# OXPHOS

## Complex I model[[1]](#footnote-20)

Assuming single electron transfer for each cycle.

| Parameter | Value | Units | Desc. |
| --- | --- | --- | --- |
|  | 8.849 | mM | Concentration of complex I(Adjustable) |
|  | 50 | mV | Phase boundary potential |
|  | 6.3396E11 | Hz/mM^2 |  |
|  | 5 | Hz |  |
|  | 100 | Hz |  |
|  | 2.5119E13 | Hz/mM^2 |  |
|  | 1E7 | Hz |  |
|  | 130 | Hz |  |
|  | 3886.7 | Hz/mM^{1/2} |  |
|  | 9.1295E6 | Hz |  |
|  | 639.1364 | Hz |  |
|  | 3.2882 | Hz/mM^{1/2} |  |
|  | 1.5962E7 | Hz/mM |  |
|  | 65.2227 | Hz |  |
|  | 24615 | Hz |  |
|  | 1166.7 | Hz/mM^{1/2} |  |
|  | 6.0318 | Hz/mM |  |
|  | -375 | mV | Midpoint potential of flavin mononucleotide |
|  | -150 | mV | Midpoint potential of superoxide |

## Complex II (Succinate dehydrogenase)[[2]](#footnote-23)

| Parameter | Value | Units | Desc. |
| --- | --- | --- | --- |
|  | 4.167 | mM \* Hz | Maximum rate of SDH |
|  | 0.150 | mM | Inhibition constant for oxaloacetate |
|  | 0.6 | - | Michaelis constant for CoQ |

## Complex III[[3]](#footnote-25)

| Parameter | Value | Unit | Desc. |
| --- | --- | --- | --- |
|  | 1,666.63 | Hz/mM | Reverse rate constant for reaction 3 |
|  | 0.6877 | - | Equilibrium constant for reaction 3 |
|  | 60.67 | Hz/mM | Reverse rate constant for reaction 4 |
|  | 129.9853 | - | Equilibrium constant for reaction 4 (bH oxidized) |
|  | 13.7484 | - | Equilibrium constant for reaction 4 (bH reduced) |
|  | 0.5 | - |  |
|  | 0.2497 | - |  |
|  | 22000 | Hz | Rate of diffusion across the membrane for Q and QH2 |
|  | 166.67 | Hz/mM | Reverse rate constant for reaction 6 |
|  | 9.4596 | - | Equilibrium constant for reaction 6 |
|  | 0.5 | - |  |
|  | 0.5006 | - |  |
|  | 13.33 | Hz/mM | Reverse rate constant for reaction 7 (bL oxidized) |
|  | 3.0748 | - | Equilibrium constant for reaction 7 (bL oxidized) |
|  | 1.667 | Hz/mM | Reverse rate constant for reaction 7 (bL reduced) |
|  | 29.0714 | - | Equilibrium constant for reaction 7 (bL reduced) |
|  | 0.5 | - |  |
|  | 0.2497 | - |  |
|  | 83.33 | Hz/mM | Reverse rate constant for reaction 8 (bL oxidized) |
|  | 129.9853 | - | Equilibrium constant for reaction 8 (bL oxidized) |
|  | 8.333 | Hz/mM | Reverse rate constant for reaction 8 (bL reduced) |
|  | 9.4596 | - | Equilibrium constant for reaction 8 (bL reduced) |
|  | 833 | Hz/mM | Reverse rate constant for reaction 9 |
|  | 0.2697 | - | Equilibrium constant for reaction 9 |
|  | 0.8333 | Hz/mM | Reverse rate constant for reaction 10 |
|  | 1.4541 | - | Equilibrium constant for reaction 10 |
|  | 2469.13 | Hz/mM | Reverse rate constant for reaction 33 |
|  | 2.1145 | - | Equilibrium constant for reaction 33 |
|  | 0.325 | mM | Total complex III protein |

