

Assignment Rules

$$\text{alphaps} = \exp(\log_{\text{alphaps}})$$

$$\text{Eps} = kT \cdot \text{Eps}_{kT}$$

$$\text{alphapstilde} = \exp(\log_{\text{alphapstilde}})$$

$$\text{Epstilde} = kT \cdot \text{Epstilde}_{kT}$$

$$\text{alphadps} = \exp(\log_{\text{alphadps}})$$

$$\text{Edps} = kT \cdot \text{Edps}_{kT}$$

$$\text{alphadpstilde} = \exp(\log_{\text{alphadpstilde}})$$

$$\text{Edpstilde} = kT \cdot \text{Edpstilde}_{kT}$$

$$\text{kps} = \text{alphaps} \cdot \exp\left(\frac{-\text{Eps}}{T}\right)$$

$$\text{kpstilde} = \text{alphapstilde} \cdot \exp\left(\frac{-\text{Epstilde}}{T}\right)$$

$$\text{kdps} = \text{alphadps} \cdot \exp\left(\frac{-\text{Edps}}{T}\right)$$

$$\text{kdpstilde} = \text{alphadpstilde} \cdot \exp\left(\frac{-\text{Edpstilde}}{T}\right)$$

$$\text{alphaf0} = \exp(\log_{\text{alphaf0}})$$

$$\text{Ef0} = kT \cdot \text{Ef0}_{kT}$$

$$\text{alphab0} = \exp(\log_{\text{alphab0}})$$

$$\text{Eb0} = kT \cdot \text{Eb0}_{kT}$$

$$\text{f0} = \text{alphaf0} \cdot \exp\left(\frac{-\text{Ef0}}{T}\right)$$

$$\text{b0} = \text{alphab0} \cdot \exp\left(\frac{-\text{Eb0}}{T}\right)$$

$$\text{alphaf1} = \exp(\log_{\text{alphaf1}})$$

$$\text{Ef1} = kT \cdot \text{Ef1}_{kT}$$

$$\text{alphab1} = \exp(\log_{\text{alphab1}})$$

$$\begin{aligned}
\text{Eb1} &= kT \cdot \text{Eb1}_{kT} \\
f1 &= \text{alphaf1} \cdot \exp\left(\frac{-Ef1}{T}\right) \\
b1 &= \text{alphab1} \cdot \exp\left(\frac{-Eb1}{T}\right) \\
\text{alphaf2} &= \exp(\log_{\text{alphaf2}}) \\
Ef2 &= kT \cdot Ef2_{kT} \\
\text{alphab2} &= \exp(\log_{\text{alphab2}}) \\
Eb2 &= kT \cdot Eb2_{kT} \\
f2 &= \text{alphaf2} \cdot \exp\left(\frac{-Ef2}{T}\right) \\
b2 &= \text{alphab2} \cdot \exp\left(\frac{-Eb2}{T}\right) \\
\text{alphaf3} &= \exp(\log_{\text{alphaf3}}) \\
Ef3 &= kT \cdot Ef3_{kT} \\
\text{alphab3} &= \exp(\log_{\text{alphab3}}) \\
Eb3 &= kT \cdot Eb3_{kT} \\
f3 &= \text{alphaf3} \cdot \exp\left(\frac{-Ef3}{T}\right) \\
b3 &= \text{alphab3} \cdot \exp\left(\frac{-Eb3}{T}\right) \\
\text{alphaf4} &= \exp(\log_{\text{alphaf4}}) \\
Ef4 &= kT \cdot Ef4_{kT} \\
\text{alphab4} &= \exp(\log_{\text{alphab4}}) \\
Eb4 &= kT \cdot Eb4_{kT} \\
f4 &= \text{alphaf4} \cdot \exp\left(\frac{-Ef4}{T}\right) \\
b4 &= \text{alphab4} \cdot \exp\left(\frac{-Eb4}{T}\right) \\
\text{alphaf5} &= \exp(\log_{\text{alphaf5}})
\end{aligned}$$

