Problemi e domande sulla Termodinamica Chimica

- Qual è la variazione di energia libera di una reazione all'equilibrio?
- Scrivete l'equazione che mostra la relazione tra $\Delta G°$ e K_{eq}.
- Scrivete l'equazione che mostra la relazione tra ΔG, $\Delta G°$ e le concentrazioni dei reagenti e dei prodotti.
- Spiegate come i biochimici definiscono lo stato standard di un soluto. Perché i biochimici e i chimici usano convenzioni differenti?

SAMPLE CALCULATION 1-1

The enthalpy and entropy of the initial and final states of a reacting system are shown in the table.

	H ($\mathbf{J \cdot mol^{-1}}$)	S ($\mathbf{J \cdot K^{-1} \cdot mol^{-1}}$)
Initial state (before reaction)	54,000	22
Final state (after reaction)	60,000	43

a. Calculate the change in enthalpy and change in entropy for the reaction.

b. Calculate the change in free energy for the reaction when the temperature is 4°C. Is the reaction spontaneous?

c. Is the reaction spontaneous at 37°C?

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a. $\Delta H = H_{\text{final}} - H_{\text{initial}} = 60{,}000\ \text{J} \cdot \text{mol}^{-1} - 54{,}000\ \text{J} \cdot \text{mol}^{-1} = 6000\ \text{J} \cdot \text{mol}^{-1}$

$$\begin{aligned}\Delta S &= S_{\text{final}} - S_{\text{initial}} = \Delta S = 43\ \text{J} \cdot \text{K}^{-1} \cdot \text{mol}^{-1} - 22\ \text{J} \cdot \text{K}^{-1} \cdot \text{mol}^{-1} \\ &= 21\ \text{J} \cdot \text{K}^{-1} \cdot \text{mol}^{-1}\end{aligned}$$

b. First, convert temperature from °C to K: $4 + 273 = 277$ K. Then use Eq. 1-11.

$$\Delta G = \Delta H - T\Delta S$$

$$\begin{aligned}\Delta G &= (6000\ \text{J} \cdot \text{mol}^{-1}) - (277\ \text{K})(21\ \text{J} \cdot \text{K}^{-1} \cdot \text{mol}^{-1}) \\ &= 6000\ \text{J} \cdot \text{mol}^{-1} - 5817\ \text{J} \cdot \text{mol}^{-1} = 183\ \text{J} \cdot \text{mol}^{-1}\end{aligned}$$

The value for ΔG is greater than zero, so this is an endergonic (nonspontaneous) reaction at 4°C.

c. Convert temperature from °C to K: $37 + 273 = 310$ K.

$$\Delta G = \Delta H - T\Delta S$$

$$\begin{aligned}\Delta G &= (6000\ \text{J} \cdot \text{mol}^{-1}) - (310\ \text{K})(21\ \text{J} \cdot \text{K}^{-1} \cdot \text{mol}^{-1}) \\ &= 6000\ \text{J} \cdot \text{mol}^{-1} - 6510\ \text{J} \cdot \text{mol}^{-1} = -510\ \text{J} \cdot \text{mol}^{-1}\end{aligned}$$

The value for ΔG is less than zero, so the reaction is spontaneous (exergonic) at 37°C.

Tabella finale riassuntiva

Box 1-2 Perspectives in Biochemistry

Biochemical Conventions

Modern biochemistry generally uses Système International (SI) units, including meters (m), kilograms (kg), and seconds (s) and their derived units, for various thermodynamic and other measurements. The following lists the commonly used biochemical units, some useful biochemical constants, and a few conversion factors.

Units

Energy, heat, work	joule (J)	$kg \cdot m^2 \cdot s^{-2}$ or $C \cdot V$
Electric potential	volt (V)	$J \cdot C^{-1}$

Prefixes for units

mega (M)	10^6	nano (n)	10^{-9}
kilo (k)	10^3	pico (p)	10^{-12}
milli (m)	10^{-3}	femto (f)	10^{-15}
micro (μ)	10^{-6}	atto (a)	10^{-18}

Conversions

angstrom (Å)	10^{-10} m
calorie (cal)	4.184 J
kelvin (K)	degrees Celsius (°C) + 273.15

Constants

Avogadro's number (*N*)	6.0221×10^{23} molecules $\cdot$ mol^{-1}
Coulomb (C)	6.241×10^{18} electron charges
Faraday ($\mathcal{F}$)	96,485 $C \cdot mol^{-1}$ or 96,485 $J \cdot V^{-1} \cdot mol^{-1}$
Gas constant (*R*)	8.3145 $J \cdot K^{-1} \cdot mol^{-1}$
Boltzmann constant (k_B)	1.3807×10^{-23} $J \cdot K^{-1}$ (R/N)
Planck's constant (*h*)	6.6261×10^{-34} $J \cdot s$

Throughout this text, molecular masses of particles are expressed in units of **daltons (D),** which are defined as l/12th the mass of a ^{12}C atom (1000 D = 1 **kilodalton, kD**). Biochemists also use **molecular weight,** a dimensionless quantity defined as the ratio of the particle mass to l/12th the mass of a ^{12}C atom, which is symbolized $\boldsymbol{M_r}$ (for relative molecular mass).