1 Results

Product forming complex

$$\frac{dP}{dT} = \frac{E * B/EQk_6 - Ek_{-6}[Q]}{\sum}$$

Simplifications:

$$k_{-6}, k_{-7}, [P], [Q], k_{-2} = 0$$

Substitutions

$$k_8 = \frac{k_{-8}}{k_{ib}}$$

$$k_1 = \frac{1}{k_{ma}}(k_2 + k_{-1})$$

$$k_4 = \frac{1}{k_{ma2}}(k_7 + k_{-4})$$

$$k_3 = \frac{1}{k_{mb}}(k_6 + k_{-3})$$

Resulting equation

$$\frac{dP}{dT} = v = \frac{N}{D}$$

where

$$N = E_0[A][B]k_2k_6k_{ib}k_{ma2}$$

and

$$\begin{aligned} D = {} & [A]^2k_2k_{ib}k_{mb} + [A]^2k_7k_{ib}k_{mb} + [A][B]k_2k_{ib}k_{ma2} \\ & + [A][B]k_6k_{ib}k_{ma2} + [A][B]k_7k_{ma}k_{mb} + [A]k_2k_{ib}k_{ma2}k_{mb} \\ & + [A]k_7k_{ib}k_{ma}k_{mb} + [B]^2k_6k_{ma}k_{ma2} + [B]k_6k_{ib}k_{ma}k_{ma2} \end{aligned}$$

2 Full report

2.1 Input data

Input file name:

`UPO.txt`

File contents:

```
#mathmatical symbols used in rate constant names (e.g. k-1) must be escaped with a prece

E, k1; [A], EA/EP
EA/EP, k_-1, E
EA/EP, k2, E*
E*, k_-2, EA/EP
```

```
E*, k3; [B], E*B/EQ
E*B/EQ, k_-3, E*
E*B/EQ, k6, E
E, k_-6; [Q], E*B/EQ
E*, k4; [A], E*A/EPR
E*A/EPR, k_-4, E*
E*A/EPR, k7, E
E, k_-7; [P], E*A/EPR
E, k8; [B], EB
EB, k_-8, E

=+: E*B/EQ, k6,
=-: E, k_-6; [Q],

=0: k_-6, k_-7, [P], [Q], k_-2

subsymbols: k_ib, k_ma, k_ma2, k_mb
subs:k8, k_-8/k_ib
subs:k1, (k_-1 + k2)/k_ma
subs:k4, (k_-4+k7)/k_ma2
subs:k3, (k_-3+k6)/k_mb
```

2.2 Parsed reactions

Reactions after parsing:

$$
\begin{array}{lcr}
E & \xrightarrow{k_1[A]} & EA/EP \\
EA/EP & \xrightarrow{k_{-1}} & E \\
EA/EP & \xrightarrow{k_2} & E* \\
E* & \xrightarrow{k_{-2}} & EA/EP \\
E* & \xrightarrow{k_3[B]} & E*B/EQ \\
E*B/EQ & \xrightarrow{k_{-3}} & E* \\
E*B/EQ & \xrightarrow{k_6} & E \\
E & \xrightarrow{k_{-6}[Q]} & E*B/EQ \\
E* & \xrightarrow{k_4[A]} & E*A/EPR \\
E*A/EPR & \xrightarrow{k_{-4}} & E* \\
E*A/EPR & \xrightarrow{k_7} & E \\
E & \xrightarrow{k_{-7}[P]} & E*A/EPR \\
E & \xrightarrow{k_8[B]} & EB \\
EB & \xrightarrow{k_{-8}} & E
\end{array}
$$

2.3 Linear graph matrix

$$
\begin{bmatrix}
 & \frac{k_{-1}}{k_1[A]} & & \frac{k_{-6}[Q]}{k_6} & \frac{k_{-7}[P]}{k_7} & \frac{k_{-8}}{k_8[B]} \\
\frac{k_{-1}}{k_1[A]} & & \frac{k_{-2}}{k_2} & & & \\
 & \frac{k_{-2}}{k_2} & & \frac{k_{-3}}{k_3[B]} & \frac{k_{-4}}{k_4[A]} & \\
\frac{k_{-6}[Q]}{k_6} & & \frac{k_{-3}}{k_3[B]} & & & \\
\frac{k_{-7}[P]}{k_7} & & \frac{k_{-4}}{k_4[A]} & & & \\
\frac{k_{-8}}{k_8[B]} & & & & &
\end{bmatrix}
$$

2.4 Kinetic matrix

$$\begin{bmatrix} & k_1[A] & & k_{-6}[Q] & k_{-7}[P] & k_8[B] \\ k_{-1} & & k_2 & & & \\ & k_{-2} & & k_3[B] & k_4[A] & \\ k_6 & & k_{-3} & & & \\ k_7 & & k_{-4} & & & \\ k_{-8} & & & & & \end{bmatrix}$$

