Electronic Supplementary Information

Entropy in multiple equilibria, compounds with different sites

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ESI1. Systems $X_{rc_1}\{n_1ABn_2\}X_{rc_2}$ for which explicit solutions are reported

Table ESI1

n_1+n_2	n_1, n_2	number of objects $(n_1+1)(n_2+1)$	number of equilibria $(n_1+1)(n_2+1)-1$	$X_{rc_1}\{n_1ABn_2\}X_{rc_2}$	
				rc_1=0,1,…,n_1	rc_2=0,1,…,n_2
12	12,0	13	12	0,…,12	0
	4, 8	45	44	0,…,4	0,…,8
6	6, 0	7	6	0,…,6	0
	5, 1	12	11	0,…,5	0,1
	4, 2	15	14	0,…,4	0,1,2
	3, 3	16	15	0,1,2,3	0,1,2,3
5	5, 0	6	5	0,…,5	0
	4, 1	10	9	0,…,4	0,1
	3, 2	12	11	0,1,2,3	0,1,2
4	4, 0	5	4	0,…,4	0
	3, 1	8	7	0,1,2,3	0,1
	2, 2	9	8	0,1,2	0,1,2
3	3, 0	4	3	0,1,2,3	0
	2, 1	6	5	0,1,2	0,1
2	2, 0	3	2	0,1,2	0
	1, 1	4	3	0,1	0,1
1	1, 0	2	1	0,1	0

The solution for systems with n_2=0 correspond to the results described in ref. 1 and are not further discussed.

ESI2. Solutions for the $X_{rc_1}\{n_1ABn_2\}X_{rc_2}$ equilibrium systems

Table ESI2. {1AB1}

$X_{rc_1}\{1AB1\}X_{rc_2}$	
$\{1AB1\}X + X \rightleftharpoons X\{1AB1\}X$	K_{11}
$\{1AB1\} + X \rightleftharpoons X\{1AB1\}$	K_{10}
$\{1AB1\} + X \rightleftharpoons \{1AB1\}X$	K_{01}

$X_{rc_1}\{1AB1\}X_{rc_2}$			Lc: $K_{10} = K_{11}$	
C_1=	$[X\{1AB1\}X]$	= $K_{11}K_{10}X^2C_4$	C_1=	$K_{10}^2X^2C_4$
C_2=	$[X\{1AB1\}]$	= $K_{10}XC_4$	C_2=	$K_{10}XC_4$
C_3=	$[\{1AB1\}X]$	= $K_{01}XC_4$	C_3=	$K_{01}XC_4$
C_4=	$[\{1AB1\}]$	= $A_0 - \sum_{i=1}^{3} C_i$	C_4=	$A_0 - \sum_{i=1}^{3} C_i$

Table ESI3. $\{2AB1\}$

$X_{rc_1}\{2AB1\}X_{rc_2}$	
$X\{2AB1\}X + X \rightleftharpoons X_2\{2AB1\}X$	K_{21}
$\{2AB1\}X + X \rightleftharpoons X\{2AB1\}X$	K_{11}
$X\{2AB1\} + X \rightleftharpoons X_2\{2AB1\}$	K_{20}
$\{2AB1\} + X \rightleftharpoons X\{2AB1\}$	K_{10}
$\{2AB1\} + X \rightleftharpoons \{2AB1\}X$	K_{01}

$X_{rc_1}\{2AB1\}X_{rc_2}$			Lc: $K_{10} = K_{11}$ pd: $K_{21} = f(2,1)K_{10}$ and $K_{20} = f(2,1)K_{10}$
$C_1 =$	$[X_2\{2AB1\}X]$	$= K_{11}K_{21}K_{01}X^3C_6$	$C_1 = \frac{1}{4}K_{10}^2K_{01}X^3C_6$
$C_2 =$	$[X\{2AB1\}X]$	$= K_{21}K_{01}X^2C_6$	$C_2 = \frac{1}{4}K_{10}K_{01}X^2C_6$
$C_3 =$	$[X_2\{2AB1\}]$	$= K_{10}K_{20}X^2C_6$	$C_3 = \frac{1}{4}K_{10}^2X^2C_6$
$C_4 =$	$[X\{2AB1\}]$	$= K_{20}XC_6$	$C_4 = \frac{1}{4}K_{10}XC_6$
$C_5 =$	$[\{2AB1\}X]$	$= K_{01}XC_6$	$C_5 = K_{01}XC_6$
$C_6 =$	$[\{2AB1\}]$	$= A_0 - \sum_{i=1}^{5} C_i$	$C_6 = A_0 - \sum_{i=1}^{5} C_i$

Table ESI4. $\{3AB1\}$ and $\{2AB2\}$ (These data are reported and explained in Tables 2, 3, 4, and 5 of the main text.)

