Marks 6

- The first step in the metabolism of glucose in biological systems is the addition of a phosphate group in a dehydration-condensation reaction:

$$\text{glucose(aq)} + H_2PO_4^-\text{(aq)} \rightleftharpoons \text{[glucose phosphate]}^-\text{(aq)} + H_2O\text{(l)}$$

The free energy change associated with this reaction is $\Delta G° = 13.8$ kJ mol$^{-1}$. The reaction is driven forwards by harnessing the free energy associated with the hydrolysis of adenosine triphosphate, $ATP^{4-}$, to adenosine diphosphate, $ADP^{3-}$:

$$ATP^{4-}\text{(aq)} + H_2O\text{(l)} \rightleftharpoons ADP^{3-}\text{(aq)} + H_2PO_4^-\text{(aq)} \qquad \Delta G° = -30.5 \text{ kJ mol}^{-1}$$

The overall reaction is thus:

$$\text{glucose(aq)} + ATP^{4-}\text{(aq)} \rightleftharpoons \text{[glucose phosphate]}^-\text{(aq)} + ADP^{3-}\text{(aq)}$$

Calculate the equilibrium constant associated with this overall reaction at body temperature (37 ºC).

**The overall reaction is the sum of the two reactions:**

| Reaction | $\Delta G°$ (kJ mol$^{-1}$) |
|---|---|
| $\text{glucose(aq)} + H_2PO_4^-\text{(aq)} \rightleftharpoons \text{[glucose phosphate]}^-\text{(aq)} + H_2O\text{(l)}$ | **13.8** |
| $ATP^{4-}\text{(aq)} + H_2O\text{(l)} \rightleftharpoons ADP^{3-}\text{(aq)} + H_2PO_4^-\text{(aq)}$ | **-30.5** |
| $\text{glucose(aq)} + ATP^{4-}\text{(aq)} \rightleftharpoons \text{[glucose phosphate]}^-\text{(aq)} + ADP^{3-}\text{(aq)}$ | **-16.7** |

**For the overall reaction, $\Delta G° = ((13.8) + (-30.5))$ kJ mol$^{-1}$ = -16.7 kJ mol$^{-1}$. Using $\Delta G° = -RT\ln K$,**

$$-16.7 \times 10^3 = -8.314 \times (37 + 273)\ln K \quad \text{or } K = e^{6.48} = 652$$

Answer: ***K* = 652 (no units)**

This overall equilibrium reaction is investigated by adding 0.0100 mol of $ATP^{4-}$ to a flask containing 175 mL of a 0.0500 M aqueous solution of glucose at 37 ºC. What percentage of the $ATP^{4-}$ will have been consumed when the system reaches equilibrium?

**The initial concentration of $ATP^{4-}$ is $\frac{n}{V} = \frac{0.0100 \text{ mol}}{0.175 \text{ L}}$ = 0.0571 M. The reaction table is then:**

| | glucose(aq) | $ATP^{4-}$(aq) | $\rightleftharpoons$ | [glucose phosphate]$^-$(aq) | $ADP^{3-}$(aq) |
|---|---|---|---|---|---|
| initial | 0.0500 | 0.0571 | | 0 | 0 |
| change | -x | -x | | +x | +x |
| equilibrium | 0.0500-x | 0.0571-x | | x | x |

**At equilibrium,**

$$K = \frac{[\text{glucose-phosphate}^-\text{(aq)}][ADP^{3-}\text{(aq)}]}{[\text{glucose(aq)}][ATP^{4-}\text{(aq)}]} = \frac{x^2}{(0.0500 - x)(0.0571 - x)} = 652$$

**ANSWER CONTINUES ON THE NEXT PAGE**

**As the equilibrium constant is large so is x and this expression cannot be approximated. Instead, the full quadratic equation must be solved.**

$$\mathbf{x^2 = 652(0.0500-x)(0.0571-x)}\ \textbf{or}$$

$$\mathbf{651x^2 - 652(0.0500+0.0571) + (652\times0.0500\times0.0571) = 0}$$

**The two roots are $x_1$ = 0.0578 M and $x_2$ = 0.0495 M. As $x_1$ gives a negative [glucose(aq)], it is not physically significant. As x is the concentration consumed, using $x_2$ gives:**

$$\textbf{percentage of } \mathbf{ATP^{4-}(aq)} \textbf{ consumed} = \mathbf{\frac{0.0495\,M}{0.0571\,M}\times100\% = 87\%}$$

Answer: **87%**

Suggest two simple ways of further reducing the remaining percentage of $ATP^{4-}$.

**The remaining $ATP^{4-}$ can be reduced by (i) adding more glucose and (ii) reducing the temperature. Removal of either product would also drive the reaction to the right but would be very difficult to achieve in practice.**