Notes on HCl Transport

J. P. Keener
Department of Mathematics
University of Utah

September 26, 2023

The notation is $S_{x_1,x_2,x_3,x_4,x_5,x_6}$ where $x_j = 0, 1$. Thus, there are $2^6 = 64$ states (although not all are allowed). A possible binary representation is σ_p where

$$p = \sum_{j=1}^{6} x_j 2^{6-j}. \tag{1}$$

The states are

$$x_1 \quad = \begin{cases} 1, \text{E148 up}, \\ 0, \text{E148 down} \end{cases} \tag{2}$$

$$x_2 \quad = \begin{cases} 1, \text{E148 protonated}, \\ 0, \text{E148 deprotonated} \end{cases} \tag{3}$$

$$x_3 \quad = \begin{cases} 1, \text{E203 protonated}, \\ 0, \text{E203 deprotonated} \end{cases} \tag{4}$$

$$x_{4,5,6} \quad = \begin{cases} 1, \text{Cl bound}, \\ 0, \text{Cl unbound} \end{cases}. \tag{5}$$

However, some states are not permitted.

1. E148 down and S_{cen} occupied is not allowed. Thus, the states $S_{0,x_2,x_3,x_4,1,x_6}$ are not allowed.

2. Only one proton can be bound at a time, not two. Thus, the states $S_{x_1,1,1,x_4,x_5,x_6}$ are not allowed.

   So, there are only 36 allowed states. A possible enumeration of these 36 states is

   $$\sigma = 12(2x_2 + x_3) + 4(x_1 + x_5) + 2x_4 + x_6 + 1, \tag{6}$$

   with the requirement that $x_1 = 0$ and $x_5 = 1$ is not allowed and $x_2 = x_3 = 1$ is not allowed.

Some transitions are restricted.

1. E148 must be protonated to allow for transfer between Scen and Sout. This means the transition between $S_{x_1,0,x_3,1,0,x_6}$ and $S_{x_1,0,x_3,0,1,x_6}$ is not permitted. These are $7 \leftrightarrow 9$, $8 \leftrightarrow 10$, $19 \leftrightarrow 21$, $20 \leftrightarrow 22$.

2. The proton transfer $S_{1,1,0,0,0,x_1}$ to $S_{1,0,1,0,0,x_1}$ is not permitted. This is the transition $29 \rightarrow 17$, and $30 \rightarrow 18$.

3. The proton transfer $S_{1,0,1,x_4,0,x_6}$ to $S_{1,1,0,x_4,0,x_6}$ is not permitted . These are $17 \rightarrow 29$, $18 \rightarrow 30$, $19 \rightarrow 31$, $20 \rightarrow 32$.

4. The proton transfer $S_{1,0,1,1,x_5,x_6}$ to $S_{1,1,0,1,x_5,x_6}$ is not permitted. These are $19 \rightarrow 31$, $20 \rightarrow 32$, $23 \rightarrow 35$, $24 \rightarrow 36$.

Remark: The code has a reaction from a state that is not permitted.
There are 12 states that are never used. These are
100001 100101 1001 1101 101000 101001 101100 101101 101011 101111 110001 110101