

Parameter	Value	Description
$bc_1::k_{\text{on}}(\text{H}^+_{\text{out}})$	$10^{10} \text{ nm}^3 \text{ s}^{-1}$	rate for proton uptake from the cytoplasm by bc_1
$bc_1::k_{\text{tr}}(\text{e}:Q_0 \Rightarrow \text{FeS})$	$2.3 * 10^3 \text{ s}^{-1}$	rate for electron transfer from Q_0 to FeS
$bc_1::k_{\text{tr}}(\text{e}:c_1 \Rightarrow c_2)$	10^5 s^{-1}	electron transfer rate from c_1 to bound cytochrome c_2
$bc_1::k_{\text{tr}}(\text{e}:Q_0 \Rightarrow b_L)$	10^4 s^{-1}	electron transfer from Q_0 to b_L heme
$bc_1::k_{\text{tr}}(\text{e}:b_L \Rightarrow b_H)$	10^4 s^{-1}	electron transfer from b_L to b_H heme
$\Delta\Phi::V$	$2.65 * 10^4 \text{ nm}^3$	inner volume of the vesicle
$\Delta\Phi::A$	$5.28 * 10^3 \text{ nm}^2$	membrane area (Q pool „volume“)
$\Delta\Phi::C_{\text{Hin}}$	1.0 e	effective charge of a free proton in the vesicle
$\Delta\Phi::C_{\text{Hm}}$	1.0 e	effective charge of a proton on the titratable groups
$\Delta\Phi::C_{\text{prot}}$	-1.0 e	effective charge of an e^- translocated through an RC
$\Delta\Phi::C_{\text{cred}}$	-0.5 e	effective charge of a reduced cytochrome c_2
$\Delta\Phi::C_{\text{cox}}$	0.5 e	effective charge of an oxidized cytochrome c_2
PR:: N_p	80	number of titratable groups in the vesicle
PR::pK	5.0	pK of the titratable groups
N_{core}	10	number of dimeric core complexes (2 RC + 1 LHC)
N_{bc_1}	10	number of cytochrome bc_1 complexes
N_{ATPase}	1	number of ATPases
N_{c_2}	20	total number of cytochrome c_2
N_Q	200	total number of quinones

Table S1: Model Parameters Not Included in the Optimization Process

Parameters and stoichiometries that were not included in the optimization process with their (fixed) values. Effective charges of ± 0.5 e were used for the cytochrome c_2 to achieve a change of the total charge of the cytochrome c_2 of ± 1 e when a reduced c_2 is replaced by an oxidized one or vice versa. Note that N_{bc_1} was determined prior to the main parameterization and is thus considered a fixed parameter for the chromatophore setup.