Table ESI5. $\{4AB1\}$ and $\{3AB2\}$

$X_{rc_1}\{4AB1\}X_{rc_2}$		$X_{rc_1}\{3AB2\}X_{rc_2}$	
$X_3\{4AB1\}X + X \rightleftharpoons X_4\{4AB1\}X$	K_{41}	$X_2\{3AB2\}X_2 + X \rightleftharpoons X_3\{3AB2\}X_2$	K_{32}
$X_2\{4AB1\}X + X \rightleftharpoons X_3\{4AB1\}X$	K_{31}	$X\{3AB2\}X_2 + X \rightleftharpoons X_2\{3AB2\}X_2$	K_{22}
$X\{4AB1\}X + X \rightleftharpoons X_2\{4AB1\}X$	K_{21}	$\{3AB2\}X_2 + X \rightleftharpoons X\{3AB2\}X_2$	K_{12}
$\{4AB1\}X + X \rightleftharpoons X\{4AB1\}X$	K_{11}	$X_2\{3AB2\}X + X \rightleftharpoons X_3\{3AB2\}X$	K_{31}
$X_3\{4AB1\} + X \rightleftharpoons X_4\{4AB1\}$	K_{40}	$X\{3AB2\}X + X \rightleftharpoons X_2\{3AB2\}X$	K_{21}
$X_2\{4AB1\} + X \rightleftharpoons X_3\{4AB1\}$	K_{30}	$\{3AB2\}X + X \rightleftharpoons X\{3AB2\}X$	K_{11}
$X\{4AB1\} + X \rightleftharpoons X_2\{4AB1\}$	K_{20}	$X_2\{3AB2\} + X \rightleftharpoons X_3\{3AB2\}$	K_{30}
$\{4AB1\} + X \rightleftharpoons X\{4AB1\}$	K_{10}	$X\{3AB2\} + X \rightleftharpoons X_2\{3AB2\}$	K_{20}
$\{4AB1\} + X \rightleftharpoons \{4AB1\}X$	K_{01}	$\{3AB2\} + X \rightleftharpoons X\{3AB2\}$	K_{10}
		$\{3AB2\}X + X \rightleftharpoons \{3AB2\}X_2$	K_{02}
		$\{3AB2\} + X \rightleftharpoons \{3AB2\}X$	K_{01}

$X_{rc_1}\{4AB1\}X_{rc_2}$			$X_{rc_1}\{3AB2\}X_{rc_2}$
$C_1 =$	$[X_4\{4AB1\}X]$	$= K_{11}K_{21}K_{31}K_{41}K_{01}X^5C_{10}$	The solution of the $X_{rc_1}\{3AB2\}X_{rc_2}$ system is reported and discussed in detail in ref. 25.
$C_2 =$	$[X_3\{4AB1\}X]$	$= K_{11}K_{21}K_{31}K_{01}X^4C_{10}$	
$C_3 =$	$[X_2\{4AB1\}X]$	$= K_{11}K_{21}K_{01}X^3C_{10}$	
$C_4 =$	$[X\{4AB1\}X]$	$= K_{11}K_{01}X^2C_{10}$	
$C_5 =$	$[X_4\{4AB1\}]$	$= K_{10}K_{20}K_{30}K_{40}X^4C_{10}$	
$C_6 =$	$[X_3\{4AB1\}]$	$= K_{10}K_{20}K_{30}X^3C_{10}$	
$C_7 =$	$[X_2\{4AB1\}]$	$= K_{10}K_{20}X^2C_{10}$	
$C_8 =$	$[X\{4AB1\}]$	$= K_{10}XC_{10}$	
$C_9 =$	$[\{4AB1\}X]$	$= K_{01}XC_{10}$	
$C_{10} =$	$[\{4AB1\}]$	$= A_0 - \sum_{i=1}^{9} C_i$	

Relation between the equilibrium constants of the two $X_{rc_1}\{n_1ABn_2\}X_{rc_2}$ systems with 5 sites as a consequence of Langmuir's condition Lc and the particle distribution pd.

	$X_{rc_1}\{4AB1\}X_{rc_2}$									$X_{rc_1}\{3AB2\}X_{rc_2}$
	K_{11}	K_{21}	K_{31}	K_{41}	K_{10}	K_{20}	K_{30}	K_{40}	K_{01}	see ref. [25]
Lc	K_{10}									
pd		$f(4,1)\,K_{10}$	$f(4,1)\,f(4,2)K_{10}$	$f(4,1)\,f(4,2)\,f(4,3)K_{10}$		$f(4,1)\,K_{10}$	$f(4,1)\,f(4,2)K_{10}$	$f(4,1)\,f(4,2)\,f(4,3)K_{10}$		
	K_{10}	$\frac{3}{8}K_{10}$	$\frac{1}{6}K_{10}$	$\frac{1}{16}K_{10}$	K_{10}	$\frac{3}{8}K_{10}$	$\frac{1}{6}K_{10}$	$\frac{1}{16}K_{10}$	K_{01}	

$X_{rc_1}\{4AB1\}X_{rc_2}$	$X_{rc_1}\{3AB2\}X_{rc_2}$
$\begin{bmatrix} C_1 \\ C_2 \\ C_3 \\ C_4 \\ C_5 \\ C_6 \\ C_7 \\ C_8 \\ C_9 \end{bmatrix}(X) = \begin{bmatrix} \frac{1}{256}K_{10}^4 K_{01}[X]^5 \\ \frac{1}{16}K_{10}^3 K_{01}[X]^4 \\ \frac{3}{8}K_{10}^2 K_{01}[X]^3 \\ K_{10}K_{01}[X]^2 \\ \frac{1}{256}K_{10}^4[X]^4 \\ \frac{1}{16}K_{10}^3[X]^3 \\ \frac{3}{8}K_{10}^2[X]^2 \\ K_{10}[X] \\ K_{01}[X] \end{bmatrix} C_{10}(X)$ $C_{10}(X) = A_0 - \sum_{i=1}^{9} C_i\ (X)$	see ref. [25]