## Complex IV[[4]](#footnote-27)

| Parameter | Value | Unit | Desc. |
| --- | --- | --- | --- |
|  | 0.325 | mM | Cytochrome c pool |
|  | 0.325 | mM | Complex IV concentration |
|  | 2.9445E10 | Hz/mM^3 | @ pH = 7 |
|  | 290.03 | Hz/mM^3 | @ pH = 7 |
|  | 45000 | Hz/mM |  |
|  | 4.826E11 | Hz/mM | @ pH = 7 |
|  | 4.826 | Hz/mM | @ pH = 7 |
|  | 1.7245E8 | Hz | @ pH = 7 |
|  | 17.542 | Hz | @ pH = 7 |

## Complex V (ATP synthase) [[5]](#footnote-29)

| Parameter | Value | Unit | Desc. |
| --- | --- | --- | --- |
|  | 5 | mM | Concentration of F1-Fo ATPase |
|  | 6.47E5 | M | Apparent equilibrium constant for ATP hydrolysisFrom Golding’s work[[6]](#footnote-31) |
|  | 50 | mV | Phase boundary potential |
|  | 1.656E-5 | Hz | Sum of products of rate constants |
|  | 3.373E-7 | Hz | Sum of products of rate constants |
|  | 9.651E-14 | Hz | Sum of products of rate constants |
|  | 4.585E-14 | Hz | Sum of products of rate constants |
|  | 1.346E-4 | - | Sum of products of rate constants |
|  | 7.739E-7 | - | Sum of products of rate constants |
|  | 6.65E-15 | - | Sum of products of rate constants |

## ODE system for the Q cycle

1. Gauthier LD, Greenstein JL, O’Rourke B, Winslow RL. An Integrated Mitochondrial ROS Production and Scavenging Model: Implications for Heart Failure. Biophysical Journal. 2013;105(12):2832-2842. doi:10.1016/j.bpj.2013.11.007. [PMC3882515](https://www.ncbi.nlm.nih.gov/pmc/articles/PMC3882515) [↑](#footnote-ref-20)
2. Gauthier LD, Greenstein JL, O’Rourke B, Winslow RL. An Integrated Mitochondrial ROS Production and Scavenging Model: Implications for Heart Failure. Biophysical Journal. 2013;105(12):2832-2842. doi:10.1016/j.bpj.2013.11.007. [PMC3882515](https://www.ncbi.nlm.nih.gov/pmc/articles/PMC3882515) [↑](#footnote-ref-23)
3. Gauthier LD, Greenstein JL, O’Rourke B, Winslow RL. An Integrated Mitochondrial ROS Production and Scavenging Model: Implications for Heart Failure. Biophysical Journal. 2013;105(12):2832-2842. doi:10.1016/j.bpj.2013.11.007. [PMC3882515](https://www.ncbi.nlm.nih.gov/pmc/articles/PMC3882515) [↑](#footnote-ref-25)
4. Gauthier LD, Greenstein JL, O’Rourke B, Winslow RL. An Integrated Mitochondrial ROS Production and Scavenging Model: Implications for Heart Failure. Biophysical Journal. 2013;105(12):2832-2842. doi:10.1016/j.bpj.2013.11.007. [PMC3882515](https://www.ncbi.nlm.nih.gov/pmc/articles/PMC3882515) [↑](#footnote-ref-27)
5. Wei AC, Aon MA, O’Rourke B, Winslow RL, Cortassa S. Mitochondrial energetics, pH regulation, and ion dynamics: a computational-experimental approach. Biophys J. 2011;100(12):2894-903. [PMC3123977](https://www.ncbi.nlm.nih.gov/pmc/articles/PMC3123977/) [↑](#footnote-ref-29)
6. Golding, E. M., Teague, W. E., & Dobson, G. P. (1995). Adjustment of K’ to varying pH and pMg for the creatine kinase, adenylate kinase and ATP hydrolysis equilibria permitting quantitative bioenergetic assessment. The Journal of Experimental Biology, 198(Pt 8), 1775–1782. [↑](#footnote-ref-31)