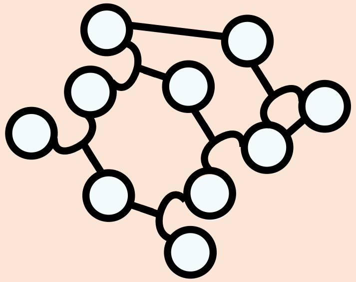
Some structural aspects of CRNS in theory and experiment

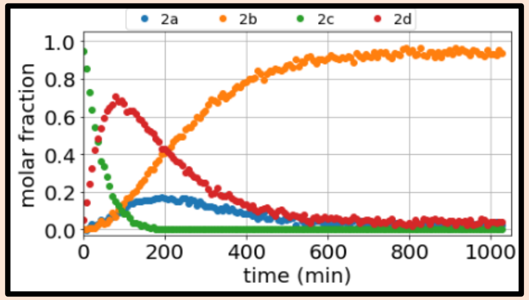
Alex Blokhuis

IMDEA Nanociencia, Madrid

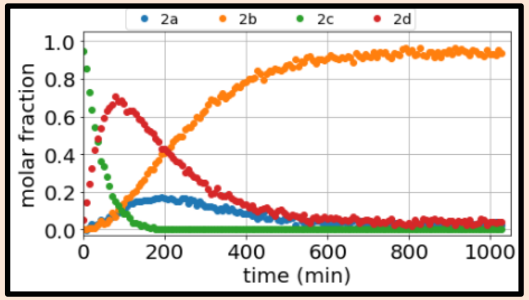
Chemical reaction networks, two problems

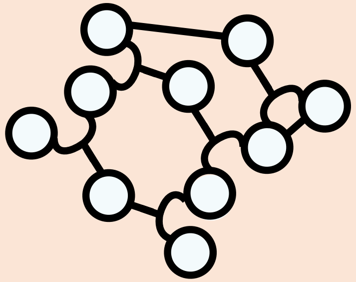
I) How does the structure of a CRN relate to what it can and cannot do?





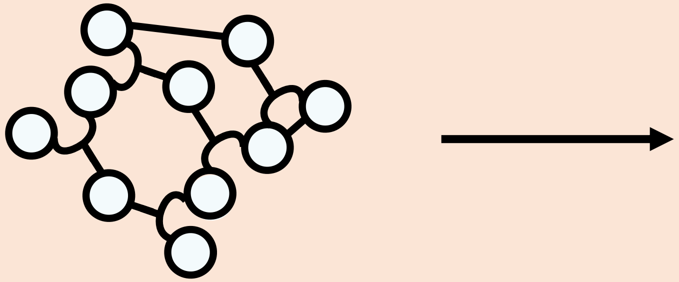
II) How do I know what CRN I'm looking at*?

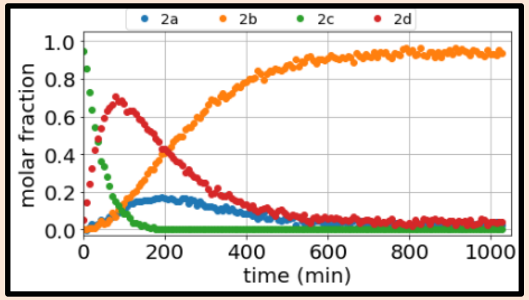




Chemical reaction networks in chemistry, two problems

I) How does the structure of a CRN relate to what it can and cannot do?

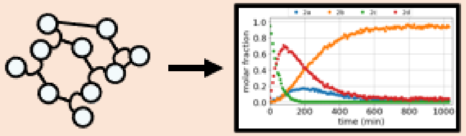




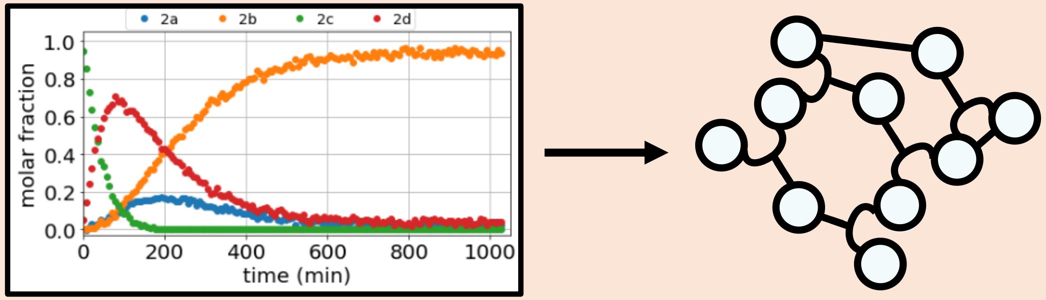
II) How do I know what CRN I'm looking at*?

*(*in a way where I can quantitatively account for all my experiments with a chemically sound description*)

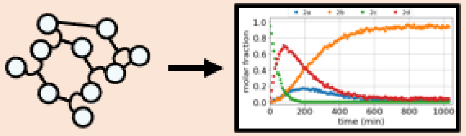
CRNs in Chemistry



- CRNs allow us to better understand chemistry.
- Chemistry provides clues towards understanding CRNs, and in turn better understanding dynamical systems.
- To pursue these goals, we need CRNs with ‘chemical’ properties



CRNs in Chemistry



What makes a reaction network “chemical”?

Stefan Müller[1], Christoph Flamm[2] and Peter F. Stadler[2,3,4,5,6,7*]

Müller *et al. Journal of Cheminformatics* (2022) 14:63
https://doi.org/10.1186/s13321-022-00621-8

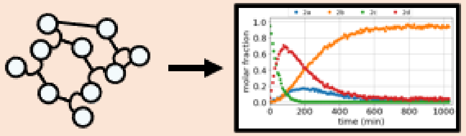
- To pursue these goals, we need CRNs with ‘chemical’ properties

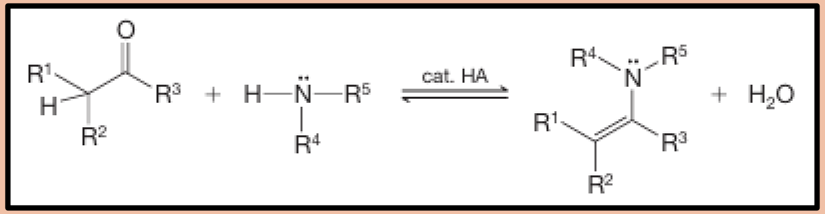
- What makes a reaction network chemical? [1]

Conservation laws with chemical interpretations, local energy conservation (detailed balance), …

- What else makes a reaction network ‘chemical’?

Chemists assume implicit detail





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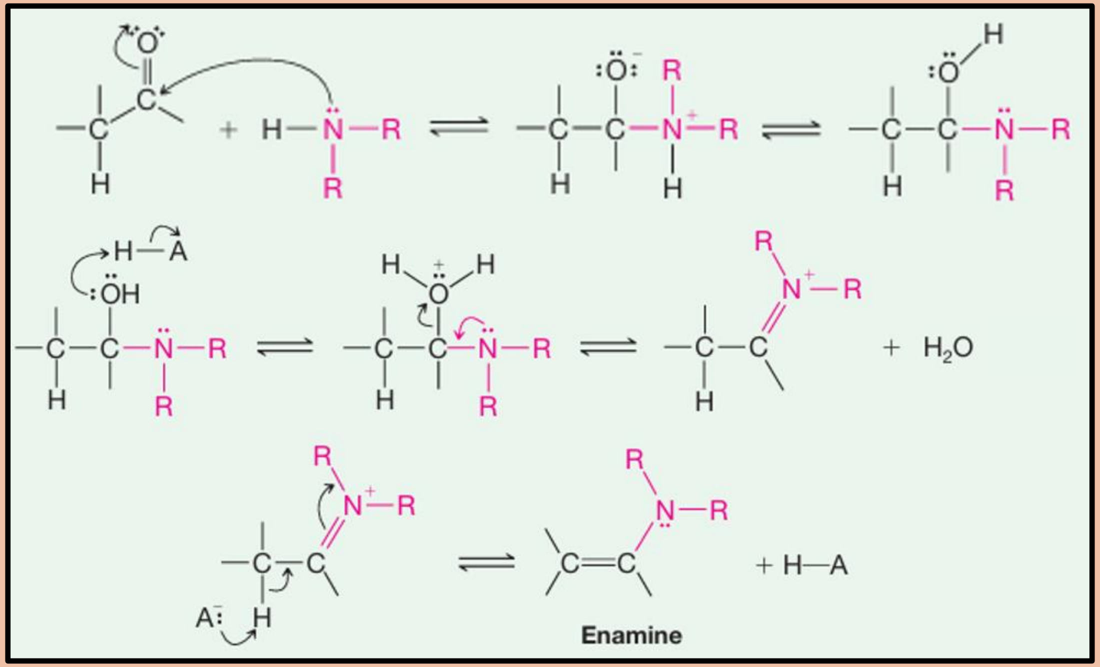
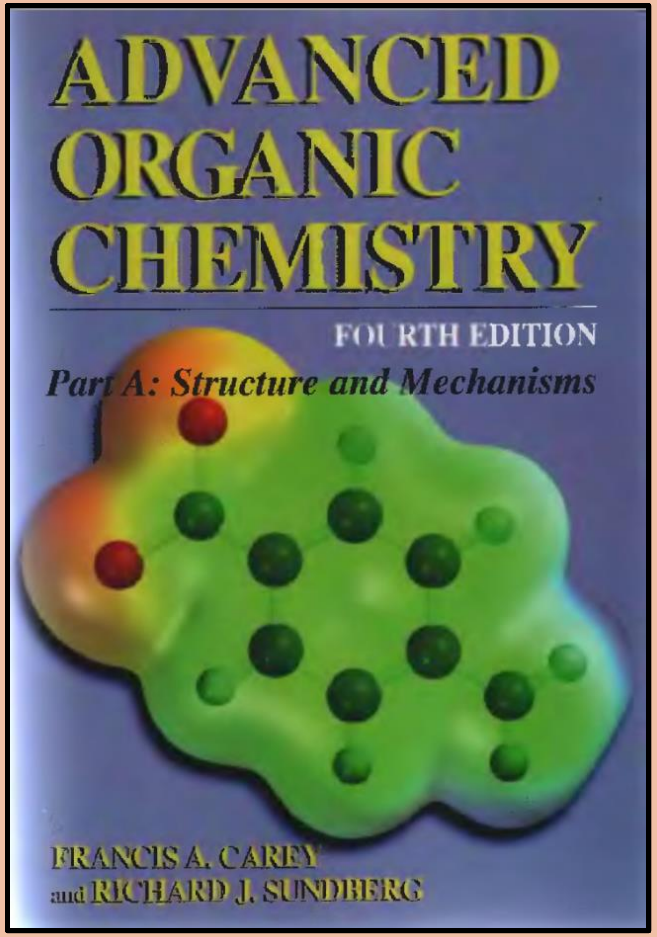
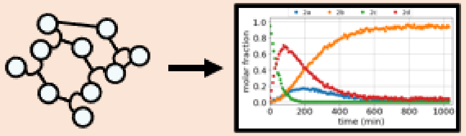
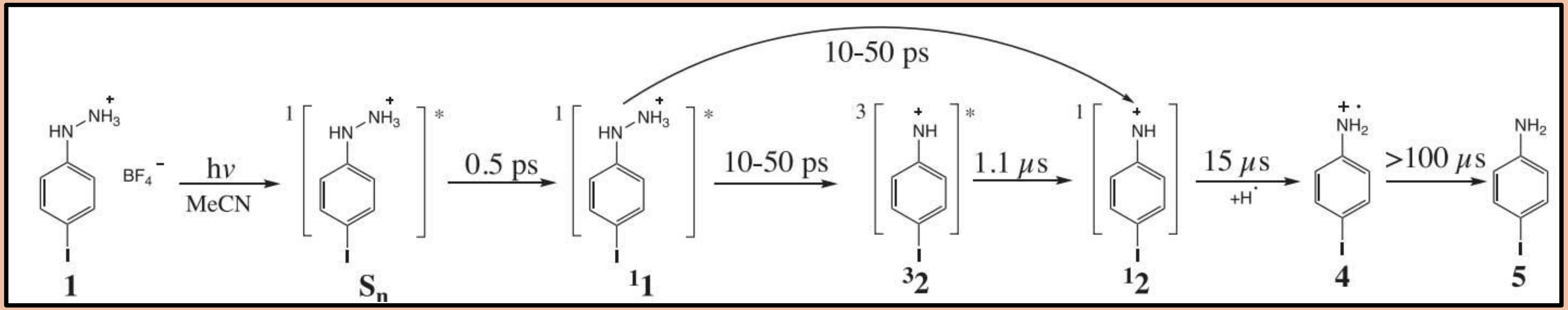
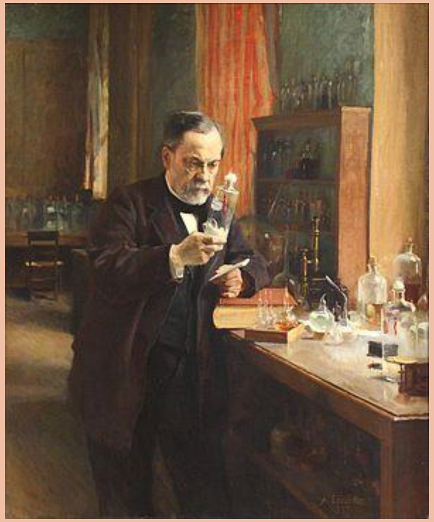