Table ESI6. {5AB1}, {4AB2} and {3AB3}

$X_{rc_1}\{5AB1\}X_{rc_2}$		$X_{rc_1}\{4AB2\}X_{rc_2}$		$X_{rc_1}\{3AB3\}X_{rc_2}$	
$X_4\{5AB1\}X + X \rightleftharpoons X_5\{5AB1\}X$	K_{51}	$X_3\{4AB2\}X_2 + X \rightleftharpoons X_4\{4AB2\}X_2$	K_{42}	$X_2\{3AB3\}X_2 + X \rightleftharpoons X_3\{3AB3\}X_3$	K_{33}
$X_3\{5AB1\}X + X \rightleftharpoons X_4\{5AB1\}X$	K_{41}	$X_2\{4AB2\}X_2 + X \rightleftharpoons X_3\{4AB2\}X_2$	K_{32}	$X\{3AB3\}X_2 + X \rightleftharpoons X_2\{3AB3\}X_3$	K_{23}
$X_2\{5AB1\}X + X \rightleftharpoons X_3\{5AB1\}X$	K_{31}	$X\{4AB2\}X_2 + X \rightleftharpoons X_2\{4AB2\}X_2$	K_{22}	$\{3AB3\}X_2 + X \rightleftharpoons X\{3AB3\}X_3$	K_{13}
$X\{5AB1\}X + X \rightleftharpoons X_2\{5AB1\}X$	K_{21}	$\{4AB2\}X_2 + X \rightleftharpoons X\{4AB2\}X_2$	K_{12}	$X_2\{3AB3\}X_2 + X \rightleftharpoons X_3\{3AB3\}X_2$	K_{32}
$\{5AB1\}X + X \rightleftharpoons X\{5AB1\}X$	K_{11}	$X_3\{4AB2\}X + X \rightleftharpoons X_4\{4AB2\}X$	K_{41}	$X\{3AB3\}X + X \rightleftharpoons X_2\{3AB3\}X_2$	K_{22}
$X_4\{5AB1\} + X \rightleftharpoons X_5\{5AB1\}$	K_{50}	$X_2\{4AB2\}X + X \rightleftharpoons X_3\{4AB2\}X$	K_{31}	$\{3AB3\}X + X \rightleftharpoons X\{3AB3\}X_2$	K_{12}
$X_3\{5AB1\} + X \rightleftharpoons X_4\{5AB1\}$	K_{40}	$X\{4AB2\}X + X \rightleftharpoons X_2\{4AB2\}X$	K_{21}	$X_2\{3AB3\}X + X \rightleftharpoons X_3\{3AB3\}X$	K_{31}
$X_2\{5AB1\} + X \rightleftharpoons X_3\{5AB1\}$	K_{30}	$\{4AB2\}X + X \rightleftharpoons X\{4AB2\}X$	K_{11}	$X\{3AB3\}X + X \rightleftharpoons X_2\{3AB3\}X$	K_{21}
$X\{5AB1\} + X \rightleftharpoons X_2\{5AB1\}$	K_{20}	$X_3\{4AB2\} + X \rightleftharpoons X_4\{4AB2\}$	K_{40}	$\{3AB3\}X + X \rightleftharpoons X\{3AB3\}X$	K_{11}
$\{5AB1\} + X \rightleftharpoons X\{5AB1\}$	K_{10}	$X_2\{4AB2\} + X \rightleftharpoons X_3\{4AB2\}$	K_{30}	$X_2\{3AB3\} + X \rightleftharpoons X_3\{3AB3\}$	K_{30}
$\{5AB1\} + X \rightleftharpoons \{5AB1\}X$	K_{01}	$X\{4AB2\} + X \rightleftharpoons X_2\{4AB2\}$	K_{20}	$X\{3AB3\} + X \rightleftharpoons X_2\{3AB3\}$	K_{20}
		$\{4AB2\} + X \rightleftharpoons X\{4AB2\}$	K_{10}	$\{3AB3\} + X \rightleftharpoons X\{3AB3\}$	K_{10}
		$\{4AB2\}X + X \rightleftharpoons \{4AB2\}X_2$	K_{02}	$\{3AB3\}X_2 + X \rightleftharpoons \{3AB3\}X_3$	K_{03}
		$\{4AB2\} + X \rightleftharpoons \{4AB2\}X$	K_{01}	$\{3AB3\}X + X \rightleftharpoons \{3AB3\}X_2$	K_{02}
				$\{3AB3\} + X \rightleftharpoons \{3AB3\}X$	K_{01}

