

## Electronic Supplementary Information for: Stoichiometric Network Analysis in Reaction Networks Yielding Spontaneous Mirror Symmetry Breaking in Prebiotic Atmosphere

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The extreme currents matrix  $\mathbf{E}$  and the explicit extreme currents of KNS-LES, KNSCI and KNSCI-LES models

Extreme currents matrix  $\mathbf{E}$  of KNS-LES model.

$$\mathbf{E} = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 1 & 0 & 0 & 0 & 1 & 0 & 1 \\ 0 & 1 & 0 & 0 & 1 & 1 \\ 0 & 0 & 1 & 0 & 0 & 1 & 0 & 0 & 0 & 1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 1 & 0 & 0 & 0 & 1 & 0 & 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 & 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 1 & 0 & 0 & 0 & 1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 1 & 0 & 0 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 1 & 0 & 0 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 1 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 1 & 1 & 0 \end{pmatrix},$$

here, the columns are the extreme currents  $E_p$  ( $p = 1, \dots, 24$ ), from left to right, and the rows denote the reactions  $R_j$  ( $j = 1, \dots, 14$ ) from top to bottom. We verified that  $\nu\mathbf{E} = \mathbf{0}$  ( $\Leftrightarrow \nu\mathbf{v} = \mathbf{0}$ ). The explicit extreme currents of the stoichiometric network of KNS-LES model are in Table S1.

**Table S1.** Extreme currents of KNS - LES model.

$E_i$	Subnetwork	Reactions
$E_1$	$INH + HCN + L-CN \rightarrow L-CN + D-CN, D-CN \rightarrow D-AA + NH_3$	$R_{11}, R_{14}$
$E_2$	$INH + HCN + D-CN \rightarrow 2D-CN, D-CN \rightarrow D-AA + NH_3$	$R_7, R_{14}$
$E_3$	$INH + HCN \rightarrow D-CN, D-CN \rightarrow D-AA + NH_3$	$R_3, R_{14}$
$E_4$	$INH + HCN + L-CN \rightarrow L-CN + D-CN, L-CN + D-CN \rightarrow INH + HCN + L-CN$	$R_{11}, R_{12}$
$E_5$	$INH + HCN + D-CN \rightarrow 2D-CN, D-CN + L-CN \rightarrow L-CN + INH + HCN$	$R_7, R_{12}$
$E_6$	$INH + HCN \rightarrow D-CN, D-CN + L-CN \rightarrow L-CN + INH + HCN$	$R_3, R_{12}$
$E_7$	$INH + HCN + L-CN \rightarrow L-CN + D-CN, 2D-CN \rightarrow INH + HCN + D-CN$	$R_{11}, R_8$
$E_8$	$INH + HCN + L-CN \rightarrow L-CN + D-CN, D-CN \rightarrow INH + HCN$	$R_{11}, R_4$
$E_9$	$INH + HCN + D-CN \rightarrow 2D-CN, 2D-CN \rightarrow INH + HCN + D-CN$	$R_7, R_8$
$E_{10}$	$INH + HCN \rightarrow D-CN, 2D-CN \rightarrow INH + HCN + D-CN$	$R_3, R_8$
$E_{11}$	$INH + HCN + D-CN \rightarrow 2D-CN, D-CN \rightarrow INH + HCN$	$R_7, R_4$
$E_{12}$	$INH + HCN \rightarrow D-CN, D-CN \rightarrow INH + HCN$	$R_3, R_4$
$E_{13}$	$INH + HCN + D-CN \rightarrow D-CN + L-CN, L-CN \rightarrow L-AA + NH_3$	$R_9, R_{13}$
$E_{14}$	$INH + HCN + L-CN \rightarrow 2L-CN, L-CN \rightarrow L-AA + NH_3$	$R_5, R_{13}$
$E_{15}$	$INH + HCN \rightarrow L-CN, L-CN \rightarrow L-AA + NH_3$	$R_1, R_{13}$
$E_{16}$	$INH + HCN + D-CN \rightarrow D-CN + L-CN, D-CN + L-CN \rightarrow INH + HCN + D-CN$	$R_9, R_{10}$
$E_{17}$	$INH + HCN + L-CN \rightarrow 2L-CN, L-CN + D-CN \rightarrow D-CN + INH + HCN$	$R_5, R_{10}$
$E_{18}$	$INH + HCN \rightarrow L-CN, L-CN + D-CN \rightarrow D-CN + INH + HCN$	$R_1, R_{10}$
$E_{19}$	$INH + HCN + D-CN \rightarrow D-CN + L-CN, 2L-CN \rightarrow INH + HCN + L-CN$	$R_9, R_6$
$E_{20}$	$INH + HCN + D-CN \rightarrow D-CN + L-CN, L-CN \rightarrow INH + HCN$	$R_9, R_2$
$E_{21}$	$INH + HCN + L-CN \rightarrow 2L-CN, 2L-CN \rightarrow INH + HCN + L-CN$	$R_5, R_6$
$E_{22}$	$INH + HCN \rightarrow L-CN, 2L-CN \rightarrow INH + HCN + L-CN$	$R_1, R_6$
$E_{23}$	$INH + HCN + L-CN \rightarrow 2L-CN, L-CN \rightarrow INH + HCN$	$R_5, R_2$
$E_{24}$	$INH + HCN \rightarrow L-CN, L-CN \rightarrow INH + HCN$	$R_1, R_2$