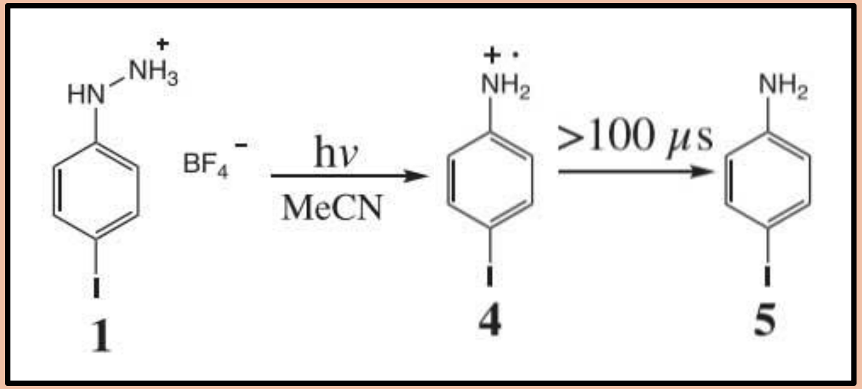


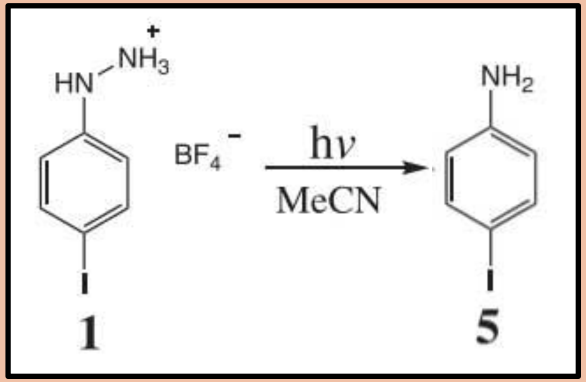
“My colleagues can see more”

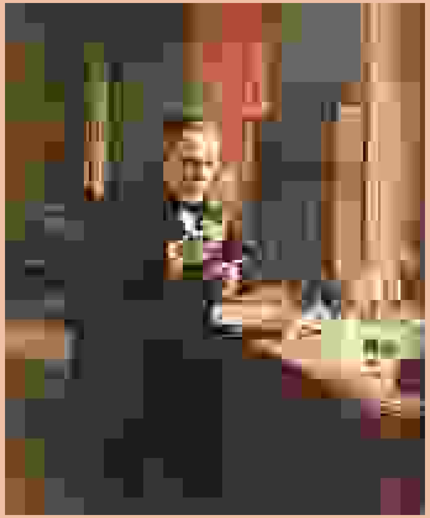






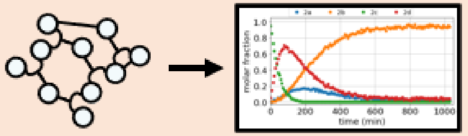


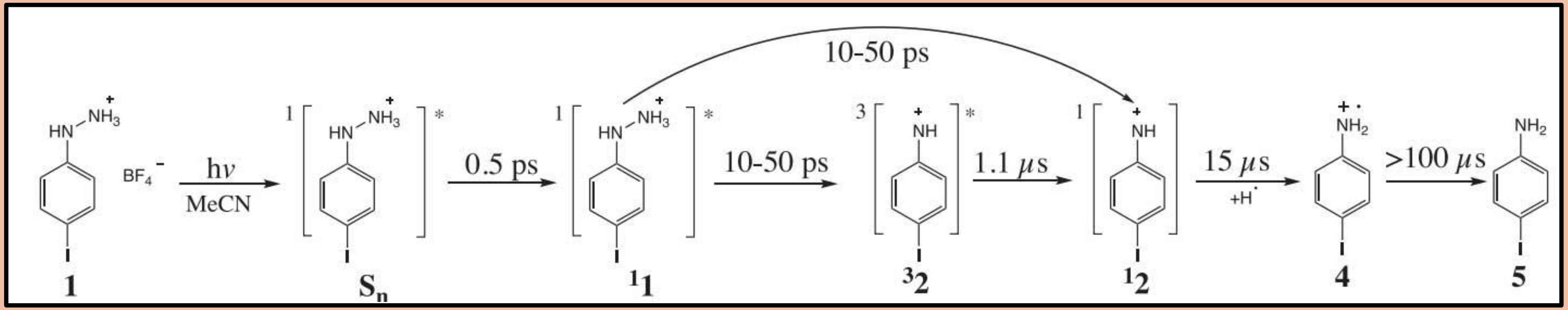


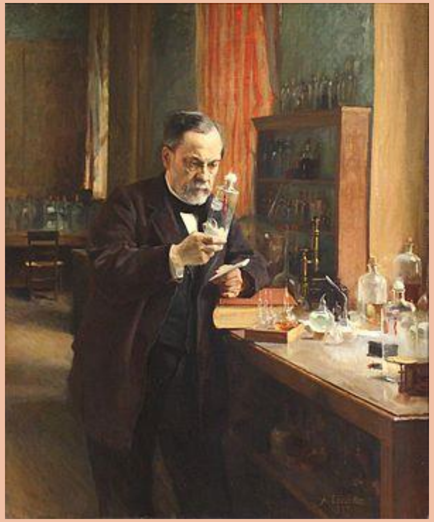


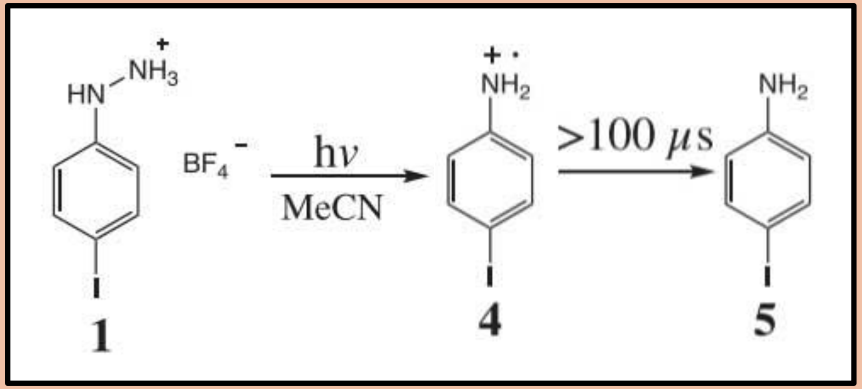
Different representations, but not contradictory: we’re talking about the same thing

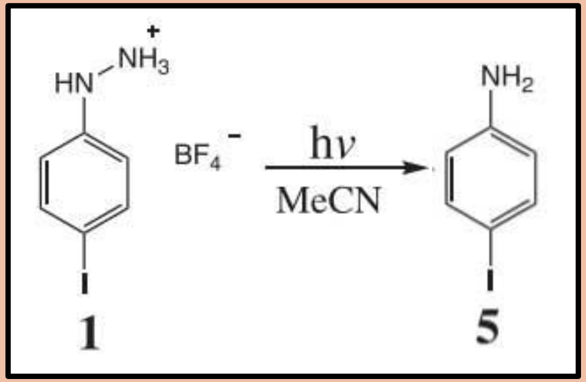
Resolution of CRNs: no 'absolute' representation

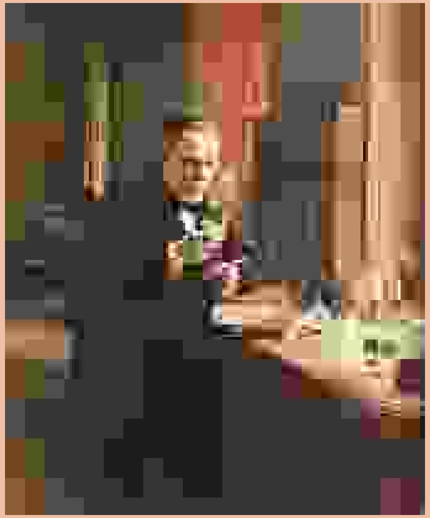












Different representations, but not contradictory: we're talking about the same thing

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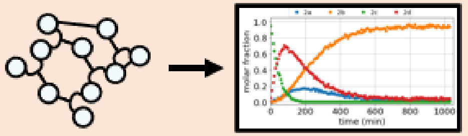

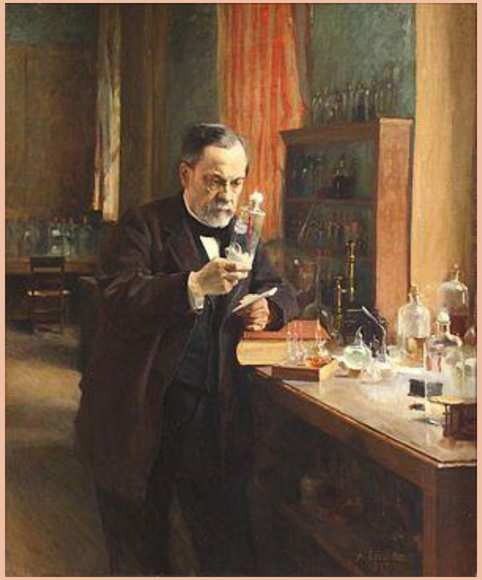

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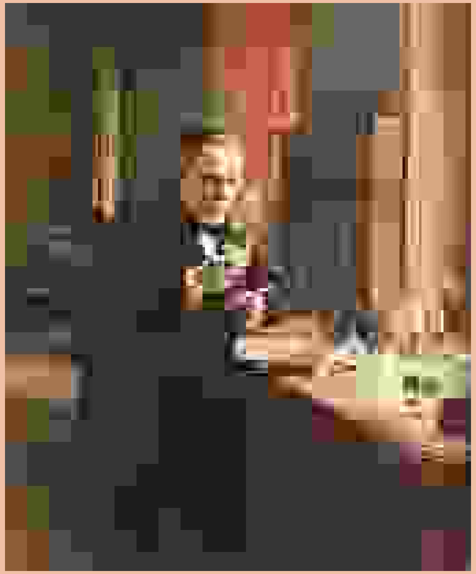

L. Pasteur,
A. Edelfelt (1885)

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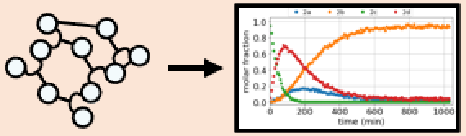
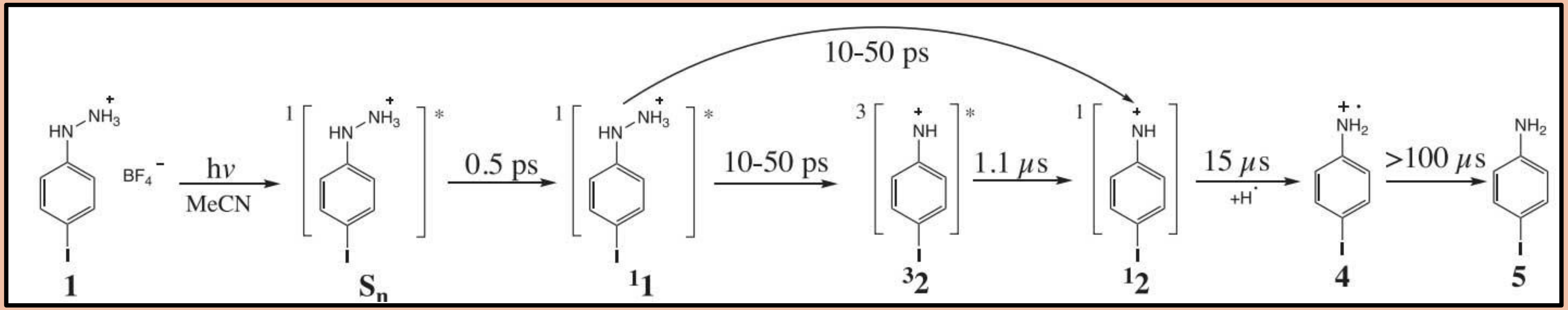
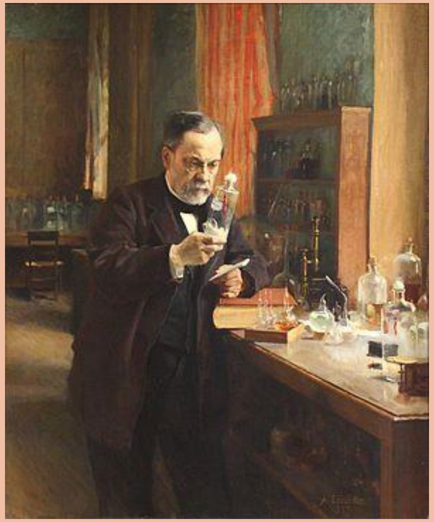
Different representations, but not contradictory: we’re talking about the same thing