2.5 King-Altman Patterns

0	$\frac{k_{-1}}{k_1[A]}$	$\frac{k_{-2}}{k_2}$	$\frac{k_{-6}[Q]}{k_6}$	$\frac{k_{-7}[P]}{k_7}$	$\frac{k_{-8}}{k_8[B]}$
1	$\frac{k_{-1}}{k_1[A]}$	$\frac{k_{-2}}{k_2}$	$\frac{k_{-6}[Q]}{k_6}$	$\frac{k_{-4}}{k_4[A]}$	$\frac{k_{-8}}{k_8[B]}$
2	$\frac{k_{-1}}{k_1[A]}$	$\frac{k_{-2}}{k_2}$	$\frac{k_{-3}}{k_3[B]}$	$\frac{k_{-7}[P]}{k_7}$	$\frac{k_{-8}}{k_8[B]}$
3	$\frac{k_{-1}}{k_1[A]}$	$\frac{k_{-2}}{k_2}$	$\frac{k_{-3}}{k_3[B]}$	$\frac{k_{-4}}{k_4[A]}$	$\frac{k_{-8}}{k_8[B]}$
4	$\frac{k_{-6}[Q]}{k_6}$	$\frac{k_{-1}}{k_1[A]}$	$\frac{k_{-3}}{k_3[B]}$	$\frac{k_{-7}[P]}{k_7}$	$\frac{k_{-8}}{k_8[B]}$
5	$\frac{k_{-6}[Q]}{k_6}$	$\frac{k_{-1}}{k_1[A]}$	$\frac{k_{-3}}{k_3[B]}$	$\frac{k_{-4}}{k_4[A]}$	$\frac{k_{-8}}{k_8[B]}$
6	$\frac{k_{-6}[Q]}{k_6}$	$\frac{k_{-2}}{k_2}$	$\frac{k_{-3}}{k_3[B]}$	$\frac{k_{-7}[P]}{k_7}$	$\frac{k_{-8}}{k_8[B]}$
7	$\frac{k_{-6}[Q]}{k_6}$	$\frac{k_{-2}}{k_2}$	$\frac{k_{-3}}{k_3[B]}$	$\frac{k_{-4}}{k_4[A]}$	$\frac{k_{-8}}{k_8[B]}$
8	$\frac{k_{-7}[P]}{k_7}$	$\frac{k_{-1}}{k_1[A]}$	$\frac{k_{-6}[Q]}{k_6}$	$\frac{k_{-4}}{k_4[A]}$	$\frac{k_{-8}}{k_8[B]}$
9	$\frac{k_{-7}[P]}{k_7}$	$\frac{k_{-1}}{k_1[A]}$	$\frac{k_{-3}}{k_3[B]}$	$\frac{k_{-4}}{k_4[A]}$	$\frac{k_{-8}}{k_8[B]}$
10	$\frac{k_{-7}[P]}{k_7}$	$\frac{k_{-2}}{k_2}$	$\frac{k_{-6}[Q]}{k_6}$	$\frac{k_{-4}}{k_4[A]}$	$\frac{k_{-8}}{k_8[B]}$
11	$\frac{k_{-7}[P]}{k_7}$	$\frac{k_{-2}}{k_2}$	$\frac{k_{-3}}{k_3[B]}$	$\frac{k_{-4}}{k_4[A]}$	$\frac{k_{-8}}{k_8[B]}$

2.6 Directed Patterns

2.6.1 Directed Pattern for E*B/EQ

0	$k_{-6}[Q]$	k_{-1}	k_7	k_{-8}	k_{-2}
1	$k_{-6}[Q]$	k_{-1}	k_{-8}	k_{-2}	k_{-4}
2	$k_3[B]$	k_2	$k_1[A]$	k_7	k_{-8}
3	$k_3[B]$	k_2	k_{-4}	$k_1[A]$	k_{-8}
4	$k_3[B]$	$k_{-6}[Q]$	k_{-1}	k_7	k_{-8}
5	$k_3[B]$	$k_{-6}[Q]$	k_{-4}	k_{-1}	k_{-8}
6	$k_{-6}[Q]$	k_{-1}	k_7	k_{-8}	$k_4[A]$
7	$k_3[B]$	k_{-4}	$k_{-7}[P]$	k_{-1}	k_{-8}
8	$k_{-6}[Q]$	$k_3[B]$	k_7	k_{-8}	k_2
9	$k_{-6}[Q]$	$k_3[B]$	k_{-8}	k_2	k_{-4}
10	$k_{-6}[Q]$	k_7	k_{-8}	$k_4[A]$	k_2
11	$k_3[B]$	k_2	k_{-4}	$k_{-7}[P]$	k_{-8}

2.6.2 Directed Pattern for E

0	k_{-1}	k_6	k_7	k_{-8}	k_{-2}
1	k_{-1}	k_6	k_{-8}	k_{-2}	k_{-4}
2	k_{-1}	k_7	k_{-8}	k_{-2}	k_{-3}
3	k_{-1}	k_{-8}	k_{-2}	k_{-3}	k_{-4}
4	k_6	k_{-1}	k_7	k_{-8}	$k_3[B]$
5	k_6	k_{-1}	k_{-8}	$k_3[B]$	k_{-4}
6	k_6	k_7	k_{-8}	$k_3[B]$	k_2
7	k_6	k_{-8}	$k_3[B]$	k_2	k_{-4}
8	k_7	k_{-1}	k_6	k_{-8}	$k_4[A]$
9	k_7	k_{-1}	k_{-8}	$k_4[A]$	k_{-3}
10	k_7	k_6	k_{-8}	$k_4[A]$	k_2
11	k_7	k_{-8}	$k_4[A]$	k_2	k_{-3}

