Additional material for: Network Thermodynamics of Biological Systems: A Bond Graph Approach. *Part 1: Reaction modelling*

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Contents

1 Introduction

- This document contains additional material for the paper: *Network Thermodynamics of Biological Systems: A Bond Graph Approach* by Peter Gawthrop and Michael Pan.
- It illustrates how the Python package BondGraphTools can be used to create and analyse chemical reaction networks.
- It provides background to Section 3, Chemical Reactions.
- This document is **Reactions.pdf** (see also **Chloroplast.pdf**).
- The document is available as the Jupyter notebook **Reactions.ipynb**.
- Code is available at https://github.com/gawthrop/GawPan22

1.1 Some useful imports

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

## Stoichiometric analysis
import stoich as st

## SVG bg representation conversion
import svgBondGraph as sbg

## Modular bond graphs
import modularBondGraph as mbg

## Display (eg disp.SVG(), disp.
import IPython.display as disp

## Data
import phiData
import redoxData

import importlib as imp

## Some switches
chemformula = True
quiet = True
```

2 Basic reactions

2.1 A ⇔ B

2.1.1 Graphical bond graph representation

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

[2]:

2.1.2 Convert graphical representation to BondGraphTools representation

[3]:
```
# imp.reload(sbg)
sbg.model('ABbasic_abg.svg',quiet=quiet)
import ABbasic_abg
# imp.reload(ABbasic_abg)
```