“reactions are not absolute”



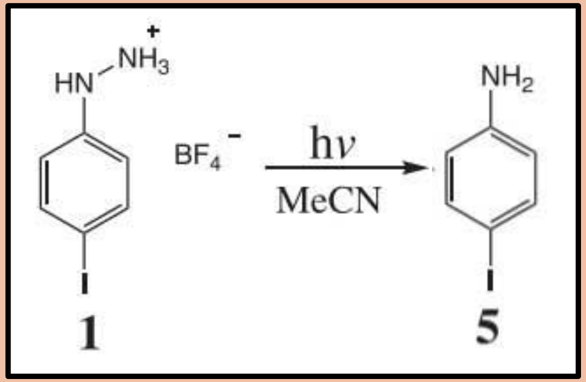


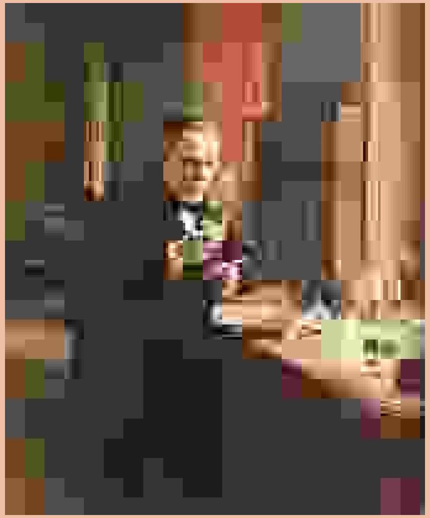


What else makes a reaction network ‘chemical’?

A system doesn’t have ‘one reaction network’, but a family of <u>agreeing</u> reaction networks of varying detail

Experimental resolution dictates the CRN we can see.





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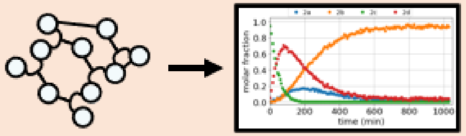

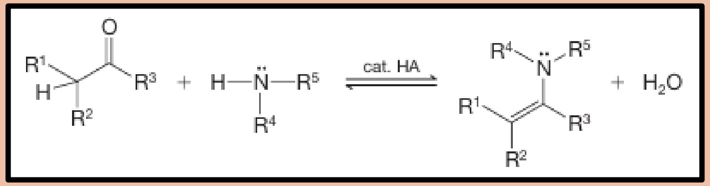

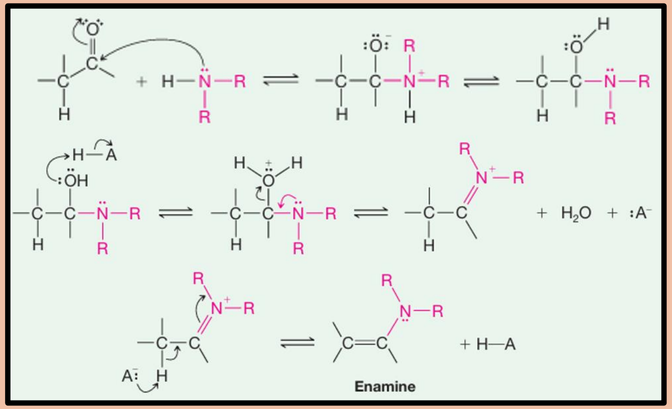

* Robustness to detail: predicted phenomenology is not expected to be altered by adding in more intermediates.

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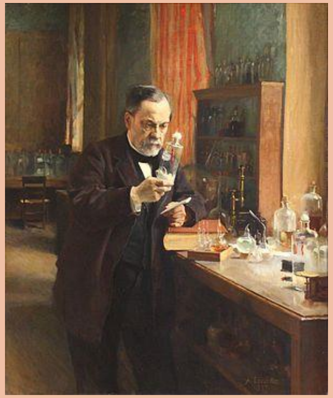

L. Pasteur, A. Edelfelt (1885)

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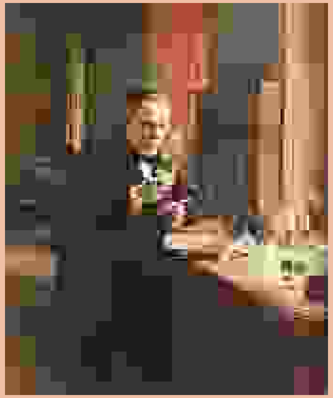

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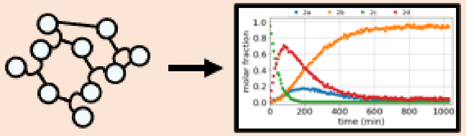
Nonrobustness, a very small example



* Robustness to detail: predicted phenomenology is not expected to be altered by adding in more intermediates.

$2X \rightarrow 3X$

Blows up in finite time

$\mathbf{N_X = 2}$

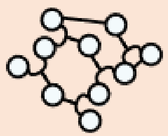
$< \boldsymbol{t_{2\rightarrow 3}} > = < \boldsymbol{t_{3\rightarrow \emptyset}} >$

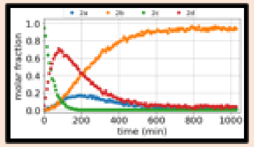
$2\,X \rightarrow X_2 \rightarrow 3\,X$

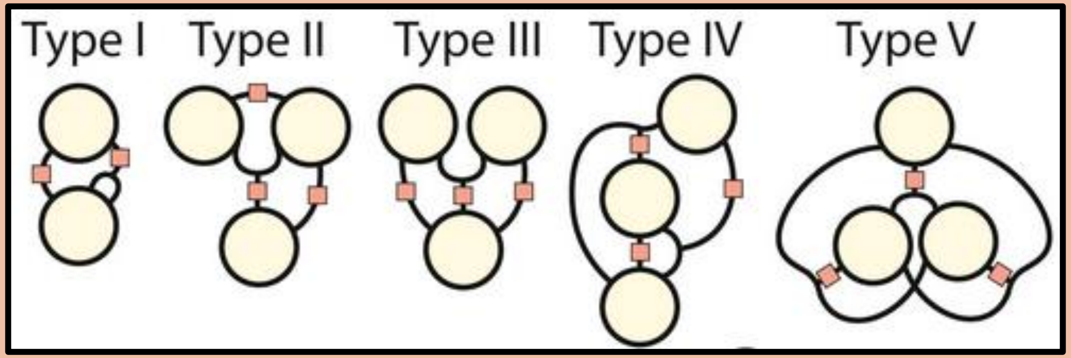
No blow up in finite time

$2X \rightarrow 3X$ intrinsically fails to be a good approximation on all but the shortest times.

No “absolute” CRN as a theoretical requirement







Universal motifs and the diversity of autocatalytic systems

Alex Blokhuis, David Lacoste, and Philippe Nghe Authors Info & Affiliations

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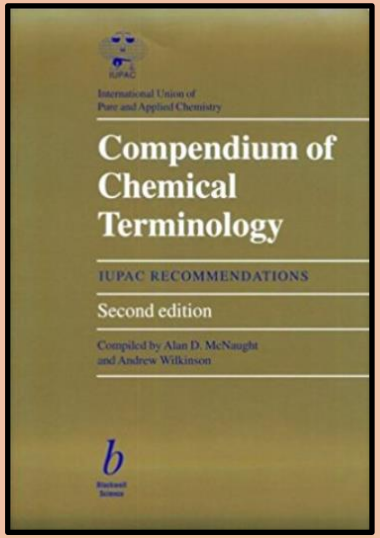
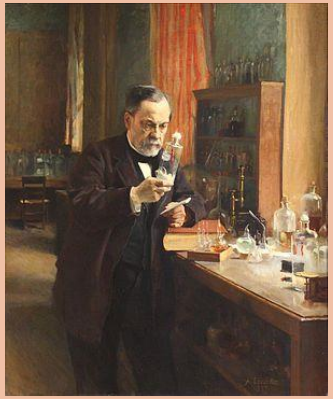
September 28, 2020 117 (41) 25230-25236 https://doi.org/10.1073/pnas.2013527117



Several concepts in chemistry (e.g. catalysis) are explicitly defined in terms of hierarchy of descriptions.



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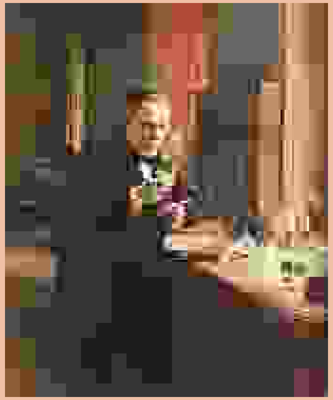

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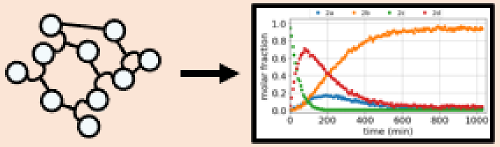

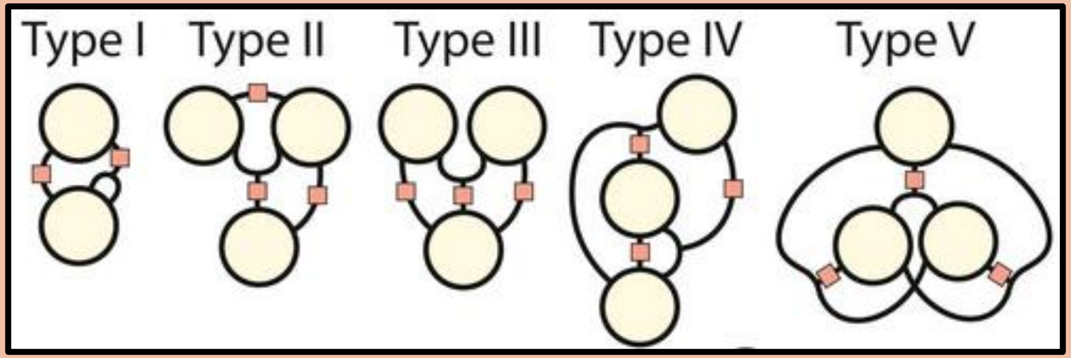

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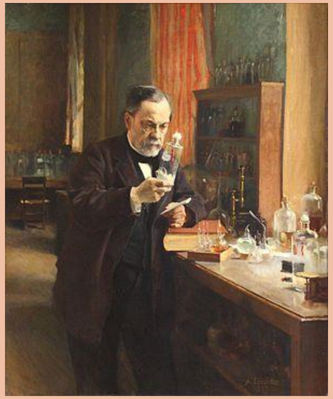
E.g. to formalize autocatalysis in chemistry we use that reaction networks have family of representations.



