

# Bond Graph Representation of Complexes: Bringing Graph Theory to Bond Graphs

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Note: this is the `Complexes.ipynb` notebook. The PDF version "Bond Graph Representation of Complexes: Bringing Graph Theory to Bond Graphs" is available [here](#).

## 1 Introduction

Chemical Reaction Network theory (Feinberg, 1972; Horn and Jackson, 1972; Feinberg and Horn, 1974; van der Schaft et al., 2013, 2015, 2016) uses the formal concept of *complexes*.

Complexes are the combination of chemical species forming the substrate and products of the network reactions. In particular, the stoichiometric matrix  $N$  can be decomposed as:

$$N = ZD \quad (1)$$

where  $Z$  relates complexes to species and  $D$  is the *incidence matrix* of the directed graph formed by taking the complexes to be vertices and the reactions to be edges. This digraph can then be analysed using standard graph theory.

This notion can be given a bond graph interpretation (Gawthrop and Crampin, 2018). This notebook illustrates complexes using examples from this paper; please see the paper for further explanation.

As noted by (Gawthrop and Crampin, 2018) the digraphs for systems with and without chemostats are very different and so both are shown in the following examples. The digraphs associated with chemostats are related to bond graph pathway analysis (Gawthrop and Crampin, 2017); for each of the three examples the corresponding pathways are given.

### 1.1 Import some python code

The bond graph analysis uses a number of Python modules:

```
In [1]: ## Some useful imports
import BondGraphTools as bgt
import numpy as np
import sympy as sp
import matplotlib.pyplot as plt
import IPython.display as disp

## Stoichiometric analysis
import stoich as st

## SVG bg representation conversion
import svgBondGraph as sbg

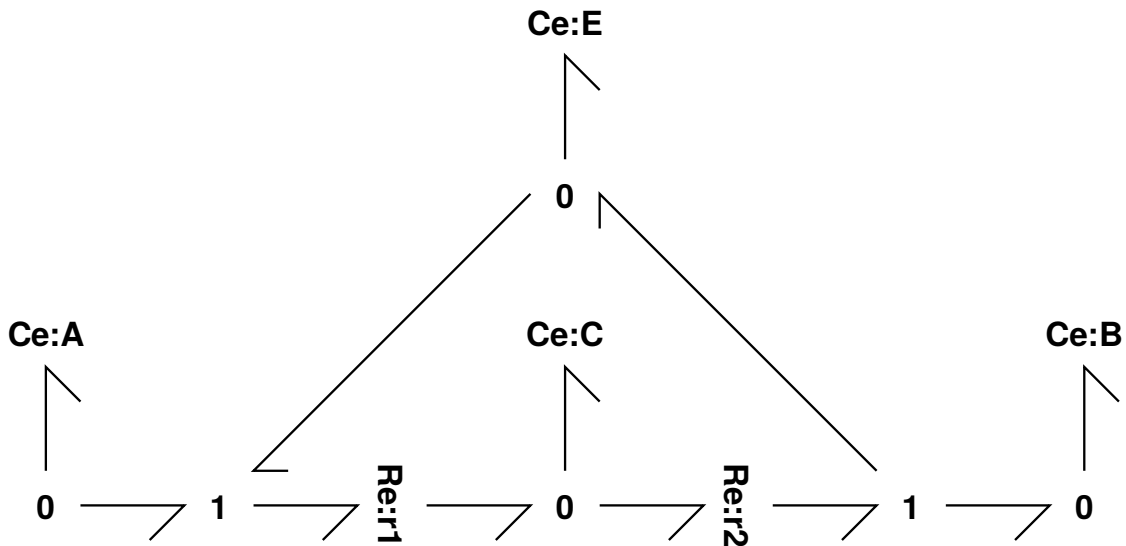
## Set quiet=False for verbose output
quiet = True
```

## 2 Example 1: enzyme-catalysed reaction

The bond graph representation of the (reversible) enzyme-catalysed reaction is (Gawthrop and Crampin, 2018):

```
In [2]: disp.SVG('RE_abg.svg')
```