Extreme currents matrix  $\mathbf{E}$  of KNSCI model.

$$\mathbf{E} = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 1 & 1 & 1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 1 & 0 & 0 \\ 0 & 1 & 0 & 1 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 1 \\ 0 & 0 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 1 & 1 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 1 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 1 & 0 \\ 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 1 & 0 & 1 & 1 & 1 \end{pmatrix},$$

each extreme current  $E_p$  ( $p = 1, \dots, 12$ ) represents a column vector of the matrix  $\mathbf{E}$ . The explicit extreme currents of KNSCI model are in Table S2.

**Table S2.** Extreme currents of KNSCI model.

$E_i$	Subnetwork	Reactions
$E_1$	$INH + HCN + D-CN \rightarrow 2D-CN \rightarrow INH + HCN + D-CN$	$R_7, R_8$
$E_2$	$INH + HCN \rightarrow D-CN \xrightarrow{D-CN} INH + HCN + D-CN$	$R_3, R_8$
$E_3$	$INH + HCN + D-CN \rightarrow 2D-CN \xrightarrow{-D-CN} INH + HCN$	$R_7, R_4$
$E_4$	$INH + HCN \rightarrow D-CN \rightarrow INH + HCN$	$R_3, R_4$
$E_5$	$INH + HCN + L-CN \rightarrow 2L-CN \rightarrow INH + HCN + L-CN$	$R_5, R_6$
$E_6$	$INH + HCN \rightarrow L-CN \xrightarrow{L-CN} INH + HCN + L-CN$	$R_1, R_6$
$E_7$	$INH + HCN + L-CN \rightarrow 2L-CN \xrightarrow{-L-CN} INH + HCN$	$R_5, R_2$
$E_8$	$INH + HCN + D-CN \rightarrow 2D-CN$ $\xrightarrow{-D-CN, -L-CN} D, L-ADCN + NH_3$	$R_5, R_7, R_9$
$E_9$	$INH + HCN + L-CN \rightarrow 2L-CN$ $\xrightarrow{-L-CN} D, L-ADCN + NH_3$	$R_3, R_5, R_9$
$E_{10}$	$INH + HCN \rightarrow L-CN \rightarrow INH + HCN$ $INH + HCN \rightarrow L-CN$	$R_1, R_2$
$E_{11}$	$INH + HCN + D-CN \rightarrow 2D-CN$ $\xrightarrow{-D-CN} D, L-ADCN + NH_3$ $INH + HCN \rightarrow D-CN$	$R_1, R_7, R_9$
$E_{12}$	$\xrightarrow{\quad} D, L-ADCN + NH_3$ $INH + HCN \rightarrow L-CN$	$R_1, R_3, R_9$

Extreme currents matrix  $\mathbf{E}$  of KNSCI-LES model.

$$\mathbf{E} = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 1 & 1 & 1 & 1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 1 & 1 & 1 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 1 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 1 & 1 & 1 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 1 & 0 & 0 \\ 1 & 1 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 1 & 1 & 0 & 0 & 0 & 1 & 1 & 1 & 0 & 1 & 1 & 1 \end{pmatrix},$$

each extreme current  $E_p$  ( $p = 1, \dots, 27$ ) represents a column vector of matrix  $\mathbf{E}$ . The explicit extreme currents of KNSCI-LES model are in Table S3.