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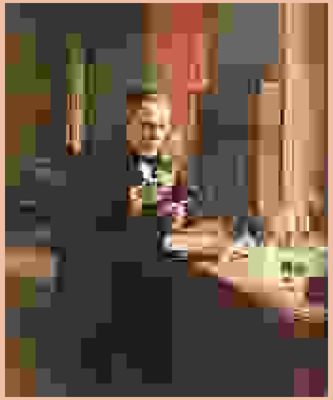

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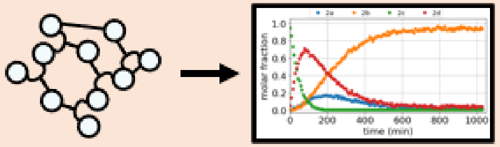
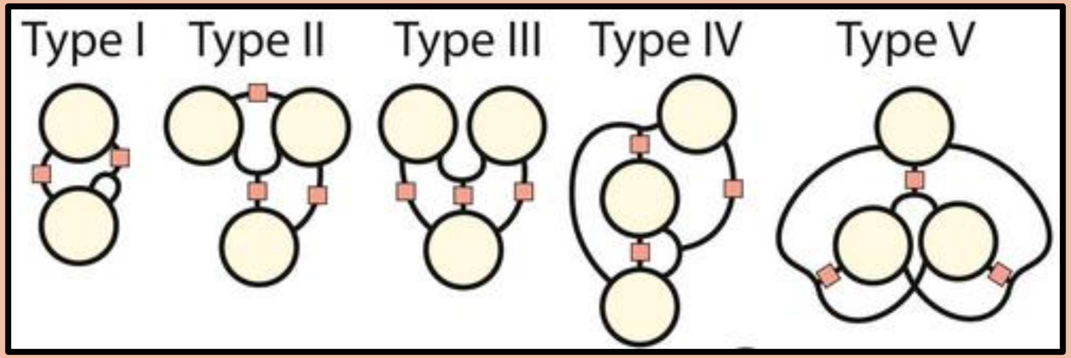
See also:

Defining Autocatalysis in Chemical Reaction Networks

Jakob L. Andersen, Christoph Flamm, Daniel Merkle, Peter F. Stadler

No "absolute" CRN as a theoretical requirement





Nonambiguity:
reactants ≠ products in the same reaction

$A+B \rightleftarrows 2\,A\,;\quad A+B \rightleftarrows AB \rightleftarrows 2\,A$

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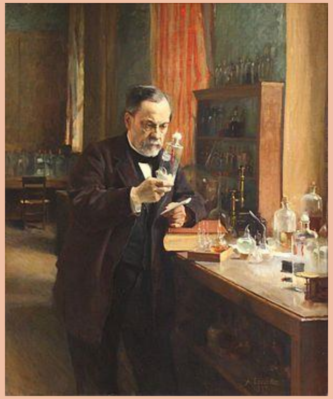

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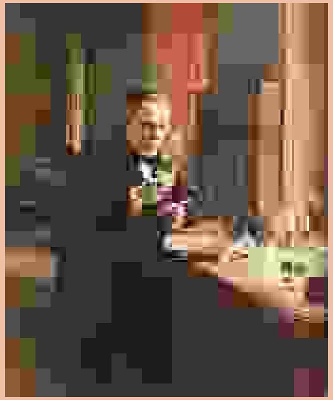

L. Pasteur, A. Edelfelt (1885) = L. Pasteur, A. Edelfelt (1885)

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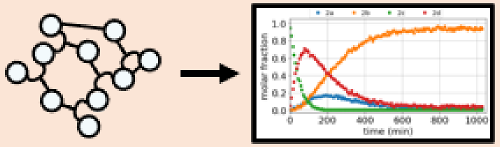

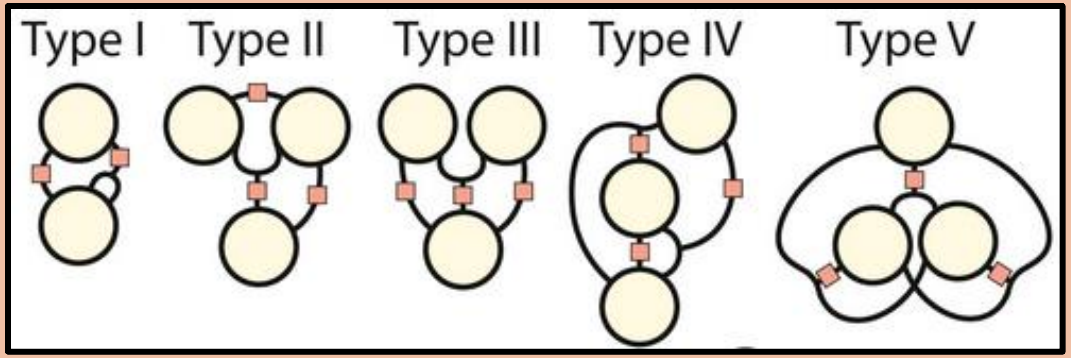

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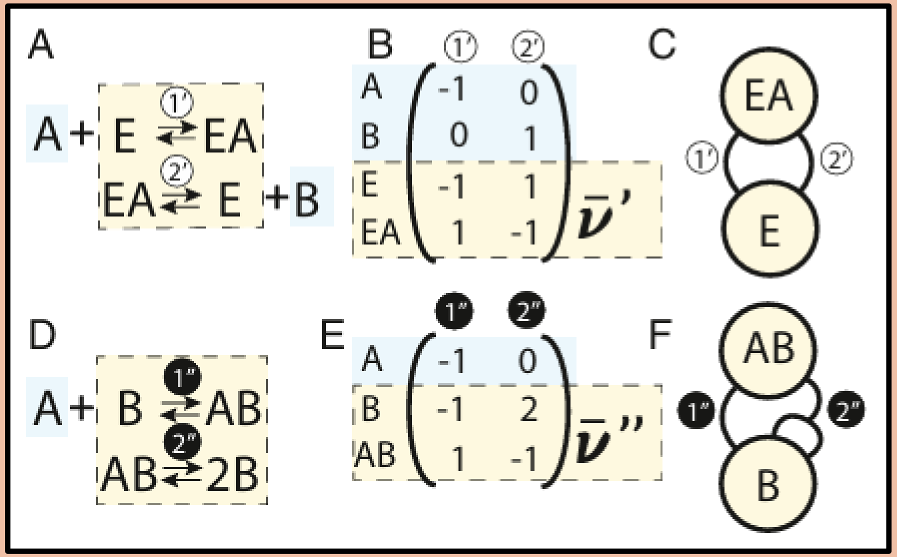
A methodological advantage:

→ Under **nonambiguity**, list of reactions maps 1-to-1 to stoichiometric matrix.



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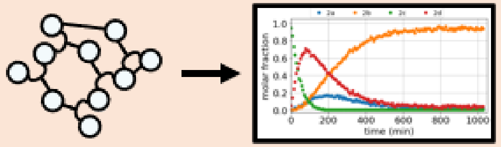

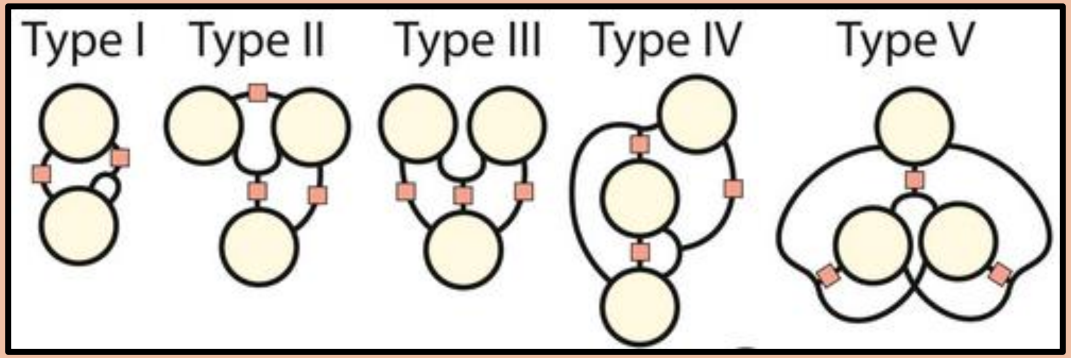

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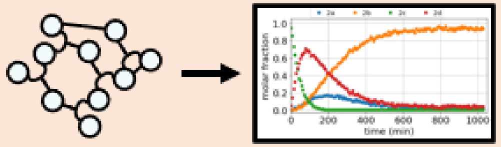
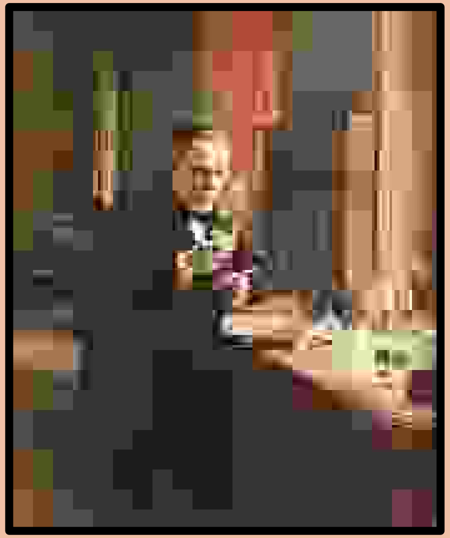
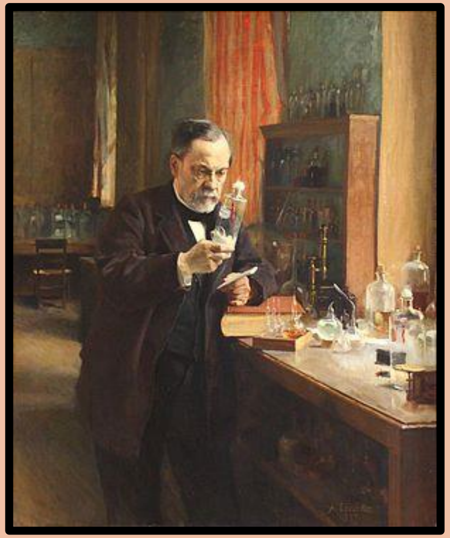
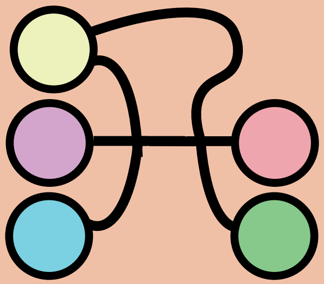
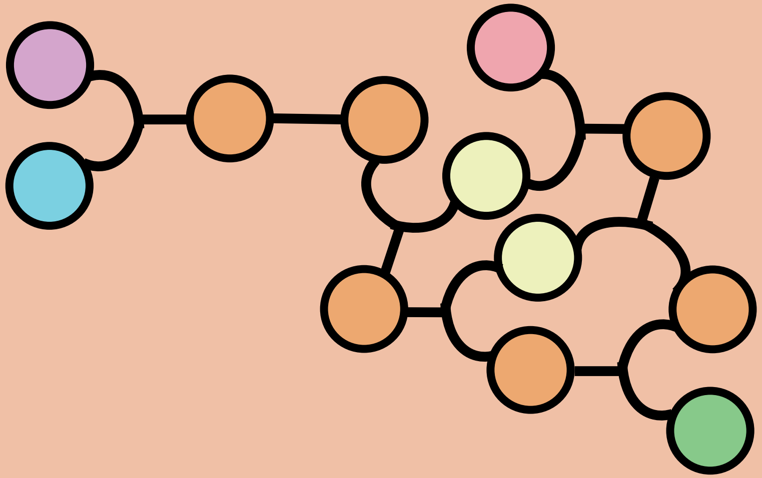
More steps, simpler steps

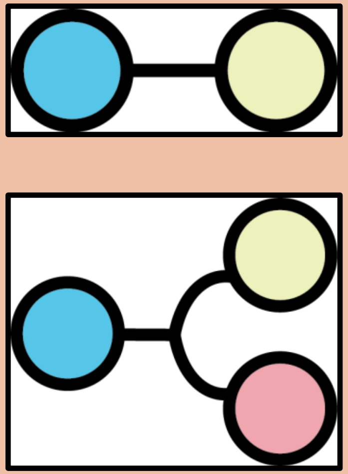






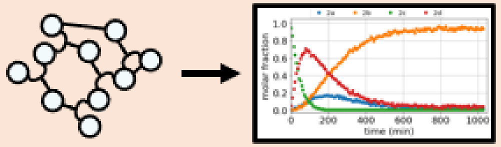


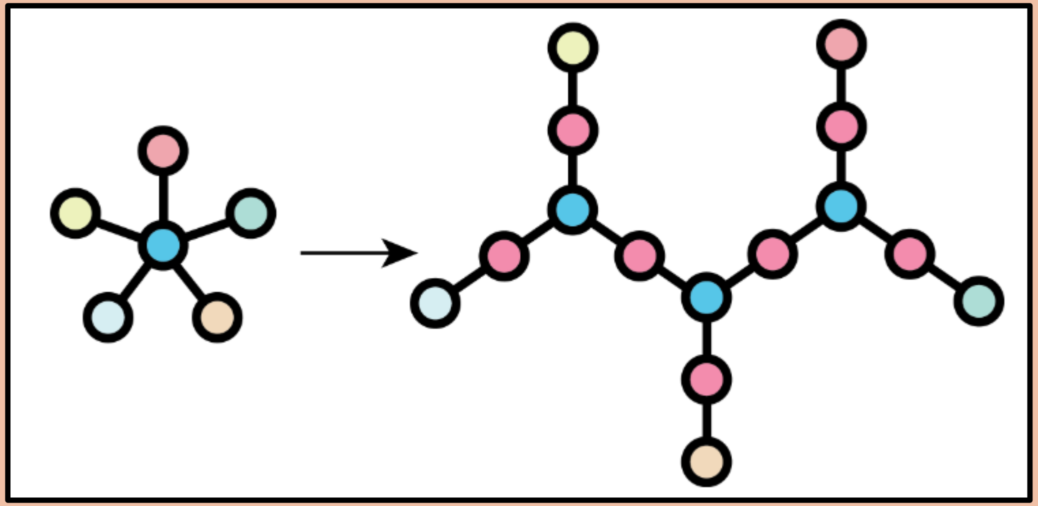




We only need two types of reactions

More steps, simpler steps



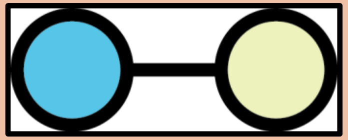


$s^{(3)} = 3$

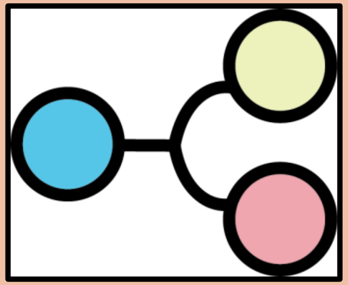
A species involved in >3 reactions can be reduced to several triconnected species