Out[2]:



This graphical representation may be converted to [bond-graph tools](#) format using

```
In [3]: sbg.model('RE_abg.svg')
import RE_abg
```

## 2.1 Reactions

The reactions corresponding to this system are:

```
In [4]: s = st.stoich(RE_abg.model(), quiet=quiet)
disp.Latex(st.sprintrl(s, chemformula=True))
```

Out[4]:



## 2.2 Stoichiometric matrix and its decomposition

```
In [5]: disp.Latex(st.sprintrl(s, 'species'))
```

Out[5]:

$$X = \begin{pmatrix} X_A \\ X_B \\ X_C \\ X_E \end{pmatrix} \quad (4)$$

```
In [6]: disp.Latex(st.sprintl(s, 'reaction'))
```

```
Out[6]:
```

$$V = \begin{pmatrix} V_{r1} \\ V_{r2} \end{pmatrix} \quad (5)$$

```
In [7]: disp.Latex(st.sprintl(s, 'N'))
```

```
Out[7]:
```

$$N = \begin{pmatrix} -1 & 0 \\ 0 & 1 \\ 1 & -1 \\ -1 & 1 \end{pmatrix} \quad (6)$$

```
In [8]: disp.Latex(st.sprintl(s, 'Z'))
```

```
Out[8]:
```

$$Z = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \\ 1 & 0 & 1 \end{pmatrix} \quad (7)$$

```
In [9]: disp.Latex(st.sprintl(s, 'D'))
```

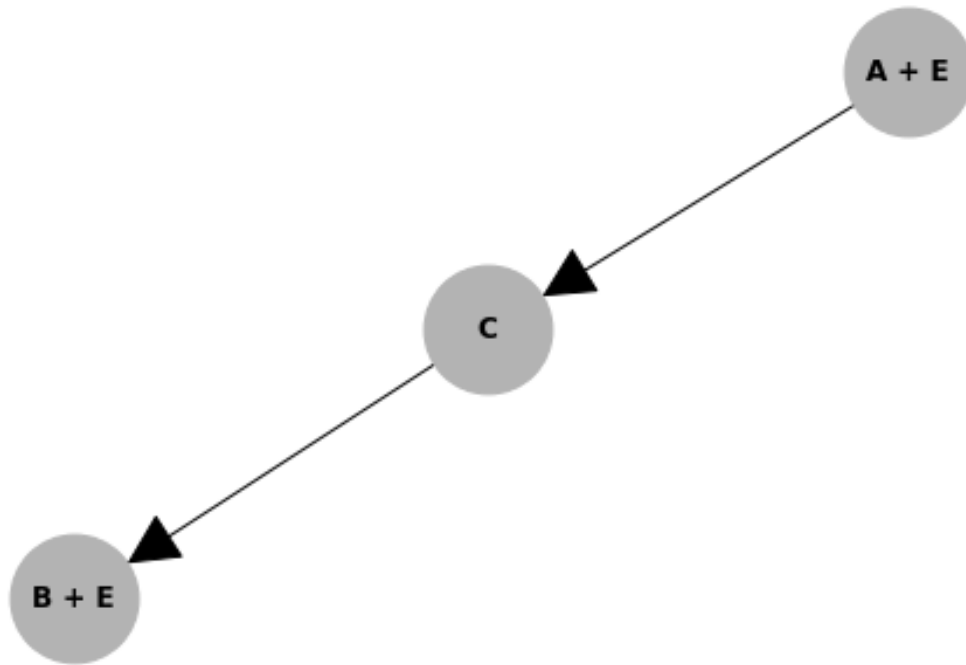
```
Out[9]:
```

$$D = \begin{pmatrix} -1 & 0 \\ 1 & -1 \\ 0 & 1 \end{pmatrix} \quad (8)$$

## 2.3 System digraph

```
In [10]: st.draw(s)
```

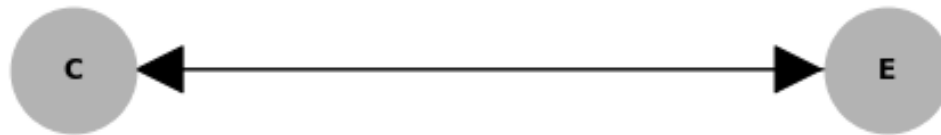
RE (0 cycles)