$X_{rc_1}\{5AB1\}X_{rc_2}$			$X_{rc_1}\{4AB2\}X_{rc_2}$			
$C_1 =$	$[X_5\{4AB1\}X]$	$= K_{11}K_{21}K_{31}K_{41}K_{51}K_{01}X^6C_{12}$	$C_1 =$	$[X_4\{4AB1\}X_2]$	$= K_{12}K_{22}K_{32}K_{42}K_{01}K_{02}X^6C_{15}$	
$C_2 =$	$[X_4\{4AB1\}X]$	$= K_{11}K_{21}K_{31}K_{41}K_{01}X^5C_{12}$	$C_2 =$	$[X_3\{4AB1\}X_2]$	$= K_{12}K_{22}K_{32}K_{01}K_{02}X^5C_{15}$	
$C_3 =$	$[X_3\{4AB1\}X]$	$= K_{11}K_{21}K_{31}K_{01}X^4C_{12}$	$C_3 =$	$[X_2\{4AB1\}X_2]$	$= K_{12}K_{22}K_{01}K_{02}X^4C_{15}$	
$C_4 =$	$[X_2\{4AB1\}X]$	$= K_{11}K_{21}K_{01}X^3C_{12}$	$C_4 =$	$[X\{4AB1\}X_2]$	$= K_{12}K_{01}K_{02}X^3C_{15}$	
$C_5 =$	$[X\{4AB1\}]$	$= K_{11}K_{01}X^2C_{12}$	$C_5 =$	$[X_4\{4AB1\}X]$	$= K_{11}K_{21}K_{31}K_{41}K_{01}X^5C_{15}$	
$C_6 =$	$[X_5\{4AB1\}]$	$= K_{10}K_{20}K_{30}K_{40}K_{50}X^5C_{12}$	$C_6 =$	$[X_3\{4AB1\}X]$	$= K_{11}K_{21}K_{31}K_{01}X^4C_{15}$	
$C_7 =$	$[X_4\{4AB1\}]$	$= K_{10}K_{20}K_{30}K_{40}X^4C_{12}$	$C_7 =$	$[X_2\{4AB1\}X]$	$= K_{11}K_{21}K_{01}X^3C_{15}$	
$C_8 =$	$[X_3\{4AB1\}]$	$= K_{10}K_{20}K_{30}X^3C_{12}$	$C_8 =$	$[X\{4AB1\}X]$	$= K_{11}K_{01}X^2C_{15}$	
$C_9 =$	$[X_2\{4AB1\}]$	$= K_{10}K_{20}X^2C_{12}$	$C_9 =$	$[X_4\{4AB1\}]$	$= K_{10}K_{20}K_{30}K_{40}X^4C_{15}$	
$C_{10} =$	$[X\{4AB1\}]$	$= K_{10}XC_{12}$	$C_{10} =$	$[X_3\{4AB1\}]$	$= K_{10}K_{20}K_{30}X^3C_{15}$	
$C_{11} =$	$[\{4AB1\}]X$	$= K_{01}XC_{12}$	$C_{11} =$	$[X_2\{4AB1\}]$	$= K_{10}K_{20}X^2C_{15}$	
$C_{12} =$	$[\{4AB1\}]$	$= A_0 - \sum_{i=1}^{11} C_i$	$C_{12} =$	$[X\{4AB1\}]$	$= K_{10}XC_{15}$	
			$C_{13} =$	$[\{4AB1\}]X_2$	$= K_{01}K_{02}X^2C_{15}$	
			$C_{14} =$	$[\{4AB1\}X]$	$= K_{01}XC_{15}$	
			$C_{15} =$	$[\{4AB1\}]$	$= A_0 - \sum_{i=1}^{14} C_i$	…

$X_{rc_1}\{3AB3\}X_{rc_2}$			
$C_1 =$	$[X_3\{3AB3\}X_3]$	$=$	$K_{13}K_{23}K_{33}K_{01}K_{02}K_{03}X^6C_{16}$
$C_2 =$	$[X_2\{3AB3\}X_3]$	$=$	$K_{13}K_{23}K_{01}K_{02}K_{03}X^5C_{16}$
$C_3 =$	$[X\{3AB3\}X_3]$	$=$	$K_{13}K_{01}K_{02}K_{03}X^4C_{16}$
$C_4 =$	$[X_3\{3AB3\}X_2]$	$=$	$K_{12}K_{22}K_{32}K_{01}K_{02}X^5C_{16}$
$C_5 =$	$[X_2\{3AB3\}X_2]$	$=$	$K_{12}K_{22}K_{01}K_{02}X^4C_{16}$
$C_6 =$	$[X\{3AB3\}X_2]$	$=$	$K_{12}K_{01}K_{02}X^3C_{16}$
$C_7 =$	$[X_3\{3AB3\}X]$	$=$	$K_{11}K_{21}K_{31}K_{01}X^4C_{16}$
$C_8 =$	$[X_2\{3AB3\}X]$	$=$	$K_{11}K_{21}K_{01}X^3C_{16}$
$C_9 =$	$[X\{3AB3\}X]$	$=$	$K_{11}K_{01}X^2C_{16}$
$C_{10} =$	$[X_3\{3AB3\}]$	$=$	$K_{10}K_{20}K_{30}X^3C_{16}$
$C_{11} =$	$[X_2\{3AB3\}]$	$=$	$K_{10}K_{20}X^2C_{16}$
$C_{12} =$	$[X\{3AB3\}]$	$=$	$K_{10}XC_{16}$
$C_{13} =$	$[\{3AB3\}X_3]$	$=$	$K_{01}K_{02}K_{03}X^3C_{16}$
$C_{14} =$	$[\{3AB3\}X_2]$	$=$	$K_{01}K_{02}X^2C_{16}$
$C_{15} =$	$[\{3AB3\}X]$	$=$	$K_{01}XC_{16}$
$C_{16} =$	$[\{3AB3\}]$	$=$	$A_0 - \sum_{i=1}^{15} C_i$

Relations between the equilibrium constants of the two $X_{rc_1}\{n_1ABn_2\}X_{rc_2}$ systems with 6 sites as a consequence of Langmuir's condition Lc and the particle distribution pd.