2 Fundamental building blocks

$A \rightleftarrows B$

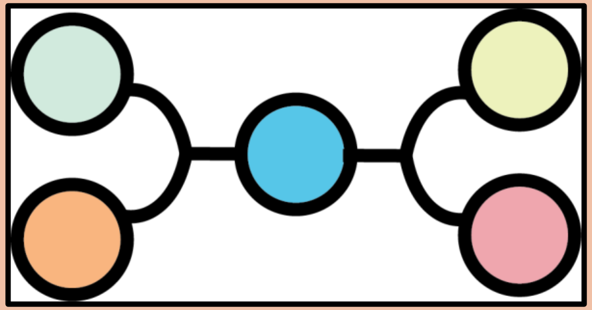


$A \rightleftarrows B + C$



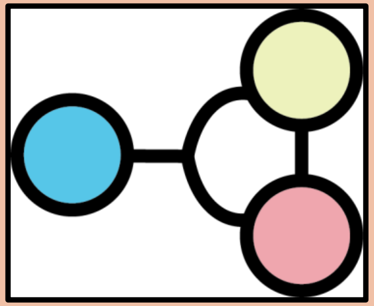
$A + B \rightleftarrows D + E$

$A + B \rightleftarrows C$
$C \rightleftarrows D + E$



$A \rightleftarrows 2B$

$A \rightleftarrows B + C$
$B \rightleftarrows C$

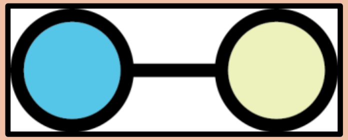
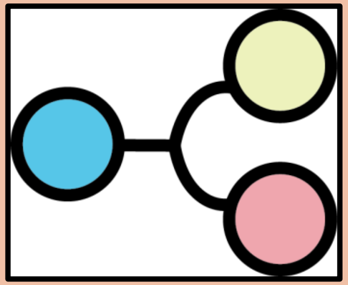


A methodological advantage

More variables, reactions ⇔ less structural elements, more regularity

- Dramatically reduces # cases to check in proofs
- Facilitates constructions
- Endows mathematical constructions with ‘nice’ properties

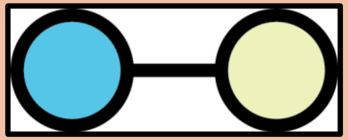
Simple building blocks ⇔ Many equivalent representations

 +  + Mass action (+Nonambiguity)

Normally in CRN Theory,
Stoichiometric matrix ≠ hypergraph ≠ dynamic equations ≠reaction list ≠ characteristic polynomial(s) ≠

Upon regularizing structure, **representations become equivalent**, **and new representations become available**
Stoichiometric matrix = hypergraph = dynamic equations = Reaction list = characteristic polynomial(s) = Big polynomial = generalized Jacobian = Jacobian for currents = Hamiltonian = ...

Simple building blocks ⇔ Many equivalent representations



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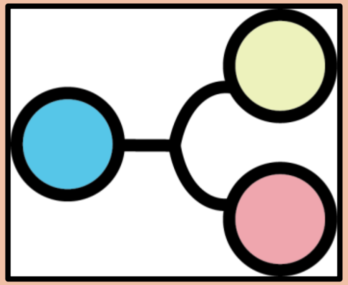
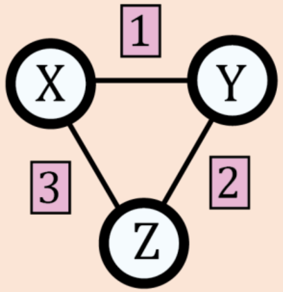


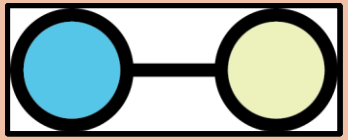
+ Mass action

(+Nonambiguity)

Directed* Hypergraph	Dynamic Equations	Reaction List	Stoichiometric Matrix	Big Polynomial	Hamiltonian
	$\mathcal{J}_1=\kappa_1^+[X]-\kappa_1^-[Y]$ $\mathcal{J}_2=\kappa_2^+[Y]-\kappa_2^-[Z]$ $\mathcal{J}_3=\kappa_3^+[Z]-\kappa_3^-[X]$ $d_t[X]= -\mathcal{J}_1 + \mathcal{J}_3$ $d_t[Y]= -\mathcal{J}_2 + \mathcal{J}_1$ $d_t[Z]= -\mathcal{J}_3 + \mathcal{J}_2$	1 $X \rightleftarrows Y$ 2 $Y \rightleftarrows Z$ 3 $Z \rightleftarrows X$	1 2 3 $\mathbb{S}=\begin{pmatrix}-1 & 0 & 1\\ 1 & -1 & 0\\ 0 & 1 & -1\end{pmatrix}\begin{matrix}X\\Y\\Z\end{matrix}$	$\mathcal{B}=\mathcal{Q}_1^+\mathcal{J}_1^++\mathcal{Q}_2^+\mathcal{J}_2^++\mathcal{Q}_3^+\mathcal{J}_3^+$ $+\mathcal{Q}_1^-\mathcal{J}_1^-+\mathcal{Q}_2^-\mathcal{J}_2^-+\mathcal{Q}_3^-\mathcal{J}_3^-$ $\mathcal{Q}_1^+=[X]^2/6-[Y]^2/2$ $\mathcal{Q}_1^-=[X]^2/6-[Y]^2/2$ $\mathcal{Q}_2^+=[Y]^2/6-[Z]^2/2$ $\mathcal{Q}_2^-=[Y]^2/6-[Z]^2/2$ $\mathcal{Q}_3^+=[Z]^2/6-[X]^2/2$ $\mathcal{Q}_3^-=[Z]^2/6-[X]^2/2$	$\mathcal{H} = \mathcal{J}_1(z_2-z_1)$ $+\mathcal{J}_2(z_3-z_2)$ $+\mathcal{J}_3(z_1-z_3)$

...

Simple building blocks ⇔ Many equivalent representations



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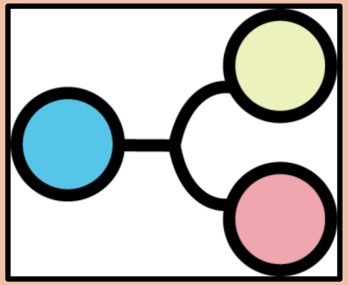


+ Mass action

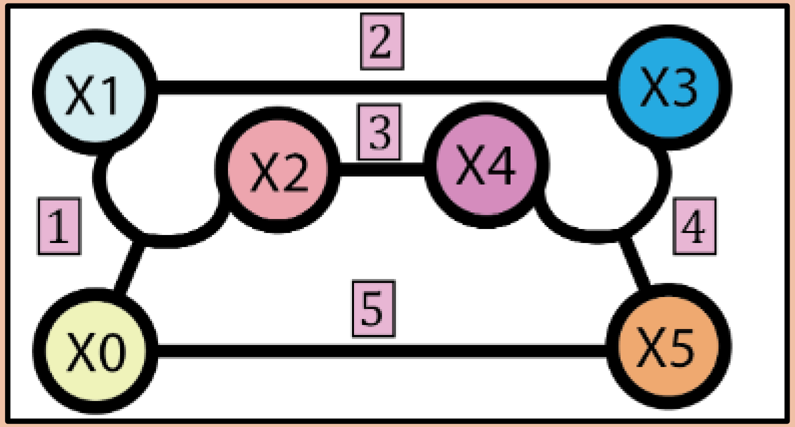
(+Nonambiguity)

Upon regularizing structure, **representations become equivalent, and new representations become available**
Stoichiometric matrix = hypergraph = dynamic equations = Reaction list = characteristic polynomial(s) = Big polynomial = generalized Jacobian = Jacobian for currents = Hamiltonian = …

Ipso facto,
→ questions can be reformulated as questions about the object of our choice.
→ representations acquire deeper, more regular structure
→ we can go back and forth between representations to look for easy insights, simple(r) proofs

Big polynomial

$$d_t x_k = \frac{\partial^2 \mathrm{B}}{\partial x_k^2}$$



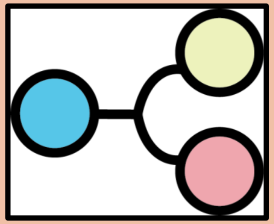
$$\mathcal{B} = \kappa_1^+ x_0 \left(\frac{x_1^2}{2} + \frac{x_2^2}{2} - \frac{x_0^2}{6} \right) + \kappa_1^- x_1 x_2 \left(\frac{x_0^2}{2} - \frac{x_1^2}{6} - \frac{x_2^2}{6} \right) + \kappa_2^+ x_1 \left(\frac{x_3^2}{2} - \frac{x_1^2}{6} \right) + \kappa_2^- x_3 \left(\frac{x_1^2}{2} - \frac{x_3^2}{6} \right)$$
$$+ \kappa_3^+ x_2 \left(\frac{x_4^2}{2} - \frac{x_2^2}{6} \right) + \kappa_3^- x_4 \left(\frac{x_2^2}{2} - \frac{x_4^2}{6} \right) + \kappa_4^+ x_3 x_4 \left(\frac{x_5^2}{2} - \frac{x_3^2}{6} - \frac{x_4^2}{6} \right) + \kappa_4^- x_5 \left(\frac{x_3^2}{2} + \frac{x_4^2}{2} - \frac{x_5^2}{2} \right)$$
$$+ \kappa_5^+ x_5 \left(\frac{x_0^2}{2} - \frac{x_5^2}{6} \right) + \kappa_5^- x_0 \left(\frac{x_0^2}{2} - \frac{x_5^2}{6} \right)$$

Regularized CRNs are never divergence-free

$$d_t x_k = \frac{\partial^2 \mathrm{B}}{\partial \mathrm{X}_\mathrm{k}^2}$$

$$\mathrm{div}(d_t \boldsymbol{x}) = \sum_k \frac{\partial^3 \mathrm{B}}{\partial \mathrm{X}_\mathrm{k}^3} < 0$$

$$\mathcal{B} = \sum_{k=1}^{r} \mathcal{B}_k = \sum_{k=1}^{r} \left(Q_k^+ J_k^+ + Q_k^- J_k^-\right)$$



$$\mathcal{B} = \kappa_1^+ x_0 \left(\frac{x_1^2}{2} + \frac{x_2^2}{2} - \frac{x_0^2}{6}\right) + \kappa_1^- x_1 x_2 \left(\frac{x_0^2}{2} - \frac{x_1^2}{6} - \frac{x_2^2}{6}\right)$$

CRN properties that critically rely on divergence-free dynamics are not robust and should not be expected in chemistry (nor ecology)

Regularized CRNs are <u>never</u> divergence-free

Lotka-Volterra
oscillates
$X \to 2X$, $X + Y \to 2Y$,
$Y \to \emptyset$
Rock-Paper-Scissers (RPS-3)
oscillates
$X + Y \to 2X$, $Y + Z \to 2Y$,
$Z + X \to 2Z$
(RPS-4)
quasi-periodic
$X + Y \to 2X$, $Y + Z \to 2Y$,
$Z + W \to 2Z$, $W + X \to 2W$

Stable, but not asymptotically stable

CRN properties that critically rely on divergence-free dynamics are not robust and should not be expected in chemistry

Regularized CRNs are never divergence-free

Lotka-Volterra

oscillates

$X \to 2X,\ X + Y \to 2Y,$

$Y \to \emptyset$

Rock-Paper-Scissers (RPS-3)

oscillates

$X + Y \to 2X, Y + Z \to 2Y,$

$Z + X \to 2Z$

(RPS-4)

quasi-periodic

$X + Y \to 2X, Y + Z \to 2Y,$

$Z + W \to 2Z, W + X \to 2W$

→

Lotka-Volterra

Fixed point, extinction

$X \to 2X,$

$X + Y \to XY \to 2Y,$

$Y \to \emptyset$

Rock-Paper-Scissers (RPS-3)

Fixed point, extinction

.