## 2.4 System digraph (with chemostats)

```
In [11]: chemostats = ['A', 'B']  
         sc = st.statify(s, chemostats=chemostats)  
         st.draw(sc)
```

RE (1 cycle)



## 2.5 Pathway analysis

```
In [12]: sp = st.path(s,sc)
         print(st.sprintp(sc))
         disp.Latex(st.sprintrl(sp,chemformula=True))
```

```
1 pathways
0: + r1 + r2
```

Out[12]:

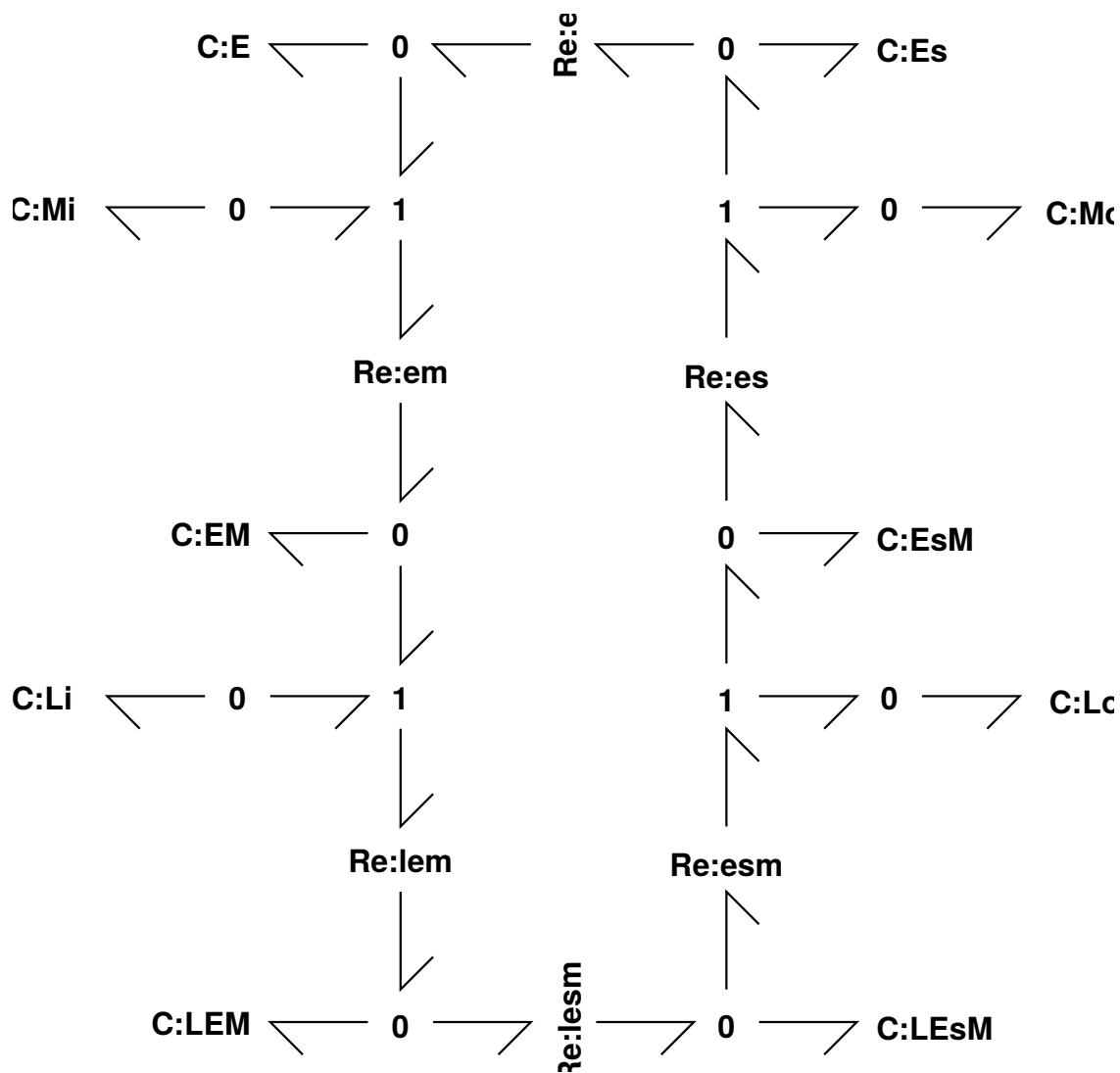


## 3 Example 2: Transporter

This example looks at bond graph representation of a membrane transporter which is discussed in detail by (Gawthrop and Crampin, 2017) and analysed by (Gawthrop and Crampin, 2018).

```
In [13]: disp.SVG('Hill_abg.svg')
```

Out[13]:



This graphical representation may be converted to [bond-graph tools](#) format using

```
In [14]: sbg.model('Hill_abg.svg')
import Hill_abg
```

### 3.1 Reactions

The reactions corresponding to this system are:

```
In [15]: s = st.stoich(Hill_abg.model(), quiet=True)
disp.Latex(st.sprintrl(s, chemformula=True))
```

Out[15]:



### 3.2 Stoichiometric matrix and its decomposition

In [16]: `disp.Latex(st.sprintl(s, 'species'))`

