta E_B}}{e^{-\beta E_C}} = e^{-\beta(E_B-E_C)} = e^{-\beta \cdot 0} = 1$$

✓

(b) State the expression for the probability (P_A) that the molecule will exist in the lowest conformational energy state (i.e. state A) at a temperature T_1. Probability $\propto e^{-\beta E_j}$

$$\therefore P_j = \frac{e^{-\beta E_j}}{\Sigma\, e^{-\beta E_j}}$$

$$P_A = \frac{e^{-\beta E_A}}{e^{-\beta(E_A+E_B+E_C)}}$$

✗

$$P_A = \frac{e^{-\beta E_A}}{e^{-\beta E_A}+e^{-\beta E_B}+e^{-\beta E_C}}$$

$$= \frac{e^{-\beta E_A}}{e^{-\beta(0.5E_B+E_B+E_B)}}$$

$E_A = \frac{1}{2} E_B$

$E_B = E_C$

$$= \frac{e^{-\beta E_A}}{e^{-2.5\beta E_B}}$$

$$= e^{-\beta E_A + 2.5\beta E_B}$$

$$= e^{-0.5E_B\beta + 2.5\beta E_B}$$

$$= e^{\cancel{2.5}\,\beta E_B} = e^{2\beta E_B}$$