2.6.3 Directed Pattern for EA/EP

0	$k_1[A]$	k_{-2}	k_6	k_7	k_{-8}
1	$k_1[A]$	k_{-2}	k_6	k_{-8}	k_{-4}
2	$k_1[A]$	k_{-2}	k_7	k_{-8}	k_{-3}
3	$k_1[A]$	k_{-2}	k_{-8}	k_{-3}	k_{-4}
4	$k_1[A]$	k_6	k_7	k_{-8}	$k_3[B]$
5	$k_1[A]$	k_6	k_{-8}	$k_3[B]$	k_{-4}
6	$k_1[A]$	k_6	k_7	k_{-8}	$k_4[A]$
7	$k_1[A]$	k_7	k_{-8}	$k_4[A]$	k_{-3}
8	k_{-2}	k_{-3}	$k_{-6}[Q]$	k_7	k_{-8}
9	k_{-2}	k_{-3}	k_{-4}	$k_{-6}[Q]$	k_{-8}
10	k_{-2}	k_{-4}	$k_{-7}[P]$	k_6	k_{-8}
11	k_{-2}	k_{-4}	k_{-3}	$k_{-7}[P]$	k_{-8}

2.6.4 Directed Pattern for E*

0	k_2	$k_1[A]$	k_{-8}	k_6	k_7
1	k_2	k_{-4}	$k_1[A]$	k_{-8}	k_6
2	k_2	k_{-3}	$k_1[A]$	k_{-8}	k_7
3	k_2	k_{-3}	k_{-4}	$k_1[A]$	k_{-8}
4	k_{-3}	$k_{-6}[Q]$	k_{-8}	k_{-1}	k_7
5	k_{-3}	k_{-4}	$k_{-6}[Q]$	k_{-8}	k_{-1}
6	k_{-4}	$k_{-7}[P]$	k_{-8}	k_{-1}	k_6
7	k_{-4}	k_{-3}	$k_{-7}[P]$	k_{-8}	k_{-1}
8	k_2	k_{-3}	$k_{-6}[Q]$	k_{-8}	k_7
9	k_2	k_{-3}	k_{-4}	$k_{-6}[Q]$	k_{-8}
10	k_2	k_{-4}	$k_{-7}[P]$	k_{-8}	k_6
11	k_2	k_{-4}	k_{-3}	$k_{-7}[P]$	k_{-8}

2.6.5 Directed Pattern for E*A/EPR

0	$k_{-7}[P]$	k_{-8}	k_{-1}	k_6	k_{-2}
1	$k_4[A]$	k_2	$k_1[A]$	k_{-8}	k_6
2	$k_{-7}[P]$	k_{-8}	k_{-1}	k_{-2}	k_{-3}
3	$k_4[A]$	k_2	k_{-3}	$k_1[A]$	k_{-8}
4	$k_{-7}[P]$	k_{-8}	k_{-1}	k_6	$k_3[B]$
5	$k_4[A]$	k_{-3}	$k_{-6}[Q]$	k_{-8}	k_{-1}
6	$k_4[A]$	$k_{-7}[P]$	k_{-8}	k_{-1}	k_6
7	$k_4[A]$	$k_{-7}[P]$	k_{-3}	k_{-8}	k_{-1}
8	$k_{-7}[P]$	k_{-8}	k_6	$k_3[B]$	k_2
9	$k_4[A]$	k_2	k_{-3}	$k_{-6}[Q]$	k_{-8}
10	$k_4[A]$	$k_{-7}[P]$	k_2	k_{-8}	k_6
11	$k_4[A]$	$k_{-7}[P]$	k_2	k_{-3}	k_{-8}

2.6.6 Directed Pattern for EB

0	$k_8[B]$	k_{-1}	k_7	k_{-2}	k_{-3}
1	$k_8[B]$	k_{-1}	k_{-2}	k_{-3}	k_{-4}
2	$k_8[B]$	k_6	k_{-1}	k_7	k_{-2}
3	$k_8[B]$	k_6	k_{-1}	k_{-2}	k_{-4}
4	$k_8[B]$	k_6	k_{-1}	k_7	$k_3[B]$
5	$k_8[B]$	k_6	k_{-1}	$k_3[B]$	k_{-4}
6	$k_8[B]$	k_6	k_{-1}	k_7	$k_4[A]$
7	$k_8[B]$	k_6	k_7	$k_3[B]$	k_2
8	$k_8[B]$	k_6	$k_3[B]$	k_2	k_{-4}
9	$k_8[B]$	k_6	k_7	$k_4[A]$	k_2
10	$k_8[B]$	k_7	k_{-1}	$k_4[A]$	k_{-3}
11	$k_8[B]$	k_7	$k_4[A]$	k_2	k_{-3}