$X_{rc_1}\{5AB1\}X_{rc_2}$

	K_{11}	K_{21}	K_{31}	K_{41}	K_{51}	K_{10}	K_{20}	K_{30}	K_{40}	K_{50}	K_{01}
Lc	K_{10}										
pd		f(5,1) K_{10}	f(5,1) f(5,2) K_{10}	f(5,1) f(5,2) f(5,3) K_{10}	f(5,1) f(5,2) f(5,3) f(5,4) K_{10}		f(5,1) K_{10}	f(5,1) f(5,2) K_{10}	f(5,1) f(5,2) f(5,3) K_{10}	f(5,1) f(5,2) f(5,3) f(5,4) K_{10}	
	K_{10}	$\frac{2}{5}K_{10}$	$\frac{1}{5}K_{10}$	$\frac{1}{10}K_{10}$	$\frac{1}{25}K_{10}$	K_{10}	$\frac{2}{5}K_{10}$	$\frac{1}{5}K_{10}$	$\frac{1}{10}K_{10}$	$\frac{1}{25}K_{10}$	K_{01}

$X_{rc_1}\{4AB2\}X_{rc_2}$

	K_{12}	K_{22}	K_{32}	K_{42}	K_{11}	K_{21}	K_{31}	K_{41}	K_{10}	K_{20}	K_{30}	K_{40}	K_{01}	K_{02}
Lc	K_{10}				K_{10}									
pd		f(4,1) K_{10}	f(4,1) f(4,2) K_{10}	f(4,1) f(4,2) f(4,3) K_{10}		K_{22}	K_{32}	K_{42}		K_{22}	K_{32}	K_{42}		f(2,1) K_{01}
	K_{10}	$\frac{3}{8}K_{10}$	$\frac{1}{6}K_{10}$	$\frac{1}{16}K_{10}$	K_{10}	$\frac{3}{8}K_{10}$	$\frac{1}{6}K_{10}$	$\frac{1}{16}K_{10}$	K_{10}	$\frac{3}{8}K_{10}$	$\frac{1}{6}K_{10}$	$\frac{1}{16}K_{10}$	K_{01}	$\frac{1}{4}K_{10}$

$X_{rc_1}\{3AB3\}X_{rc_2}$

	K_{13}	K_{23}	K_{33}	K_{12}	K_{22}	K_{32}	K_{11}	K_{21}	K_{31}	K_{10}	K_{20}	K_{30}	K_{01}	K_{02}	K_{03}
Lc	K_{10}			K_{10}			K_{10}								
pd		f(3,1) K_{10}	f(3,1) f(3,2) K_{10}		K_{23}	K_{33}		K_{23}	K_{33}		K_{23}	K_{33}		f(3,1) K_{01}	f(3,1) f(3,2) K_{01}
	K_{10}	$\frac{1}{3}K_{10}$	$\frac{1}{9}K_{10}$	K_{10}	$\frac{1}{3}K_{10}$	$\frac{1}{9}K_{10}$	K_{10}	$\frac{1}{3}K_{10}$	$\frac{1}{9}K_{10}$	K_{10}	$\frac{1}{3}K_{10}$	$\frac{1}{9}K_{10}$	K_{01}	$\frac{1}{3}K_{01}$	$\frac{1}{9}K_{01}$

$X_{rc_1}\{5AB1\}X_{rc_2}$

$$\begin{bmatrix} C_1 \\ C_2 \\ C_3 \\ C_4 \\ C_5 \\ C_6 \\ C_7 \\ C_8 \\ C_9 \\ C_{10} \\ C_{11} \end{bmatrix}(X) = \begin{bmatrix} \frac{1}{3125}{K_{10}}^5 K_{01}[X]^6 \\ \frac{1}{125}{K_{10}}^4 K_{01}[X]^5 \\ \frac{2}{25}K_{10}^3 K_{01}[X]^4 \\ \frac{2}{5}K_{10}^2 K_{01}[X]^3 \\ K_{10}K_{01}[X]^2 \\ \frac{1}{3125}K_{10}^5[X]^5 \\ \frac{1}{125}K_{10}^4[X]^4 \\ \frac{2}{25}K_{10}^3[X]^3 \\ \frac{2}{5}K_{10}^2[X]^2 \\ K_{10}[X] \\ \mathrm{K}_{01}[X] \end{bmatrix} C_{12}(X)$$