Out[16]:

$$X = \begin{pmatrix} X_E \\ X_{EM} \\ X_{Es} \\ X_{EsM} \\ X_{LEM} \\ X_{LEsM} \\ X_{Li} \\ X_{Lo} \\ X_{Mi} \\ X_{Mo} \end{pmatrix} \quad (16)$$

In [17]: `disp.Latex(st.sprintl(s, 'reaction'))`

Out[17]:

$$V = \begin{pmatrix} V_e \\ V_{em} \\ V_{es} \\ V_{esm} \\ V_{lem} \\ V_{lesm} \end{pmatrix} \quad (17)$$

In [18]: `disp.Latex(st.sprintl(s, 'N'))`

Out[18]:



$$N = \begin{pmatrix} 1 & -1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & -1 & 0 \\ -1 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & -1 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & -1 \\ 0 & 0 & 0 & -1 & 0 & 1 \\ 0 & 0 & 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & -1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \end{pmatrix} \quad (18)$$

In [19]: `disp.Latex(st.sprintl(s, 'Z'))`

Out[19]:

$$Z = \begin{pmatrix} 0 & 1 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \end{pmatrix} \quad (19)$$

In [20]: `disp.Latex(st.sprintl(s, 'D'))`

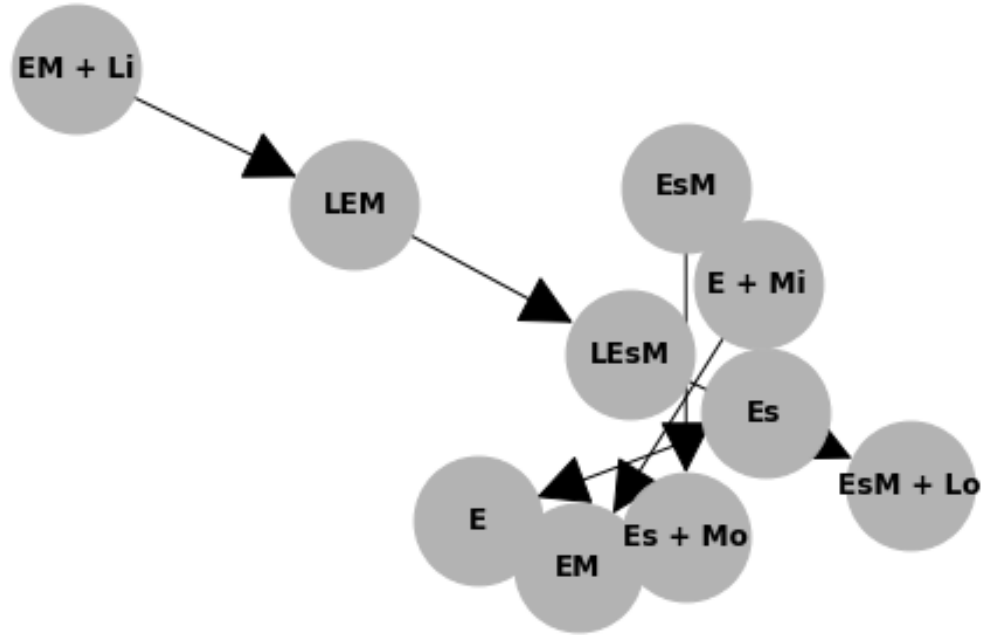
Out[20]:

$$D = \begin{pmatrix} -1 & 0 & 0 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 & 0 & 0 \\ 0 & 0 & -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 & 0 & 1 \\ 0 & 0 & 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 0 & 1 & -1 \\ 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \end{pmatrix} \quad (20)$$

### 3.3 System digraph

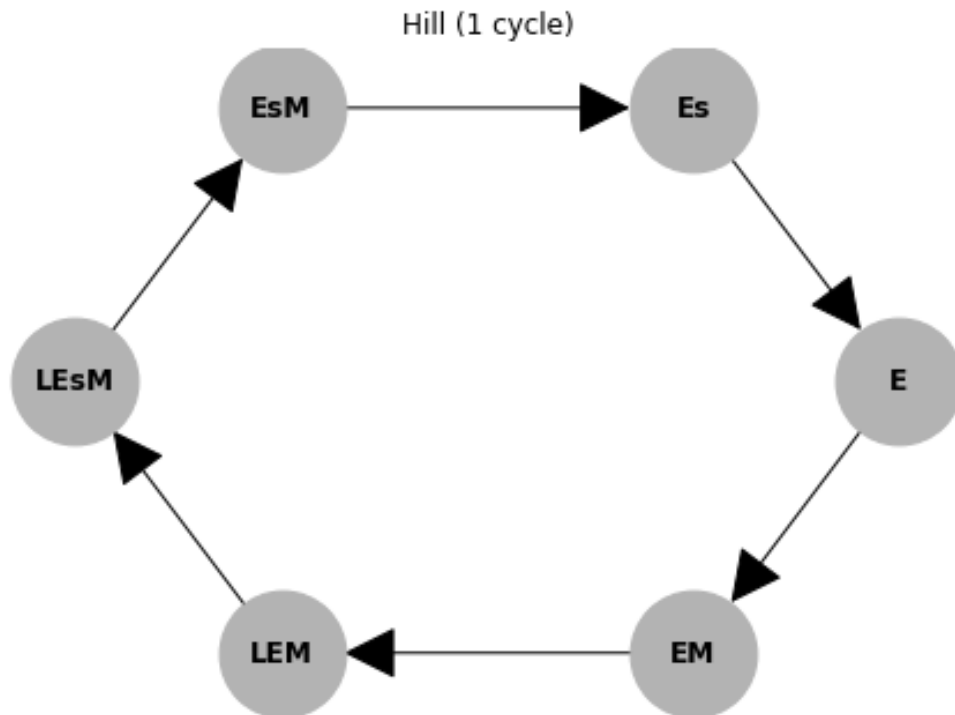
In [21]: `st.draw(s)`

Hill (0 cycles)



### 3.4 System digraph (with chemostats)

```
In [22]: chemostats = ['Mi', 'Mo', 'Li', 'Lo']  
sc = st.statify(s, chemostats=chemostats)  
st.draw(sc)
```



### 3.5 Pathway analysis

```
In [23]: sp = st.path(s,sc)
         print(st.sprintp(sc))
         disp.Latex(st.sprintrl(sp,chemformula=True))
```

