Biophysical Chemistry for Life Scientists

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Problem Set 2
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(1) Calculate $N_A k_B T$ at 25 °C, where N_A is the Avogadro number (6.0221×10^{23} molcules per mole). Express the result in calories per mole.

(2) From simple quantum mechanics, the translational energy levels of a particle in a three-dimensional cubic box of side L is given by

$$\varepsilon_{nml} = [h^2 (n^2 + m^2 + l^2)] / 32 \pi^2 M L^2$$

where n,m,l are positive integers

ε_{nml} denotes the energy of the particle when it is occupying quantum state n,m,l

M is the mass of the particle, and

h is Planck's constant (6.6262×10^{-27} erg sec) .

Estimate the degree of translational excitation, namely, the quantum state n,m,l, before $\varepsilon_{nml} \cong k_B T$ at 300 K for a molecule of molecular mass 100 amu occupying a cubic container of L = 1 cm. What is the implication of this result given that $n, m, l = 1,1,1$ in the lowest translational state?

(3) For most molecular vibrations, the force constant for vibration is sufficiently large (the bond stretch or angle deformation is sufficiently stiff) that the size of a vibration quantum $h\nu$ (energy separation between adjacent vibrational quantum states) is large compared to the thermal energy accessible to the molecule. Consequently, most molecules are not vibrationally excited and occupy the ground vibrational state only. For example, take the diatomic molecule HCl. Here, there is bond stretch only, and the energy separation between the ground and first excited vibrational states/levels is 8.26 kcal mol^{-1}. What fraction of the molecules is in the first excited vibrational level at 300 K?

(4) An essentially isothermal process within a biological cell led to an increase in the volume of the cell by ΔV. What is the pressure-volume work done on the cell by the surroundings? What could be said about the reversibility or irreversibility of the biological process? Explain.

(5) Use the following heats of combustion (reaction with O_2 to produce CO_2 and H_2O): pyruvic acid ($CH_3COCOOH$) (l), -277 kcal/mol^{-1}; and acetic acid (CH_3COOH) (l), -270 kcal mol-1 (both under standard conditions) to calculate the enthalpy change for oxidative metabolism of pyruvic acid (l) to acetic acid (l) and CO_2 under standard conditions.

(6) a. The enthalpy of unfolding of cytochrome c is 50 kcal/mole at 50 °C and 88 kcal/mole at 70 °C. Estimate ΔCp for the unfolding of this protein, assuming ΔCp is constant over this temperature range.

b. The heat capacity of denatured (unfolded) proteins is generally found to be higher than for the same proteins in their native structure. Can you think of any reasons for this observation?