$$C_{12}(X) = A_0 - \sum_{i=1}^{11} C_i\ (X)$$

$X_{rc_1}\{4AB2\}X_{rc_2}$

$$\begin{bmatrix} C_1 \\ C_2 \\ C_3 \\ C_4 \\ C_5 \\ C_6 \\ C_7 \\ C_8 \\ C_9 \\ C_{10} \\ C_{11} \\ C_{12} \\ C_{13} \\ C_{14} \end{bmatrix}(X) = \begin{bmatrix} \frac{1}{16^2}{K_{10}}^4 \frac{1}{4}{K_{01}}^2[X]^6 \\ \frac{1}{16}{K_{10}}^3 \frac{1}{4}{K_{01}}^2[X]^5 \\ \frac{3}{8}{K_{10}}^2 \frac{1}{4}{K_{01}}^2[X]^4 \\ K_{10}\frac{1}{4}{K_{01}}^2[X]^3 \\ \frac{1}{16^2}K_{10}{}^4K_{01}[X]^5 \\ \frac{1}{16}{K_{10}}^3K_{01}[X]^4 \\ \frac{3}{8}{K_{10}}^2K_{01}[X]^3 \\ K_{10}K_{01}[X]^2 \\ \frac{1}{16^2}K_{10}{}^4[X]^4 \\ \frac{1}{16}K_{10}{}^3[X]^3 \\ \frac{3}{8}{K_{10}}^2[X]^2 \\ \mathrm{K}_{10}[X] \\ \frac{1}{4}{K_{01}}^2[X]^2 \\ \mathrm{K}_{01}[X] \end{bmatrix} C_{15}(X)$$

$$C_{15}(X) = A_0 - \sum_{i=1}^{14} C_i\ (X)$$

$X_{rc_1}\{3AB3\}X_{rc_2}$

$$\begin{bmatrix} C_1 \\ C_2 \\ C_3 \\ C_4 \\ C_5 \\ C_6 \\ C_7 \\ C_8 \\ C_9 \\ C_{10} \\ C_{11} \\ C_{12} \\ C_{13} \\ C_{14} \\ C_{15} \end{bmatrix}(X) = \begin{bmatrix} \frac{1}{729}[X]^6{\mathrm{K}_{10}}^3{\mathrm{K}_{01}}^3 \\ \frac{1}{81}[X]^5{\mathrm{K}_{10}}^2{\mathrm{K}_{01}}^3 \\ \frac{1}{27}[X]^4\mathrm{K}_{10}{\mathrm{K}_{01}}^3 \\ \frac{1}{81}[X]^5\mathrm{K}_{10}{}^3\mathrm{K}_{01}{}^2 \\ \frac{1}{9}[X]^4\mathrm{K}_{10}{}^2\mathrm{K}_{01}{}^2 \\ \frac{1}{3}[X]^3\mathrm{K}_{10}\mathrm{K}_{01}{}^2 \\ \frac{1}{27}[X]^4\mathrm{K}_{10}{}^3\mathrm{K}_{01} \\ \frac{1}{3}[X]^3\mathrm{K}_{10}{}^2\mathrm{K}_{01} \\ [X]^2\mathrm{K}_{10}\mathrm{K}_{01} \\ \frac{1}{27}[X]^3{\mathrm{K}_{10}}^3 \\ \frac{1}{3}[X]^2{\mathrm{K}_{10}}^2 \\ [X]\mathrm{K}_{10} \\ \frac{1}{27}[X]^3{\mathrm{K}_{01}}^3 \\ \frac{1}{3}[X]^2{\mathrm{K}_{01}}^2 \\ [X]\mathrm{K}_{01} \end{bmatrix} C_{16}(X)$$

