

$$\Delta G^\circ = c * 1.36 * (pK_a - pH) - n(E_h - E_m)$$

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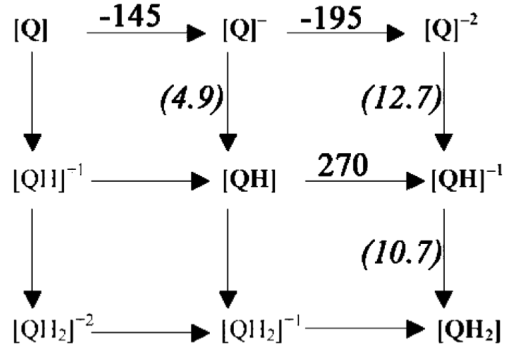
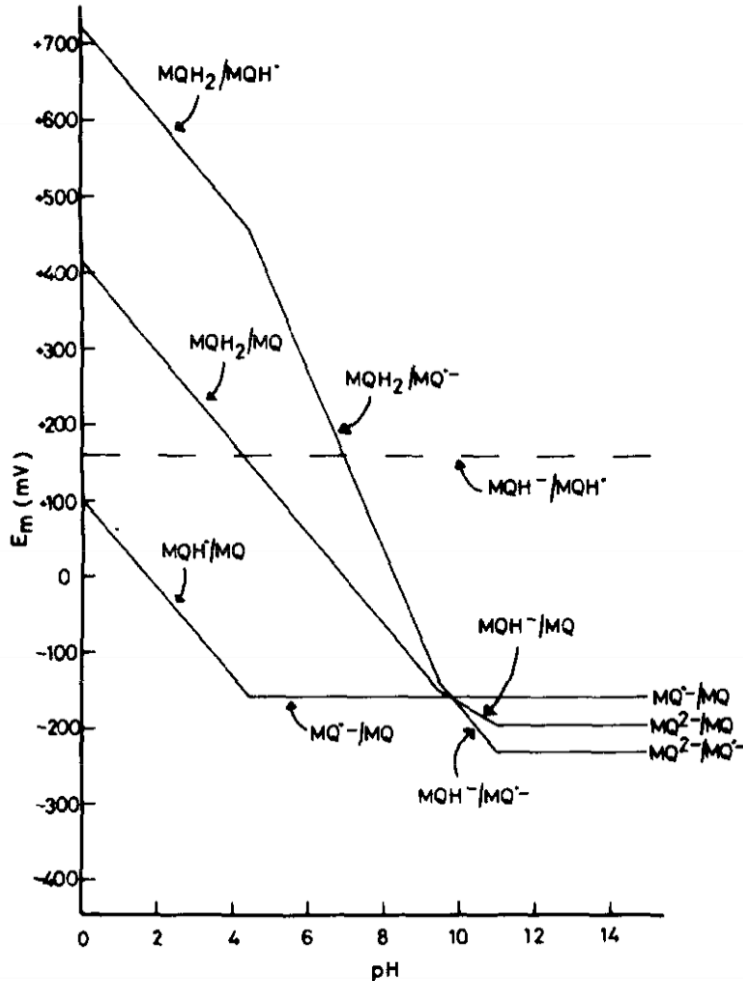


FIGURE 1: Ubiquinone redox and protonation states. States in bold are intermediates considered in coupled electron (horizontal) and proton (vertical) transfer reactions in RCs. The sources for the $E_{m,sol}$ and $pK_{a,sol}$ (in parentheses) at pH 7 are given in Table 1. The ΔG for proton transfer (vertical lines) can be obtained from $\Delta G = 59.3 \cdot (pH - pK_a)$ (eq 9).

Table 1: Reference E_m and pK_a Values for Ubiquinone 10

half-reactions	$pK_{a,sol}$	$E_{m,sol,7}^\circ$ (mV)	ΔG_{sol}° (meV)
$Q + e^- \rightarrow Q^-$		-145 ^b	145
$Q + 2e^- \rightarrow Q^{2-}$		-170 ^b	340
$Q^- + e^- \rightarrow Q^{2-}$		-195 ^c	195
$QH + e^- \rightarrow QH^-$		270 ^b	-270
$Q^- + H^+ \rightarrow QH$	4.9 ^d		124
$Q^{2-} + H^+ \rightarrow QH^-$	12.7 ^e		-338
$QH^- + H^+ \rightarrow QH_2$	10.7 ^f		-218
$Q + e^- + H^+ \rightarrow QH$		-269	269
$Q + 2e^- + H^+ \rightarrow QH^-$		1	-1
$Q + 2e^- + 2H^+ \rightarrow QH_2$		110	-220
$Q^- + e^- + H^+ \rightarrow QH^-$		146	-146
$QH + e^- + H^+ \rightarrow QH_2$		488	-488
$Q^- + e^- + 2H^+ \rightarrow QH_2$		360	-360

^a ΔG_{sol} is $2.3mk_bT(pH - pK_{a,sol}) - nF(E_h - E_{m,sol})$ (eq 4), and values are given at $E_h = 0$ and pH 7, where m is the number of protons and n is the number of electrons. ^b By analogy with the E_m of trimethyl benzoquinone (67). ^c Derived from $E_{m,sol}$ (Q/Q^-) and $E_{m,sol}$ (Q^-/Q^{2-}). ^d Derived from the $pK_{a,sol}$ for Q^{2-}/QH^- and the $E_{m,sol}$ for Q^-/Q^{2-} . ^e Derived from pK_a (Q^{2-}/QH^-) being ≈ 2 units higher than pK_a (QH^-/QH_2) (69, 72). Other values are derived as appropriate sums and differences walking around the thermodynamic box (Figure 1). See the Materials and Methods for a more complete derivation of $E_{m,sol}$ and $pK_{a,sol}$ values used here. ^f ref 67.



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