.

(RPS-4)

Fixed point, extinction

.

.

CRN properties that critically rely on divergence-free dynamics are not robust and should not be expected in chemistry

Regularized CRNs are never divergence-free

Lotka-Volterra
oscillates
X → 2 X, X + Y → 2Y,
Y → Ø
Rock-Paper-Scissers (RPS-3)
oscillates
X + Y → 2 X, Y + Z → 2Y,
Z + X → 2Z
(RPS-4)
quasi-periodic
X + Y → 2 X, Y + Z → 2Y,
Z + W → 2 Z, W + X → 2W

→

Lotka-Volterra
Fixed point, extinction
X → 2 X,
X + Y → XY → 2Y,
Y → Ø
Rock-Paper-Scissers (RPS-3)
Fixed point, extinction
.
.
(RPS-4)
Fixed point, extinction
.
.

Regularization →

Lotka-Volterra
Fixed point, extinction
.
.
.
(RPS-3)
Fixed point, extinction
.
.
(RPS-4)
Fixed point, extinction
.
.

CRN properties that critically rely on divergence-free dynamics
are not robust and should not be expected in chemistry (nor ecology)

Jacobian

$$\daleth_{k,j}(\boldsymbol{x}) = \frac{\partial d_t x_k}{\partial x_j}$$

$$d_t \Delta \boldsymbol{x} = \daleth(\boldsymbol{x}) \Delta \boldsymbol{x}$$

Linearized dynamics

$$d_t \boldsymbol{x} = \daleth(\boldsymbol{x}/2)\boldsymbol{x}$$

Full dynamics

For regularized network, the Jacobian also expresses non-linearized dynamics

Jacobian

$$\gimel_{k,j}(\boldsymbol{x}) = \frac{\partial d_t x_k}{\partial x_j}$$

$$d_t \Delta \boldsymbol{x} = \gimel(\boldsymbol{x}) \Delta \boldsymbol{x}$$

Linearized dynamics

$$d_t \boldsymbol{x} = \gimel(\boldsymbol{x}/2) \boldsymbol{x}$$

Full dynamics

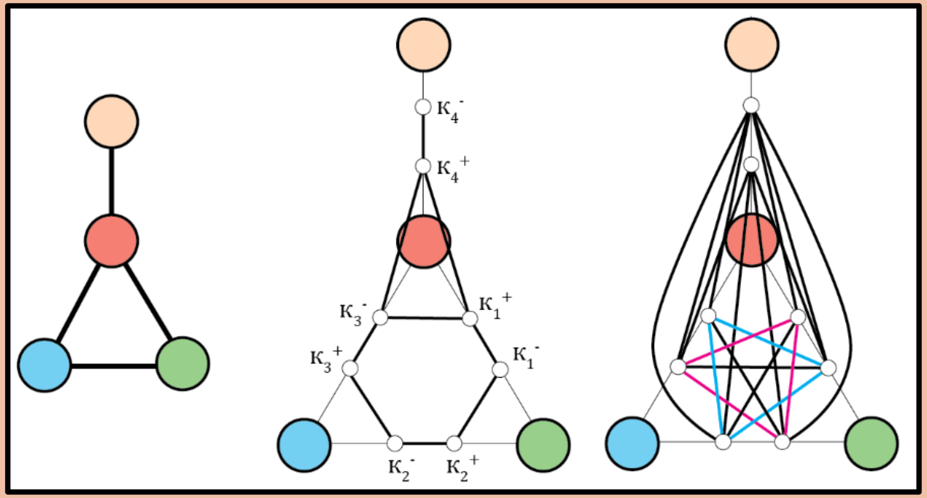
For regularized network, the Jacobian also expresses non-linearized dynamics

One can deduce simple rules to construct a characteristic polynomial $P_\lambda(J)$ from (hyper)graph, and vice versa.

A factor graph.

A factor of coefficients occurs in the characteristic polynomial if it is not **forbidden**

Forbidden: i) nearest neighbors, ii) cycles in factor graph



$\kappa_4^+ \kappa_3^-$ x , $\kappa_3^- \kappa_2^- \kappa_1^+$ x , $\kappa_4^- \kappa_3^-$

Jacobian

$$\gimel_{k,j}(\boldsymbol{x}) = \frac{\partial d_t x_k}{\partial x_j}$$

$$d_t \Delta \boldsymbol{x} = \gimel(\boldsymbol{x}) \Delta \boldsymbol{x}$$

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$$d_t \boldsymbol{x} = \gimel(\boldsymbol{x}/2) \boldsymbol{x}$$

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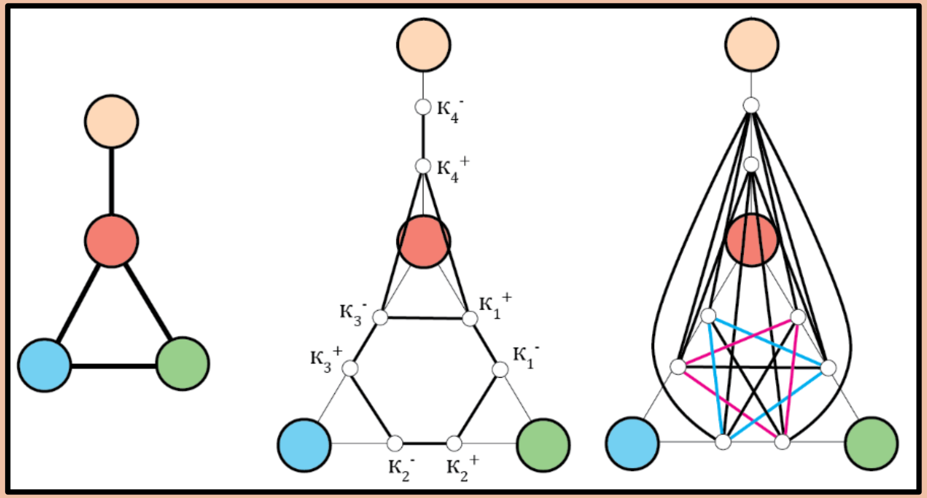


A factor graph.

A factor of coefficients occurs in the characteristic polynomial if it is not **forbidden**

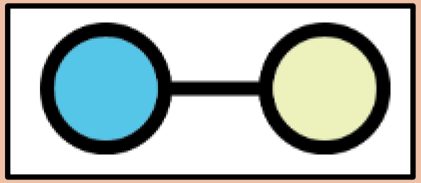
Forbidden: i) nearest neighbors, ii) cycles in factor graph

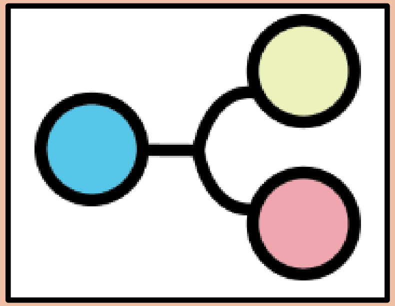
$\kappa_4^+ \kappa_3^-$ x , $\kappa_3^- \kappa_2^- \kappa_1^+$ x , $\kappa_4^- \kappa_3^-$

More elaborate rules with bimolecular reactions

Jacobian for currents

$$\aleph_{k,j}(\boldsymbol{J}) = \frac{\partial d_t J_k}{\partial J_j}$$





$$d_t x_1 = -d_t x_2 = -J_1$$

$$d_t J_1 = \kappa_1^+ d_t x_1 - \kappa_1^- d_t x_2 = -(\kappa_1^+ + \kappa_1^-) J_1$$

$$\aleph_o = \left(\frac{\partial d_t J_1}{\partial J_1} \right) = \left(-\kappa_1^+ - \kappa_1^- \right)$$

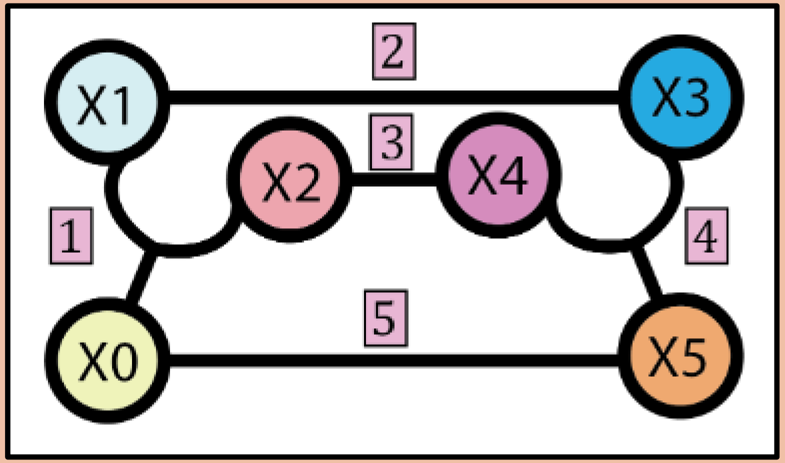
$$d_t x_1 = -d_t x_2 = -d_t x_3 = -J_1$$

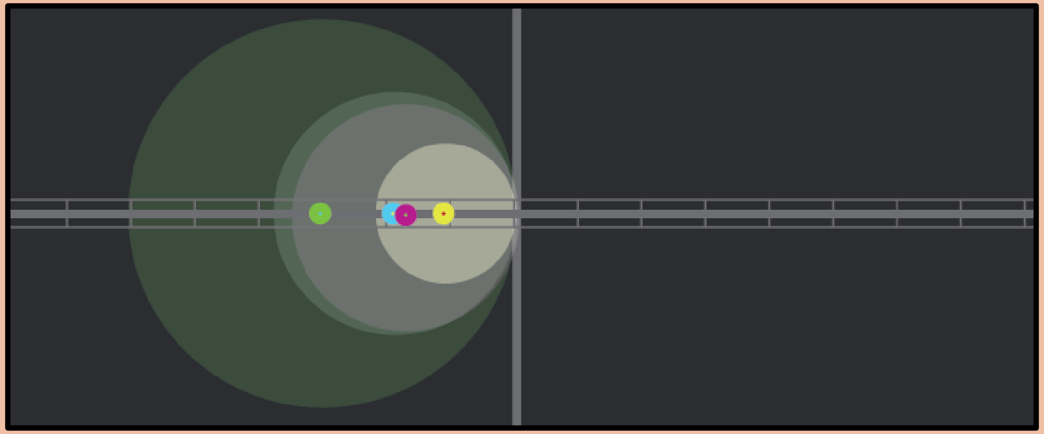
$$d_t J_1 = \kappa_1^+ d_t x_1 - \kappa_1^- x_3 d_t x_2 - \kappa_1^- x_2 d_t x_3 = -(\kappa_1^+ + \kappa_1^- (x_2 + x_3)) J_1$$

$$\aleph_{oo} = \left(\frac{\partial d_t J_1}{\partial J_1} \right) = \left(-\kappa_1^+ - \kappa_1^- (x_2 + x_3) \right)$$