$$\begin{aligned}
\text{Ef5} &= kT \cdot \text{Ef5}_{kT} \\
\text{alphab5} &= \exp(\log_{\text{alphab5}}) \\
\text{Eb5} &= kT \cdot \text{Eb5}_{kT} \\
f5 &= \text{alphaf5} \cdot \exp\left(\frac{-\text{Ef5}}{T}\right) \\
b5 &= \text{alphab5} \cdot \exp\left(\frac{-\text{Eb5}}{T}\right) \\
\text{alphaf6} &= \exp(\log_{\text{alphaf6}}) \\
\text{Ef6} &= kT \cdot \text{Ef6}_{kT} \\
\text{alphab6} &= \exp(\log_{\text{alphab6}}) \\
\text{Eb6} &= kT \cdot \text{Eb6}_{kT} \\
f6 &= \text{alphaf6} \cdot \exp\left(\frac{-\text{Ef6}}{T}\right) \\
b6 &= \text{alphab6} \cdot \exp\left(\frac{-\text{Eb6}}{T}\right) \\
p &= \frac{(0 \cdot ([C0] + [C0\text{tilde}]) + 1 \cdot ([C1] + [C1\text{tilde}]) + 2 \cdot ([C2] + [C2\text{tilde}]) + 3 \cdot ([C3] + [C3\text{tilde}]) + 4 \cdot ([C4] + [C4\text{tilde}]) + 5 \cdot ([C5] + [C5\text{tilde}]) + 6 \cdot ([C6] + [C6\text{tilde}]))}{(6 \cdot ([C0] + [C0\text{tilde}]) + 6 \cdot ([C1] + [C1\text{tilde}]) + 6 \cdot ([C2] + [C2\text{tilde}]) + 6 \cdot ([C3] + [C3\text{tilde}]) + 6 \cdot ([C4] + [C4\text{tilde}]) + 6 \cdot ([C5] + [C5\text{tilde}]) + 6 \cdot ([C6] + [C6\text{tilde}]))}
\end{aligned}$$

Differential Equations

$$\begin{aligned}
\frac{d[C0]}{dt} &= \text{kdp} \cdot [C1] \\
&\quad + b0 \cdot [C0\text{tilde}] \\
&\quad - \text{kps} \cdot [C0] \\
&\quad - f0 \cdot [C0] \\
\\
\frac{d[C0\text{tilde}]}{dt} &= \text{kdpstilde} \cdot [C1\text{tilde}] \\
&\quad + f0 \cdot [C0] \\
&\quad - \text{kpstilde} \cdot [C0\text{tilde}] \\
&\quad - b0 \cdot [C0\text{tilde}] \\
\\
\frac{d[C1]}{dt} &= \text{kps} \cdot [C0] \\
&\quad + \text{kdp} \cdot [C2] \\
&\quad + b1 \cdot [C1\text{tilde}] \\
&\quad - (\text{kps} + \text{kdp}) \cdot [C1] \\
&\quad - f1 \cdot [C1] \\
\\
\frac{d[C1\text{tilde}]}{dt} &= \text{kpstilde} \cdot [C0\text{tilde}]
\end{aligned}$$

$$\begin{aligned}
& + \text{kdpstilde} \cdot [\text{C2tilde}] \\
& + \text{f1} \cdot [\text{C1}] \\
& - (\text{kpstilde} + \text{kdpstilde}) \cdot [\text{C1tilde}] \\
& - \text{b1} \cdot [\text{C1tilde}]
\end{aligned}$$

$$\begin{aligned}
\frac{d [\text{C2}]}{dt} &= \text{kps} \cdot [\text{C1}] \\
& + \text{kdps} \cdot [\text{C3}] \\
& + \text{b2} \cdot [\text{C2tilde}] \\
& - (\text{kps} + \text{kdps}) \cdot [\text{C2}] \\
& - \text{f2} \cdot [\text{C2}]
\end{aligned}$$

$$\begin{aligned}
\frac{d [\text{C2tilde}]}{dt} &= \text{kpstilde} \cdot [\text{C1tilde}] \\
& + \text{kdpstilde} \cdot [\text{C3tilde}] \\
& + \text{f2} \cdot [\text{C2}] \\
& - (\text{kpstilde} + \text{kdpstilde}) \cdot [\text{C2tilde}] \\
& - \text{b2} \cdot [\text{C2tilde}]
\end{aligned}$$

$$\begin{aligned}
\frac{d [\text{C3}]}{dt} &= \text{kps} \cdot [\text{C2}] \\
& + \text{kdps} \cdot [\text{C4}] \\
& + \text{b3} \cdot [\text{C3tilde}] \\
& - (\text{kps} + \text{kdps}) \cdot [\text{C3}] \\
& - \text{f3} \cdot [\text{C3}]
\end{aligned}$$