2.1.3 Stoichiometric analysis and reactions

[4]:
```
## Stoichiometry
sABbasic = st.stoich(ABbasic_abg.model(),quiet=quiet)
disp.Latex(st.sprintrl(sABbasic,chemformula=chemformula))
```

[4]:

$$\mathrm{A} \underset{}{\overset{\mathrm{r}}{\rightleftharpoons}} \mathrm{B} \tag{1}$$

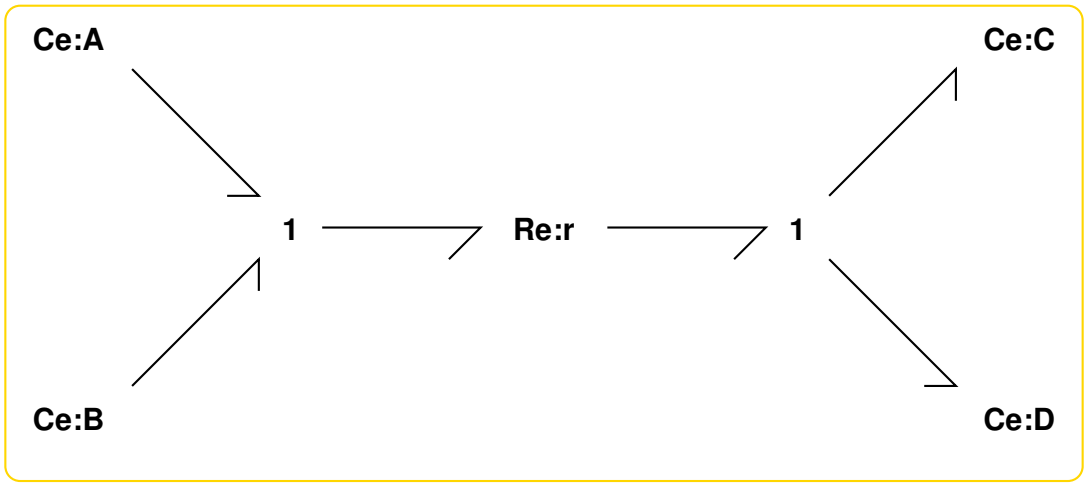
3 Reactions with connections

3.1 A + B ⇔ C + D

3.1.1 Graphical bond graph representation

[5]:
```
disp.SVG('ABCDbasic_abg.svg')
```

[5]:



3.1.2 Convert graphical representation to BondGraphTools representation

[6]:
```
# imp.reload(sbg)
sbg.model('ABCDbasic_abg.svg',quiet=quiet)
import ABCDbasic_abg
# imp.reload(ABCDbasic_abg)
```

3.1.3 Stoichiometric analysis and reactions

[7]:
```
## Stoichiometry
sABCDbasic = st.stoich(ABCDbasic_abg.model(),quiet=quiet)
disp.Latex(st.sprintrl(sABCDbasic,chemformula=chemformula))
```

[7]:

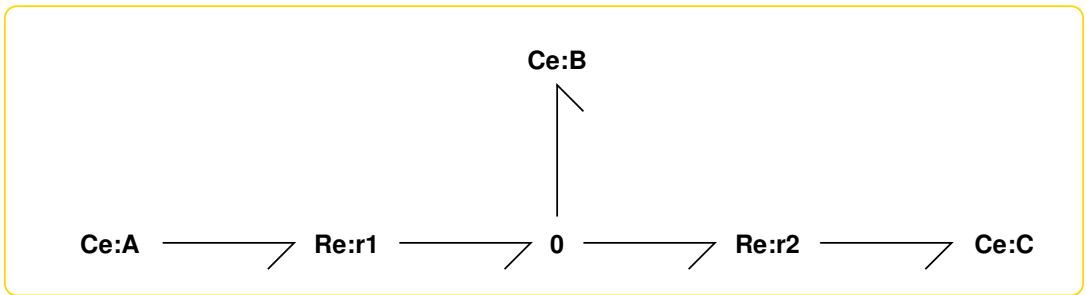
$$\mathrm{A} + \mathrm{B} \underset{}{\overset{\mathrm{r}}{\rightleftharpoons}} \mathrm{C} + \mathrm{D} \tag{2}$$

3.2 A ⇔ B ⇔ C

3.2.1 Graphical bond graph representation

[8]:
```
disp.SVG('ABCbasic_abg.svg')
```

[8]:



3.2.2 Convert graphical representation to BondGraphTools representation

[9]:
```
# imp.reload(sbg)
sbg.model('ABCbasic_abg.svg',quiet=quiet)
import ABCbasic_abg
# imp.reload(ABCbasic_abg)
```

3.2.3 Stoichiometric analysis and reactions

[10]:
```
## Stoichiometry
sABCbasic = st.stoich(ABCbasic_abg.model(),quiet=quiet)
disp.Latex(st.sprintrl(sABCbasic,chemformula=chemformula))
```

[10]:

$$\mathrm{A} \underset{}{\overset{r_1}{\rightleftharpoons}} \mathrm{B} \tag{3}$$

$$\mathrm{B} \underset{}{\overset{r_2}{\rightleftharpoons}} \mathrm{C} \tag{4}$$

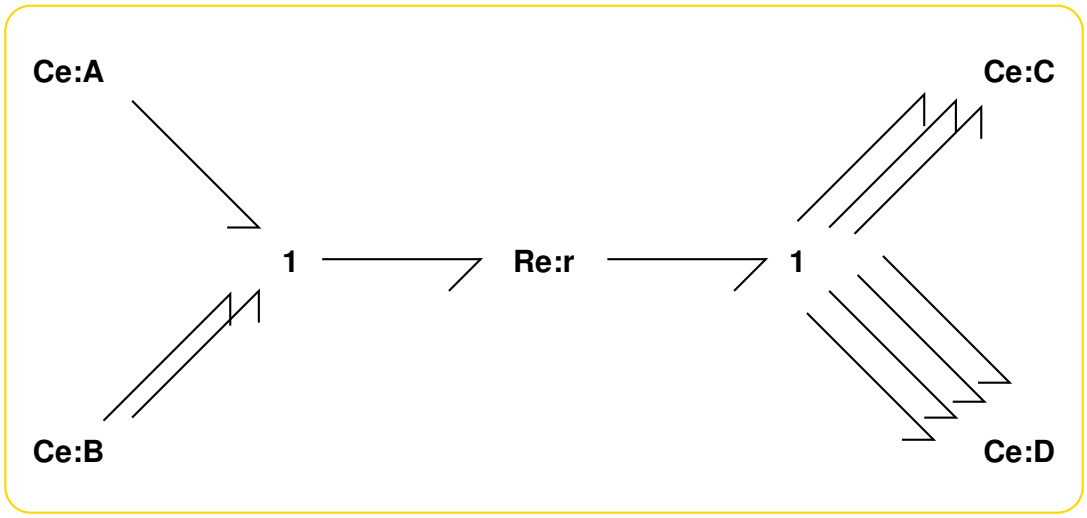
4 Multiple stoichiometry

4.1 A+2B ⇔ 3C+4D

4.1.1 Graphical bond graph representation

[11]:
```
disp.SVG('ABCDmult_abg.svg')
```

[11]:



4.1.2 Convert graphical representation to BondGraphTools representation

[12]:
```
# imp.reload(sbg)
sbg.model('ABCDmult_abg.svg',convertCe=True,quiet=quiet)
import ABCDmult_abg
# imp.reload(ABCDmult_abg)
```

4.1.3 Stoichiometric analysis and reactions

[13]:
```
## Stoichiometry
sABCDmult = st.stoich(ABCDmult_abg.model(),quiet=quiet)
disp.Latex(st.sprintrl(sABCDmult,chemformula=chemformula))
```

[13]:

$$A + 2B \underset{r}{\rightleftarrows} 3C + 4D \tag{5}$$

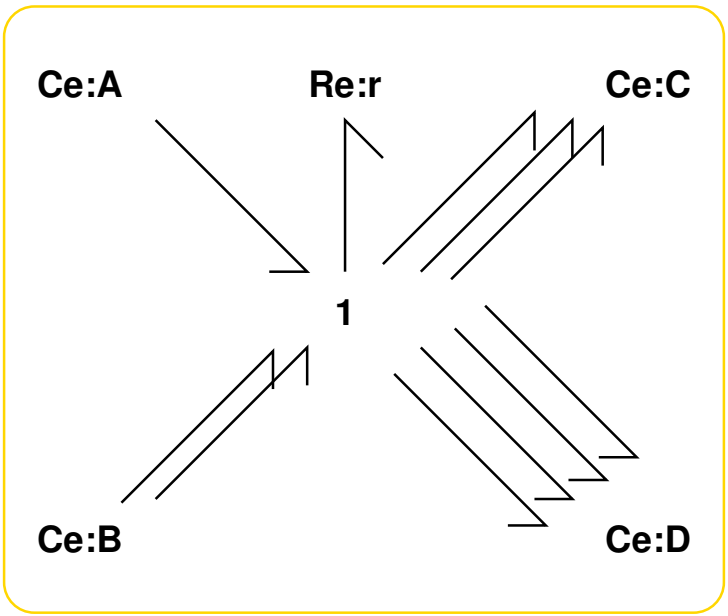
5 One-port Re component

5.1 A+2B ⇔ 3C+4D

5.1.1 Graphical bond graph representation

[14]:
```
disp.SVG('ABCDone_abg.svg')
```

[14]:



5.1.2 Convert graphical representation to BondGraphTools representation

[15]:
```
# imp.reload(sbg)
sbg.model('ABCDone_abg.svg',convertCe=True,convertR=True,quiet=quiet)
import ABCDone_abg
# imp.reload(ABCDone_abg)
```

5.1.3 Stoichiometric analysis and reactions

[16]:
```
## Stoichiometry
sABCDone = st.stoich(ABCDone_abg.model(),quiet=quiet)
disp.Latex(st.sprintrl(sABCDone,chemformula=chemformula))
```

[16]:

$$\mathrm{A} + 2\mathrm{B} \underset{}{\overset{r}{\rightleftharpoons}} 3\mathrm{C} + 4\mathrm{D} \tag{6}$$