Jacobian for currents – Handshake stability

$s^{(3)} = 0$

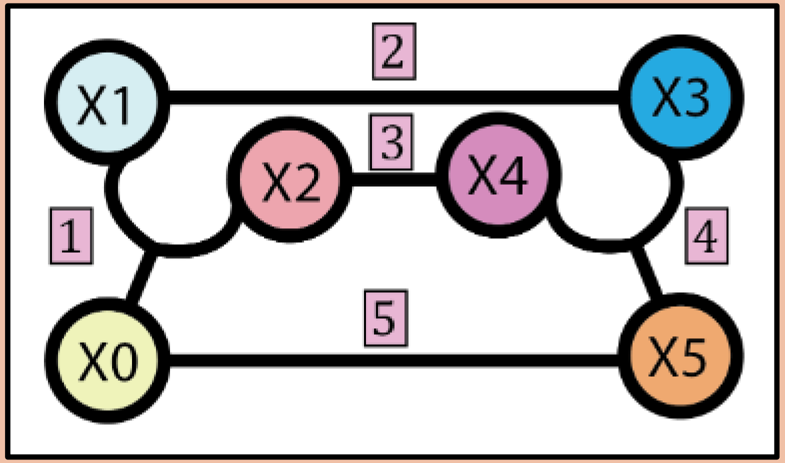


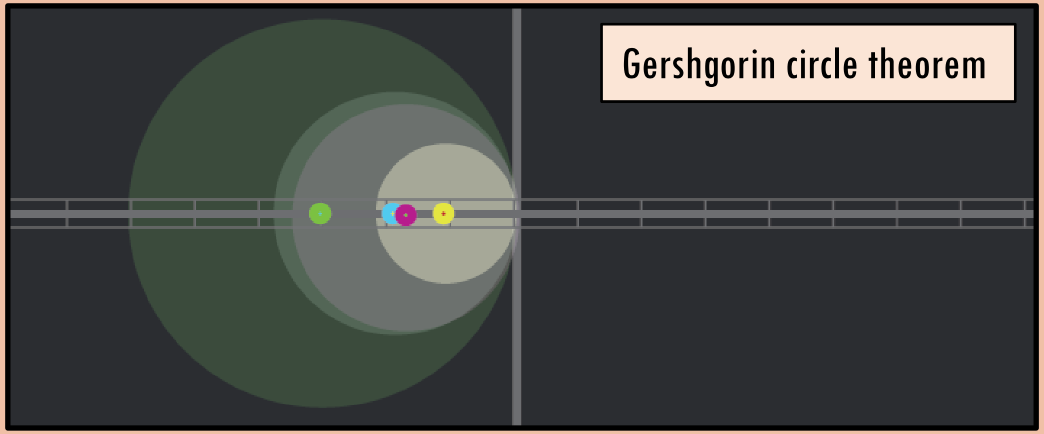


$$\aleph = \begin{pmatrix} -k_1^+ - k_1^-(x_1 + x_2) & k_1^- x_2 & k_1^- x_1 & 0 & k_1^+ \\ k_2^+ & -k_2^+ - k_2^- & 0 & k_2^- & 0 \\ k_3^+ & 0 & -k_3^+ - k_3^- & k_3^- & 0 \\ 0 & k_4^+ x_4 & k_4^+ x_3 & -k_4^+(x_3 + x_4) - k_4^- & k_4^- \\ k_5^- & 0 & 0 & k_5^+ & -k_5^+ - k_5^- \end{pmatrix}$$

Jacobian for currents – Handshake stability

$s^{(3)} = 0$

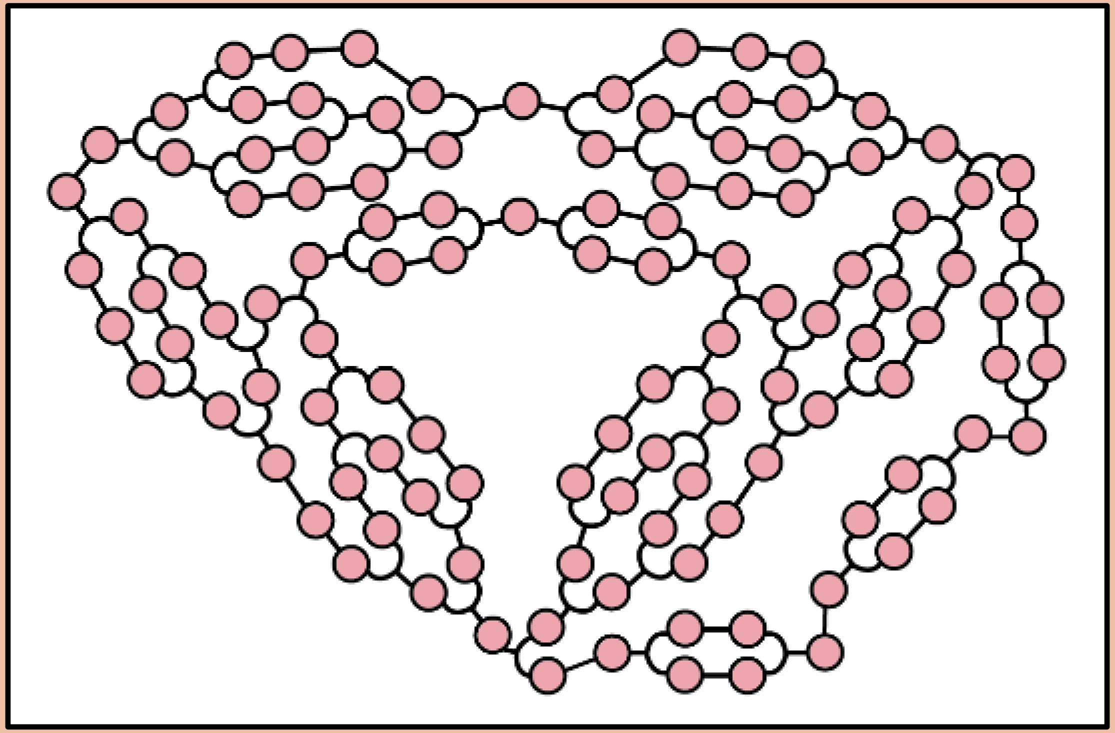




$$\aleph = \begin{pmatrix} -k_1^+ - k_1^-(x_1 + x_2) & k_1^- x_2 & k_1^- x_1 & 0 & k_1^+ \\ k_2^+ & -k_2^+ - k_2^- & 0 & k_2^- & 0 \\ k_3^+ & 0 & -k_3^+ - k_3^- & k_3^- & 0 \\ 0 & k_4^+ x_4 & k_4^+ x_3 & -k_4^+(x_3 + x_4) - k_4^- & k_4^- \\ k_5^- & 0 & 0 & k_5^+ & -k_5^+ - k_5^- \end{pmatrix}$$

Jacobian for currents – Handshake stability

If each species in a CRN engages in at most 2 reactions, then the CRN is **handshake stable**
i.e. all eigenvalues of jacobian for currents are nonpositive.



$s^{(3)} = 0$

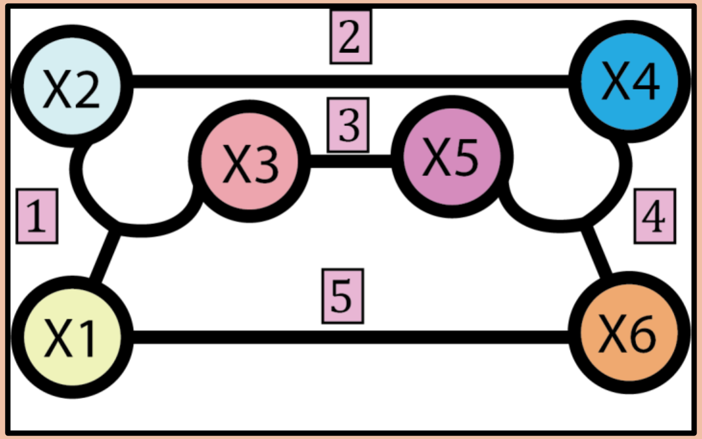
Handshake stable

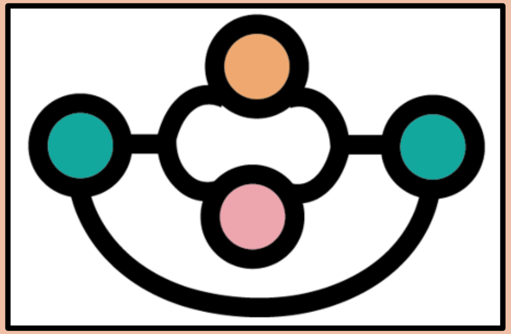
Deficiency δ, invariant deficiency δ

"properties of a system" vs "properties of a specific description"

$\delta_{\odot}, s^{(3)}$ δ

$\delta_{\odot} = c - c_o = c_{oo}$





$\delta_{\odot} = 1, \delta=1, s^{(3)} = 0$

$\delta_{\odot} = 1, \delta=0, s^{(3)} = 0$

Invariant deficiency:
nontrivial cycles
(cycles that are not purely unimolecular)

$\delta = 0$ is a well-known guarantee of stability

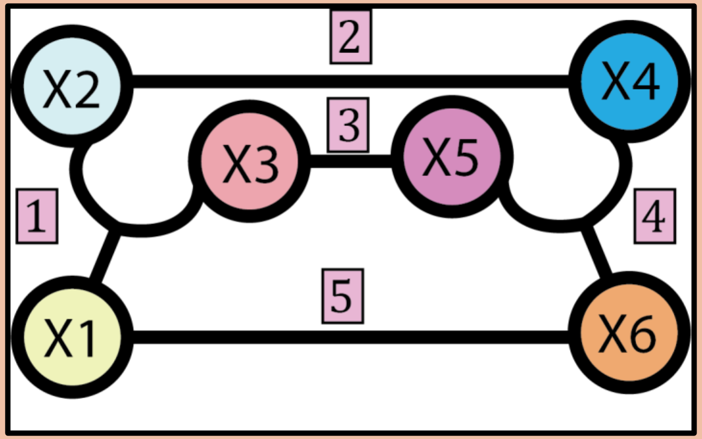
Deficiency δ, invariant deficiency δ

"properties of a system" vs "properties of a specific description"

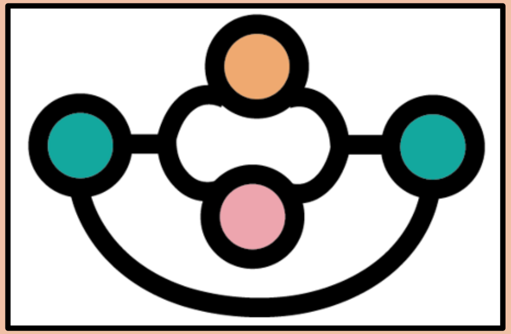
$\delta_{\odot}, s^{(3)}$ δ

$\delta_{\odot} = c - c_o = c_{oo}$

Invariant deficiency:
\# nontrivial cycles
(cycles that are not purely unimolecular)



$\delta_{\odot} = 1, \delta = 1, s^{(3)} = 0$

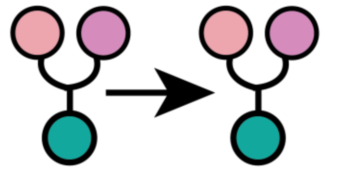
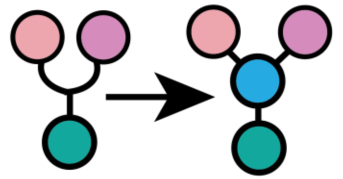
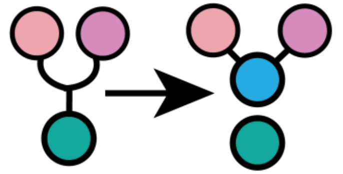
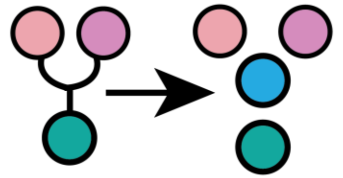


$\delta_{\odot} = 1, \delta = 0, s^{(3)} = 0$

$\delta = 0$ is a well-known guarantee of stability

Open question:
To what extent are conclusions based on deficiency robust to regularization?