$$C_{16}(X) = A_0 - \sum_{i=1}^{15} C_i\ (X)$$

Table ESI7. $\{8AB4\}$: $X_{rc_1}\{8AB4\}X_{rc_2}$

1	$X_7\{AB\}X_4 + X \rightleftharpoons X_8\{AB\}X_4$	K_{84}
2	$X_6\{AB\}X_4 + X \rightleftharpoons X_7\{AB\}X_4$	K_{74}
3	$X_5\{AB\}X_4 + X \rightleftharpoons X_6\{AB\}X_4$	K_{64}
4	$X_4\{AB\}X_4 + X \rightleftharpoons X_5\{AB\}X_4$	K_{54}
5	$X_3\{AB\}X_4 + X \rightleftharpoons X_4\{AB\}X_4$	K_{44}
6	$X_2\{AB\}X_4 + X \rightleftharpoons X_3\{AB\}X_4$	K_{34}
7	$X\{AB\}X_4 + X \rightleftharpoons X_2\{AB\}X_4$	K_{24}
8	$\{AB\}X_4 + X \rightleftharpoons X\{AB\}X_4$	K_{14}
9	$X_7\{AB\}X_3 + X \rightleftharpoons X_8\{AB\}X_3$	K_{83}
10	$X_6\{AB\}X_3 + X \rightleftharpoons X_7\{AB\}X_3$	K_{73}
11	$X_5\{AB\}X_3 + X \rightleftharpoons X_6\{AB\}X_3$	K_{63}
12	$X_4\{AB\}X_3 + X \rightleftharpoons X_5\{AB\}X_3$	K_{53}
13	$X_3\{AB\}X_3 + X \rightleftharpoons X_4\{AB\}X_3$	K_{43}
14	$X_2\{AB\}X_3 + X \rightleftharpoons X_3\{AB\}X_3$	K_{33}
15	$X_1\{AB\}X_3 + X \rightleftharpoons X_2\{AB\}X_3$	K_{23}
16	$\{AB\}X_3 + X \rightleftharpoons X\{AB\}X_3$	K_{13}
17	$X_7\{AB\}X_2 + X \rightleftharpoons X_8\{AB\}X_2$	K_{82}
18	$X_6\{AB\}X_2 + X \rightleftharpoons X_7\{AB\}X_2$	K_{72}
19	$X_5\{AB\}X_2 + X \rightleftharpoons X_6\{AB\}X_2$	K_{62}
20	$X_4\{AB\}X_2 + X \rightleftharpoons X_5\{AB\}X_2$	K_{52}
21	$X_3\{AB\}X_2 + X \rightleftharpoons X_4\{AB\}X_2$	K_{42}
22	$X_2\{AB\}X_2 + X \rightleftharpoons X_3\{AB\}X_2$	K_{32}
23	$X\{AB\}X_2 + X \rightleftharpoons X_2\{AB\}X_2$	K_{22}
24	$\{AB\}X_2 + X \rightleftharpoons X\{AB\}X_2$	K_{12}
25	$X_7\{AB\}X + X \rightleftharpoons X_8\{AB\}X$	K_{81}
26	$X_6\{AB\}X + X \rightleftharpoons X_7\{AB\}X$	K_{71}
27	$X_5\{AB\}X + X \rightleftharpoons X_6\{AB\}X$	K_{61}
28	$X_4\{AB\}X + X \rightleftharpoons X_5\{AB\}X$	K_{51}
29	$X_3\{AB\}X + X \rightleftharpoons X_4\{AB\}X$	K_{41}
30	$X_2\{AB\}X + X \rightleftharpoons X_3\{AB\}X$	K_{31}
31	$X\{AB\}X + X \rightleftharpoons X_2\{AB\}X$	K_{21}
32	$\{AB\}X + X \rightleftharpoons X\{AB\}X$	K_{11}
33	$X_7\{AB\} + X \rightleftharpoons X_8\{AB\}$	K_{80}
34	$X_6\{AB\} + X \rightleftharpoons X_7\{AB\}$	K_{70}
35	$X_5\{AB\} + X \rightleftharpoons X_6\{AB\}$	K_{60}
36	$X_4\{AB\} + X \rightleftharpoons X_5\{AB\}$	K_{50}
37	$X_3\{AB\} + X \rightleftharpoons X_4\{AB\}$	K_{40}
38	$X_2\{AB\} + X \rightleftharpoons X_3\{AB\}$	K_{30}
39	$X\{AB\} + X \rightleftharpoons X_2\{AB\}$	K_{20}
40	$\{AB\} + X \rightleftharpoons X\{AB\}$	K_{10}
41	$\{AB\}X_3 + X \rightleftharpoons \{AB\}X_4$	K_{04}
42	$\{AB\}X_2 + X \rightleftharpoons \{AB\}X_3$	K_{03}
43	$\{AB\}X + X \rightleftharpoons \{AB\}X_2$	K_{02}
44	$\{AB\} + X \rightleftharpoons \{AB\}X$	K_{01}