$$\begin{aligned}
\frac{d [\text{C3tilde}]}{dt} &= \text{kpstilde} \cdot [\text{C2tilde}] \\
& + \text{kdpstilde} \cdot [\text{C4tilde}] \\
& + \text{f3} \cdot [\text{C3}] \\
& - (\text{kpstilde} + \text{kdpstilde}) \cdot [\text{C3tilde}] \\
& - \text{b3} \cdot [\text{C3tilde}]
\end{aligned}$$

$$\begin{aligned}
\frac{d [\text{C4}]}{dt} &= \text{kps} \cdot [\text{C3}] \\
& + \text{kdps} \cdot [\text{C5}] \\
& + \text{b4} \cdot [\text{C4tilde}] \\
& - (\text{kps} + \text{kdps}) \cdot [\text{C4}] \\
& - \text{f4} \cdot [\text{C4}]
\end{aligned}$$

$$\begin{aligned}
\frac{d [\text{C4tilde}]}{dt} &= \text{kpstilde} \cdot [\text{C3tilde}] \\
& + \text{kdpstilde} \cdot [\text{C5tilde}] \\
& + \text{f4} \cdot [\text{C4}] \\
& - (\text{kpstilde} + \text{kdpstilde}) \cdot [\text{C4tilde}] \\
& - \text{b4} \cdot [\text{C4tilde}]
\end{aligned}$$

$$\begin{aligned}
\frac{d [\text{C5}]}{dt} &= \text{kps} \cdot [\text{C4}] \\
& + \text{kdps} \cdot [\text{C6}] \\
& + \text{b5} \cdot [\text{C5tilde}] \\
& - (\text{kps} + \text{kdps}) \cdot [\text{C5}]
\end{aligned}$$

$$-f5 \cdot [C5]$$

$$\begin{aligned} \frac{d[C5\text{tilde}]}{dt} = & \text{kpstilde} \cdot [C4\text{tilde}] \\ & + \text{kdpstilde} \cdot [C6\text{tilde}] \\ & + f5 \cdot [C5] \\ & - (\text{kpstilde} + \text{kdpstilde}) \cdot [C5\text{tilde}] \\ & - b5 \cdot [C5\text{tilde}] \end{aligned}$$

$$\begin{aligned} \frac{d[C6]}{dt} = & \text{kps} \cdot [C5] \\ & + b6 \cdot [C6\text{tilde}] \\ & - \text{ktps} \cdot [C6] \\ & - f6 \cdot [C6] \end{aligned}$$

$$\begin{aligned} \frac{d[C6\text{tilde}]}{dt} = & \text{kpstilde} \cdot [C5\text{tilde}] \\ & + f6 \cdot [C6] \\ & - \text{kdpstilde} \cdot [C6\text{tilde}] \\ & - b6 \cdot [C6\text{tilde}] \end{aligned}$$

Optimizable Parameters

log _{alphaps}	19.6670847171
Eps _{kT}	23.1302085335
log _{alphapstilde}	28.1790604429
Epstilde _{kT}	22.483569037
log _{alphadps}	26.6998070529
Edps _{kT}	21.1518079433
log _{alphadpstilde}	20.0002360148
Edpstilde _{kT}	23.7540865961
log _{alphaf0}	18.3985658418
Ef0 _{kT}	19.4829896692
log _{alphab0}	23.3816618327
Eb0 _{kT}	17.3118817367
log _{alphaf1}	19.5887112187
Ef1 _{kT}	21.2047859444
log _{alphab1}	21.9513036212
Eb1 _{kT}	15.9961080401
log _{alphaf2}	26.0628736509
Ef2 _{kT}	19.9611283701
log _{alphab2}	15.2282284937
Eb2 _{kT}	19.4807268335
log _{alphaf3}	21.22304938
Ef3 _{kT}	21.0483261457
log _{alphab3}	20.5275807171
Eb3 _{kT}	15.3266599034
log _{alphaf4}	22.6721612646
Ef4 _{kT}	13.7269233319

\log_{alphab4}	21.0160049046
Eb4_{kT}	14.5084060239
\log_{alphaf5}	21.0688067196
Ef5_{kT}	21.4516817705
\log_{alphab5}	20.7440933829
Eb5_{kT}	14.603008359
\log_{alphaf6}	21.2765306565
Ef6_{kT}	21.8081831576
\log_{alphab6}	18.7073910928
Eb6_{kT}	17.7747283848