

Table 4 Rate constants used by Thorneley and Lowe in the simulation of the kinetics of Kp nitrogenase at 23°, pH 7.4*

Rate constant	Value	Comment
k_1	$^a 5 \times 10^7 \text{ M}^{-1} \text{ s}^{-1}$	} Responsible for dilution effect
k_{-1}	$^a 15 \text{ s}^{-1}$	
k_2	200 s^{-1}	Electron transfer coupled to MgATP hydrolysis
k_3	$^a 4.4 \times 10^6 \text{ M}^{-1} \text{ s}^{-1}$	Responsible for inhibition at high protein concentrations
k_{-3}^b	$^a 6.4 \text{ s}^{-1}$	Rate limiting when Kp2 and substrates are saturating
k_4	$3.0 \times 10^6 \text{ M}^{-1} \text{ s}^{-1}$	Rate of reduction of $\text{Kp2}_{ox}(\text{MgADP})_2$ by SO_2^-
k_5	$^a 4.4 \times 10^6 \text{ M}^{-1} \text{ s}^{-1}$	} Responsible for inhibition of H_2 evolution when MgATP but not reductant is limiting
k_{-5}	$^a 6.4 \text{ s}^{-1}$	
k_6	$1.2 \times 10^9 \text{ M}^{-1} \text{ s}^{-1}$	} $\text{S}_2\text{O}_4^{2-} \xrightleftharpoons[k_6]{k_{-6}} 2\text{SO}_2^-$
k_{-6}	1.75 s^{-1}	
k_7	$^b 250 \text{ s}^{-1}$	Responsible for enhanced H_2 evolution at low e^- flux
k_8	$^b 8.0 \text{ s}^{-1}$	Slow in order to maximize N_2 binding to E_3
k_9	$^b, c 400 \text{ s}^{-1}$	Rapid H_2 evolution from the most reduced hydridic species
k_{10}	$4 \times 10^5 \text{ M}^{-1} \text{ s}^{-1}$	Determined from $K_m^{\text{N}_2}$ at low e^- flux
k_{-10}	$8 \times 10^4 \text{ M}^{-1} \text{ s}^{-1}$	Determined from $K_i^{\text{H}_2}$ at low e^- flux
k_{11}	$^c 2.2 \times 10^6 \text{ M}^{-1} \text{ s}^{-1}$	Determined from $K_m^{\text{N}_2}$ at high e^- flux
k_{-11}	$^c 3 \times 10^6 \text{ M}^{-1} \text{ s}^{-1}$	Determined from $K_i^{\text{H}_2}$ at high e^- flux

* Reproduced from Reference 144.

^a Kp1-Kp2 association-dissociation rates assumed to be independent of Kp1 oxidation level.

^b H_2 evolution rates. These depend on small differences between large numbers and are subject to errors of factors of about two.

^c Since these rate constants determine K_m 's and K_i 's, only their ratios are absolute values.

Note: The difference between the values of some of the rate constants shown and those reported previously are due to the more accurate determination of k_1 .