**Table S3.** Extreme currents of KNSIC-LES model.

$E_i$	Subnetwork	Reactions
$E_1$	$INH + HCN + L-CN \rightarrow D-CN + L-CN \rightarrow INH + HCN + L-CN$	$R_{11}, R_{12}$
$E_2$	$INH + HCN + D-CN \rightarrow 2D-CN \xrightarrow[-D-CN]{L-CN} INH + HCN + L-CN$	$R_7, R_{12}$
$E_3$	$INH + HCN \rightarrow D-CN \xrightarrow{L-CN} INH + HCN + L-CN$	$R_3, R_{13}$
$E_4$	$INH + HCN + L-CN \rightarrow D-CN + L-CN \xrightarrow[-L-CN]{D-CN} INH + HCN + D-CN$	$R_8, R_{11}$
$E_5$	$INH + HCN + L-CN \rightarrow D-CN + L-CN \xrightarrow[-L-CN]{L-CN} INH + HCN$	$R_4, R_{11}$
$E_6$	$INH + HCN + D-CN \rightarrow 2D-CN \rightarrow INH + HCN + D-CN$	$R_7, R_8$
$E_7$	$INH + HCN \rightarrow D-CN \xrightarrow{D-CN} INH + HCN + D-CN$	$R_3, R_8$
$E_8$	$INH + HCN + D-CN \rightarrow 2D-CN \xrightarrow{-D-CN} INH + HCN$	$R_7, R_4$
$E_9$	$INH + HCN \rightarrow D-CN \rightarrow INH + HCN$	$R_3, R_4$
$E_{10}$	$INH + HCN + D-CN \rightarrow D-CN + L-CN \rightarrow INH + HCN + D-CN$	$R_9, R_{10}$
$E_{11}$	$INH + HCN + L-CN \rightarrow 2L-CN \xrightarrow[-L-CN]{D-CN} INH + HCN + D-CN$	$R_5, R_{10}$
$E_{12}$	$INH + HCN \rightarrow L-CN \xrightarrow{D-CN} INH + HCN + D-CN$	$R_1, R_{10}$
$E_{13}$	$INH + HCN + D-CN \rightarrow D-CN + L-CN \xrightarrow[-D-CN]{L-CN} INH + HCN + L-CN$	$R_9, R_6$
$E_{14}$	$INH + HCN + D-CN \rightarrow D-CN + L-CN \xrightarrow[-D-CN]{-D-CN} INH + HCN$	$R_4, R_{11}$
$E_{15}$	$INH + HCN + D-CN \rightarrow L-CN + D-CN$ $\xrightarrow[-L-CN]{-D-CN} D, L-ADCN$ $INH + HCN + L-CN \rightarrow D-CN + L-CN$	$R_9, R_{11}, R_{13}$
$E_{16}$	$INH + HCN + D-CN \rightarrow 2D-CN$ $\xrightarrow{-2D-CN} D, L-ADCN$ $INH + HCN + D-CN \rightarrow D-CN + L-CN$ $INH + HCN \rightarrow D-CN$	$R_7, R_9, R_{13}$
$E_{17}$	$INH + HCN + D-CN \rightarrow D-CN + L-CN$ $\xrightarrow{-D-CN} D, L-ADCN$	$R_3, R_9, R_{13}$
$E_{18}$	$INH + HCN + D-CN \rightarrow 2L-CN \rightarrow INH + HCN + L-CN$	$R_5, R_6$
$E_{19}$	$INH + HCN \rightarrow L-CN \xrightarrow{L-CN} INH + HCN + L-CN$	$R_1, R_6$
$E_{20}$	$INH + HCN + L-CN \rightarrow 2L-CN \xrightarrow{-L-CN} INH + HCN$ $INH + HCN + L-CN \rightarrow 2L-CN$	$R_5, R_2$
$E_{21}$	$INH + HCN + L-CN \rightarrow L-CN + D-CN$ $\xrightarrow{-2L-CN} D, L-ADCN$ $INH + HCN + L-CN \rightarrow 2L-CN$	$R_5, R_{11}, R_{13}$
$E_{22}$	$INH + HCN + L-CN \rightarrow L-CN + D-CN$ $\xrightarrow[-L-CN]{-D-CN} D, L-ADCN$ $INH + HCN + D-CN \rightarrow 2D-CN$ $INH + HCN \rightarrow D-CN$	$R_5, R_7, R_{13}$
$E_{23}$	$INH + HCN + L-CN \rightarrow 2L-CN$ $\xrightarrow{-L-CN} D, L-ADCN$	$R_3, R_5, R_{13}$
$E_{24}$	$INH + HCN \rightarrow L-CN \rightarrow INH + HCN$ $INH + HCN \rightarrow L-CN$	$R_1, R_2$
$E_{25}$	$INH + HCN + L-CN \rightarrow L-CN + D-CN$ $\xrightarrow{-L-CN} D, L-ADCN$ $INH + HCN \rightarrow L-CN$	$R_1, R_{11}, R_{13}$
$E_{26}$	$INH + HCN + D-CN \rightarrow 2D-CN$ $\xrightarrow{-D-CN} D, L-ADCN$ $INH + HCN \rightarrow L-CN$	$R_1, R_7, R_{13}$
$E_{27}$	$INH + HCN \rightarrow D-CN$ $\rightarrow D, L-ADCN$	$R_1, R_3, R_{13}$