$C_1 =$	$[X_8\{AB\}X_4]$	=	$K_{10}^8 X^{12} Pa10(0) K_{01}^4$
$C_2 =$	$[X_7\{AB\}X_4]$	=	$K_{10}^7 X^{11} Pa10(1) K_{01}^4$
$C_3 =$	$[X_6\{AB\}X_4]$	=	$K_{10}^6 X^{10} Pa10(2) K_{01}^4$
$C_4 =$	$[X_5\{AB\}X_4]$	=	$K_{10}^5 X^9 Pa10(3) K_{01}^4$
$C_5 =$	$[X_4\{AB\}X_4]$	=	$K_{10}^4 X^8 Pa10(4) K_{01}^4$
$C_6 =$	$[X_3\{AB\}X_4]$	=	$K_{10}^3 X^7 Pa10(5) K_{01}^4$
$C_7 =$	$[X_2\{AB\}X_4]$	=	$K_{10}^2 X^6 Pa10(6) K_{01}^4$
$C_8 =$	$[X\{AB\}X_4]$	=	$K_{10} X^5 Pa10(7) K_{01}^4$
$C_9 =$	$[X_8\{AB\}X_3]$	=	$K_{10}^8 X^{11} Pa21(0) K_{01}^3$
$C_{10} =$	$[X_7\{AB\}X_3]$	=	$K_{10}^7 X^{10} Pa21(1) K_{01}^3$
$C_{11} =$	$[X_6\{AB\}X_3]$	=	$K_{10}^6 X^9 Pa21(2) K_{01}^3$
$C_{12} =$	$[X_5\{AB\}X_3]$	=	$K_{10}^5 X^8 Pa21(3) K_{01}^3$
$C_{13} =$	$[X_4\{AB\}X_3]$	=	$K_{10}^4 X^7 Pa21(4) K_{01}^3$
$C_{14} =$	$[X_3\{AB\}X_3]$	=	$K_{10}^3 X^6 Pa21(5) K_{01}^3$
$C_{15} =$	$[X_2\{AB\}X_3]$	=	$K_{10}^2 X^5 Pa21(6) K_{01}^3$
$C_{16} =$	$[X\{AB\}X_3]$	=	$K_{10} X^4 Pa21(7) K_{01}^3$
$C_{17} =$	$[X_8\{AB\}X_2]$	=	$K_{10}^8 X^{10} Pa32(0) K_{01}^2$
$C_{18} =$	$[X_7\{AB\}X_2]$	=	$K_{10}^7 X^9 Pa32(1) K_{01}^2$
$C_{19} =$	$[X_6\{AB\}X_2]$	=	$K_{10}^6 X^8 Pa32(2) K_{01}^2$
$C_{20} =$	$[X_5\{AB\}X_2]$	=	$K_{10}^5 X^7 Pa32(3) K_{01}^2$
$C_{21} =$	$[X_4\{AB\}X_2]$	=	$K_{10}^4 X^6 Pa32(4) K_{01}^2$
$C_{22} =$	$[X_3\{AB\}X_2]$	=	$K_{10}^3 X^5 Pa32(5) K_{01}^2$
$C_{23} =$	$[X_2\{AB\}X_2]$	=	$K_{10}^2 X^4 Pa32(6) K_{01}^2$
$C_{24} =$	$[X\{AB\}X_2]$	=	$K_{10} X^3 Pa32(7) K_{01}^2$
$C_{25} =$	$[X_8\{AB\}X]$	=	$K_{10}^8 X^9 Pa4(0) K_{01}$
$C_{26} =$	$[X_9\{AB\}X]$	=	$K_{10}^7 X^8 Pa4(1) K_{01}$
$C_{27} =$	$[X_6\{AB\}X]$	=	$K_{10}^6 X^7 Pa4(2) K_{01}$
$C_{28} =$	$[X_5\{AB\}X]$	=	$K_{10}^5 X^6 Pa4(3) K_{01}$
$C_{29} =$	$[X_4\{AB\}X]$	=	$K_{10}^4 X^5 Pa4(4) K_{01}$
$C_{30} =$	$[X_3\{AB\}X]$	=	$K_{10}^3 X^4 Pa4(5) K_{01}$
$C_{31} =$	$[X_2\{AB\}X]$	=	$K_{10}^2 X^3 Pa4(6) K_{01}$
$C_{32} =$	$[X\{AB\}X]$	=	$K_{10} X^2 Pa4(7) K_{01}$
$C_{33} =$	$[X_8\{AB\}]$	=	$K_{10}^8 X^8 Pa5(0)$
$C_{34} =$	$[X_7\{AB\}]$	=	$K_{10}^7 X^7 Pa5(1)$
$C_{35} =$	$[X_6\{AB\}]$	=	$K_{10}^6 X^6 Pa5(2)$
$C_{36} =$	$[X_5\{AB\}]$	=	$K_{10}^5 X^5 Pa5(3)$
$C_{37} =$	$[X_4\{AB\}]$	=	$K_{10}^4 X^4 Pa5(4)$
$C_{38} =$	$[X_3\{AB\}]$	=	$K_{10}^3 X^3 Pa5(5)$
$C_{39} =$	$[X_2\{AB\}]$	=	$K_{10}^2 X^2 Pa5(6)$
$C_{40} =$	$[X\{AB\}]$	=	$K_{10} X Pa5(7)$
$C_{41} =$	$[\{AB\}X_4]$	=	$X^4 PL(0) K_{01}^4$
$C_{42} =$	$[\{AB\}X_3]$	=	$X^3 PL(1) K_{01}^3$
$C_{43} =$	$[\{AB\}X_2]$	=	$X^2 PL(2) K_{01}^2$
$C_{44} =$	$[\{AB\}X]$	=	$X PL(3) K_{01}$
$C_{45} =$	$[\{AB\}]$	=	$A_0 - \sum_{i=1}^{44} C_i$

$\kappa := 0,1..7$

$$Pa10(\kappa) = \begin{pmatrix} \frac{1}{4294967296} \\ \frac{1}{67108864} \\ \frac{7}{16777216} \\ \frac{7}{1048576} \\ \frac{35}{524288} \\ \frac{7}{16384} \\ \frac{7}{4096} \\ \frac{1}{256} \end{pmatrix} \quad Pa21(\kappa) = \begin{pmatrix} \frac{1}{268435456} \\ \frac{1}{4194304} \\ \frac{7}{1048576} \\ \frac{7}{65536} \\ \frac{35}{32768} \\ \frac{7}{1024} \\ \frac{7}{256} \\ \frac{1}{16} \end{pmatrix} \quad Pa32(\kappa) = \begin{pmatrix} \frac{3}{134217728} \\ \frac{3}{2097152} \\ \frac{21}{524288} \\ \frac{21}{32768} \\ \frac{105}{16384} \\ \frac{21}{512} \\ \frac{21}{128} \\ \frac{3}{8} \end{pmatrix} \quad Pa4(\kappa) = \begin{pmatrix} \frac{1}{16777216} \\ \frac{1}{262144} \\ \frac{7}{65536} \\ \frac{7}{4096} \\ \frac{35}{2048} \\ \frac{7}{64} \\ \frac{7}{16} \\ 1 \end{pmatrix} \quad Pa5(\kappa) = \begin{pmatrix} \frac{1}{16777216} \\ \frac{1}{262144} \\ \frac{7}{65536} \\ \frac{7}{4096} \\ \frac{35}{2048} \\ \frac{7}{64} \\ \frac{7}{16} \\ 1 \end{pmatrix}$$

$\lambda := 0,1..3$

$$PL(\lambda) = \begin{pmatrix} \frac{1}{256} \\ \frac{1}{16} \\ \frac{3}{8} \\ 1 \end{pmatrix}$$