1 pathways

0: + e + em + es + esm + lem + lesm

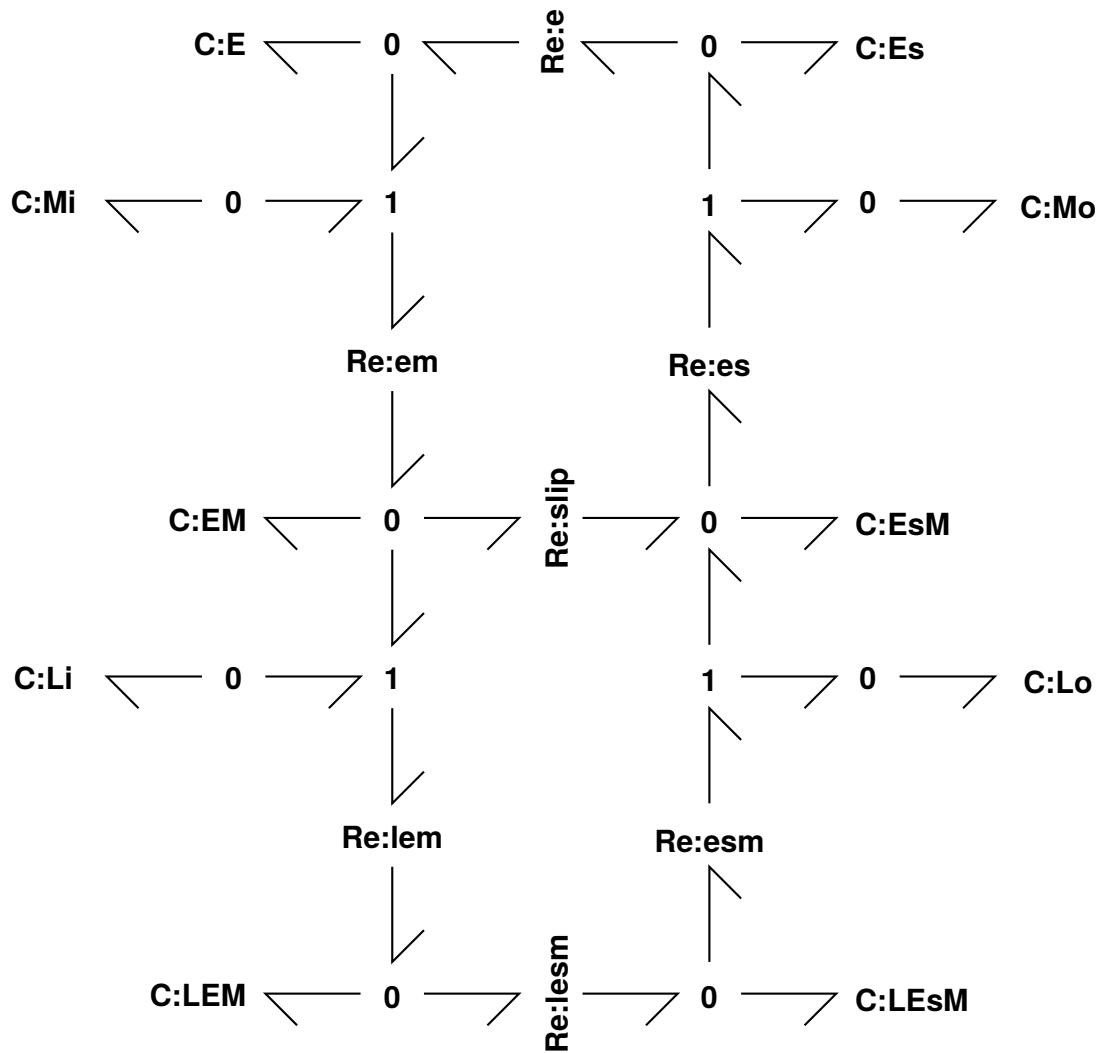
Out[23]:



## 4 Example 3: Transporter with slippage

```
In [24]: sbg.model('Hills_abg.svg')
         import Hills_abg
         disp.SVG('Hills_abg.svg')
```

Out[24]:



## 4.1 Reactions

The reactions corresponding to this system are:

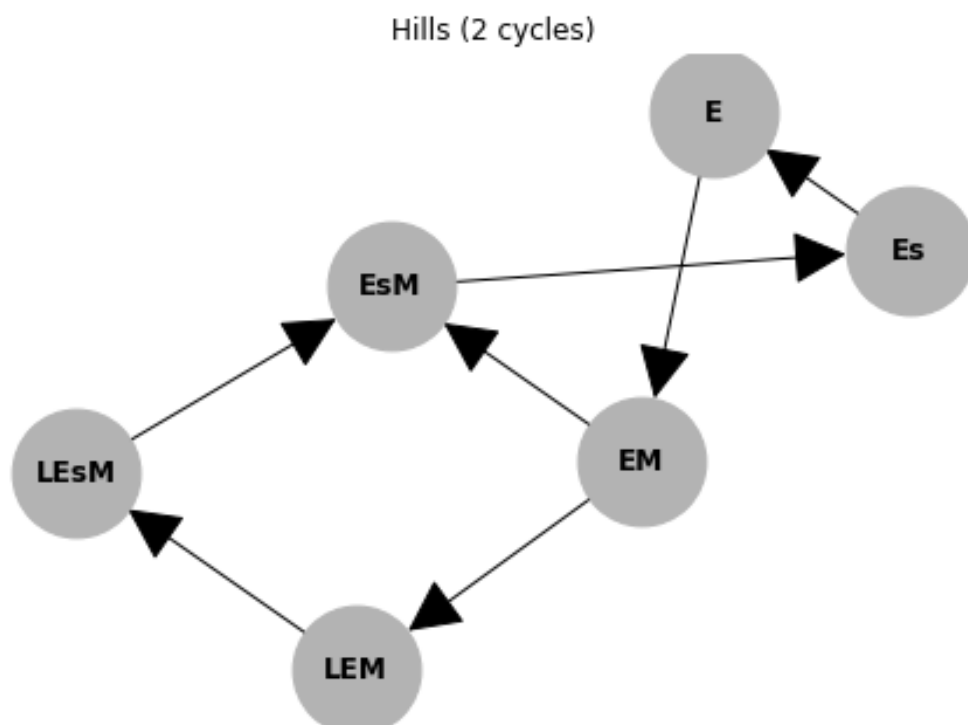
```
In [25]: s = st.stoich(Hills_abg.model(), quiet=quiet)
         disp.Latex(st.sprintrl(s, chemformula=True))
```

Out [25]:



## 4.2 System digraph (with chemostats)

```
In [26]: chemostats = ['Mi', 'Mo', 'Li', 'Lo']
         sc = st.statify(s, chemostats=chemostats)
         st.draw(sc)
```



## 4.3 Pathway analysis

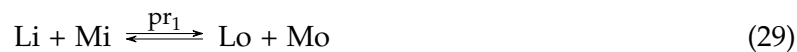
```
In [27]: sp = st.path(s, sc)
         print(st.sprintp(sc))
         disp.Latex(st.sprintrl(sp, chemformula=True))
```

2 pathways

0: + e + em + es + esm + lem + lesm

1: + e + em + es + slip

Out [27] :



## References

- Martin Feinberg. On chemical kinetics of a certain class. *Archive for Rational Mechanics and Analysis*, 46(1):1–41, 1972. ISSN 0003-9527. doi:[10.1007/BF00251866](https://doi.org/10.1007/BF00251866).
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- P. Gawthrop and E. J. Crampin. Bond graph representation of chemical reaction networks. *IEEE Transactions on NanoBioscience*, 17(4):449–455, October 2018. ISSN 1536-1241. doi:[10.1109/TNB.2018.2876391](https://doi.org/10.1109/TNB.2018.2876391). Available at arXiv:1809.00449.
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- Arjan van der Schaft, Shodhan Rao, and Bayu Jayawardhana. Complex and detailed balancing of chemical reaction networks revisited. *Journal of Mathematical Chemistry*, 53(6):1445–1458, Jun 2015. ISSN 1572-8897. doi:[10.1007/s10910-015-0498-2](https://doi.org/10.1007/s10910-015-0498-2).