Generating robust invariants & CRN index laws

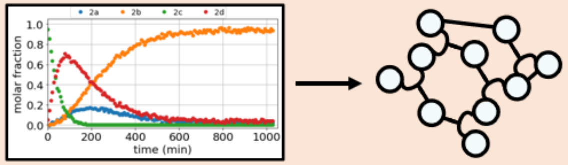
Graph transform	Structural Law	Introduced quantities
	SL1 $s - r = \ell_s - c$	s : # species r: # reactions l_s : # conserved quantities c : # cycles
	SL2 $s - r = j + r_{oo} - \gamma$	j : # disjoint networks r_{oo}: # bimolecular reactions
	SL3 $s - r = \beta - \gamma_{\triangleright} - c_0$	β : # bilinkage classes $\gamma_{\triangleright}$: # pointy loops
	SL4 $s - r = \psi - r_{oo} - c_0$	ψ : # local isomer groups c_0 : # trivial cycles

(hyper)Graph Transform +
Fundamental theorem of Linear Algebra

↓

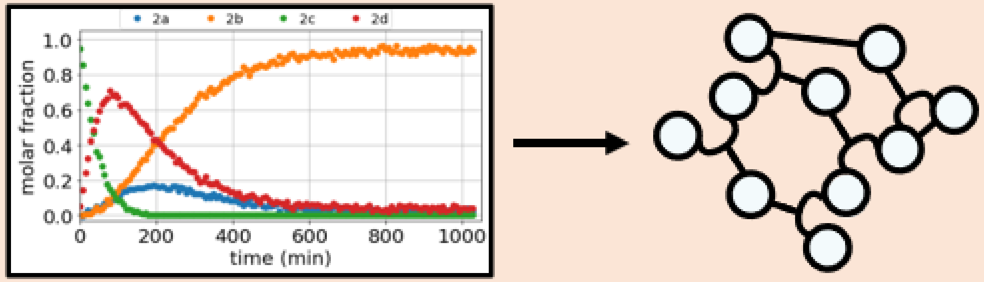
Robust topological properties of systems +
Structural laws for chemical networks

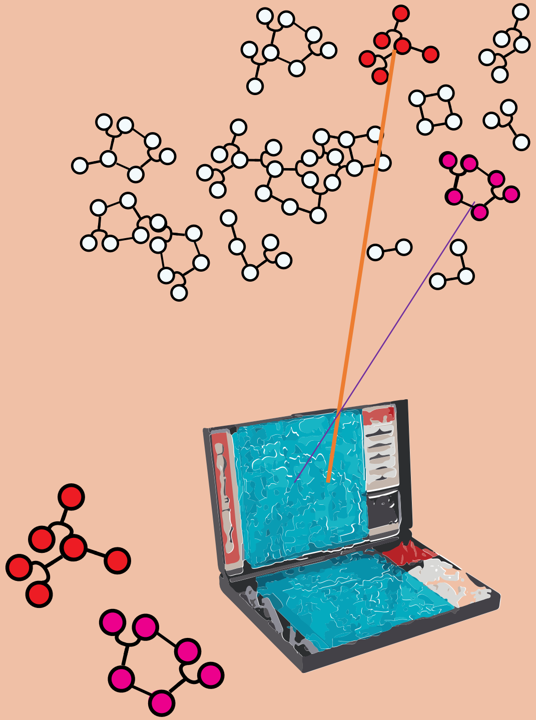
How do I know what CRN I'm looking at?

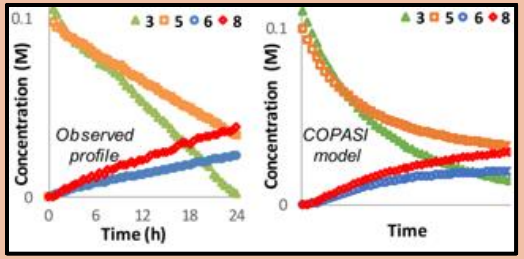


Battleship

Try to fit one specific hypothesis after another.



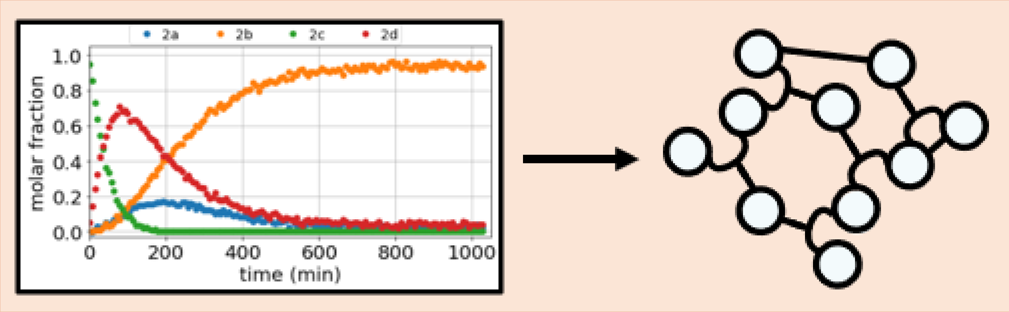




How do I know what CRN I'm looking at?

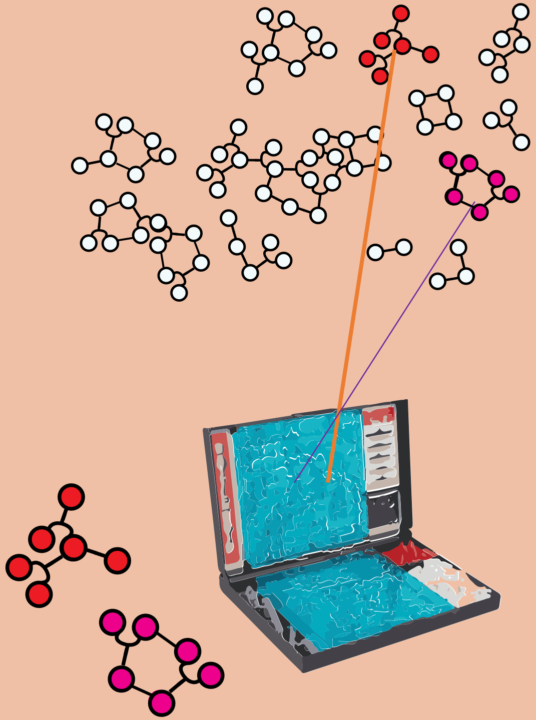
Battleship

Try to fit one specific hypothesis after another.

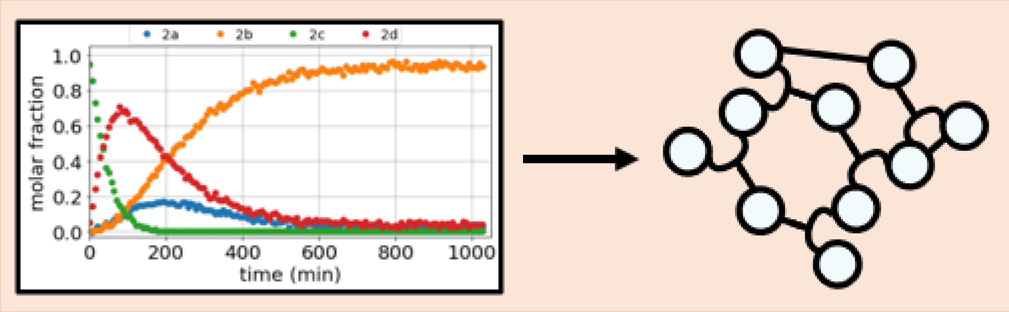


Guess who?

Exponentially narrow down the options

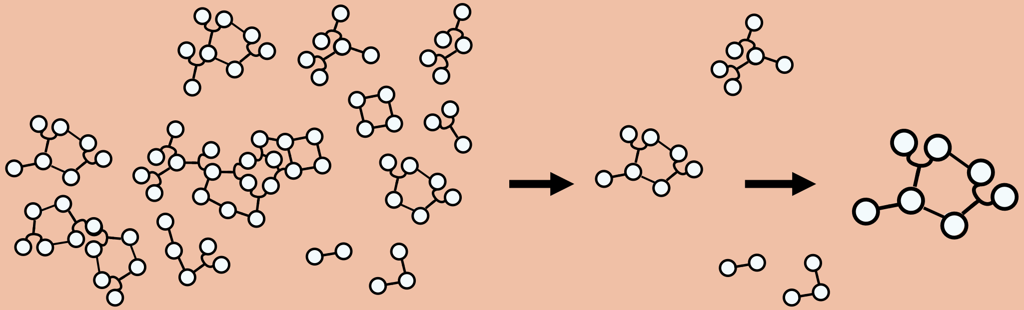


Measurable indices



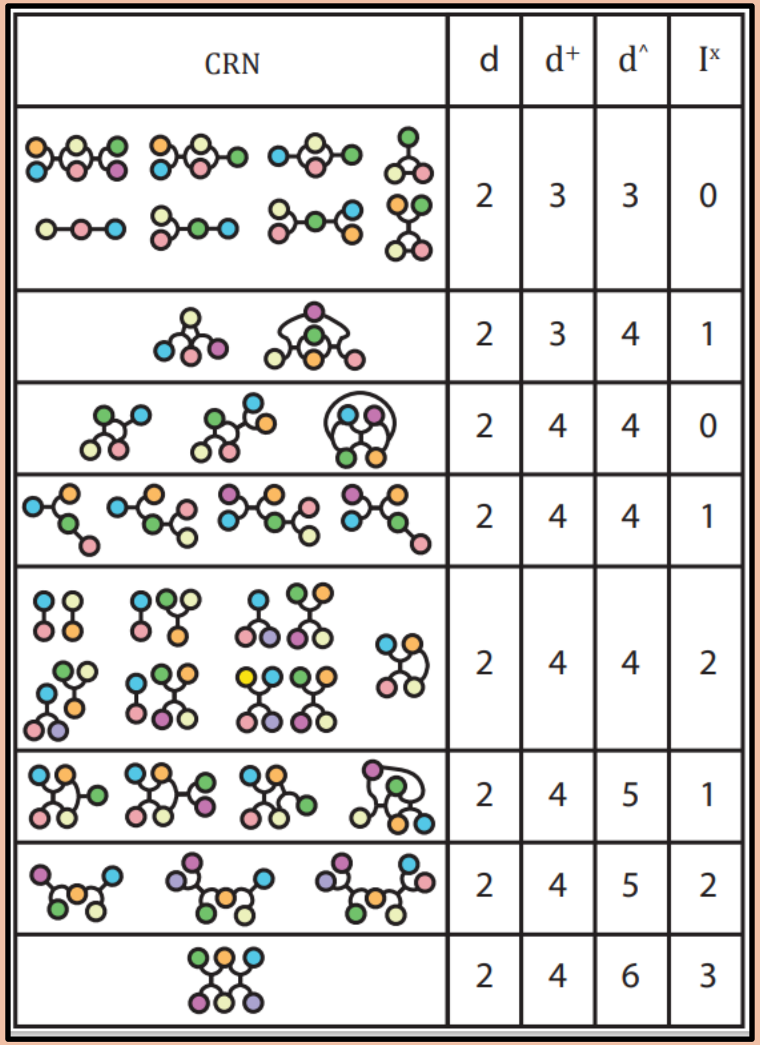
Guess who?

Exponentially narrow down the options

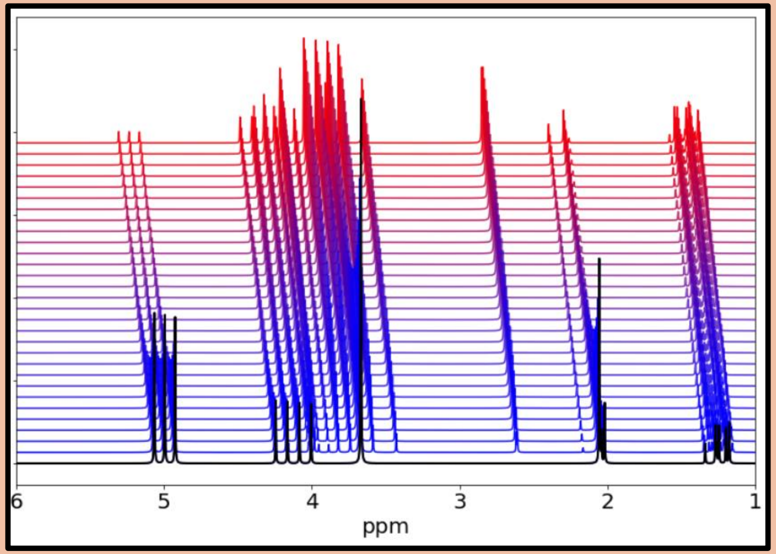


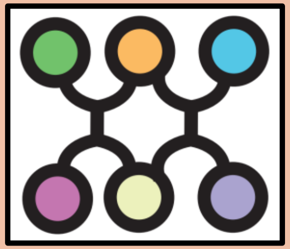
Exponentially narrow down the options by measuring various families of indices characterizing CRN

Measurable indices



CRN	d	d^+	$d^\wedge$	I^x
	2	3	3	0
	2	3	4	1
	2	4	4	0
	2	4	4	1
	2	4	4	2
	2	4	5	1
	2	4	5	2
	2	4	6	3

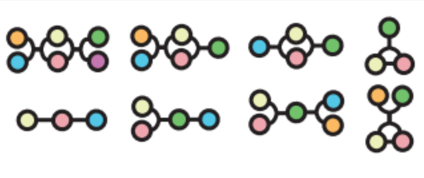
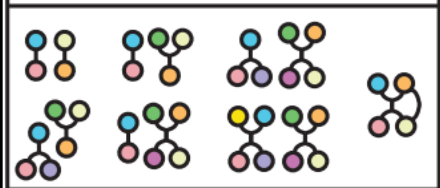


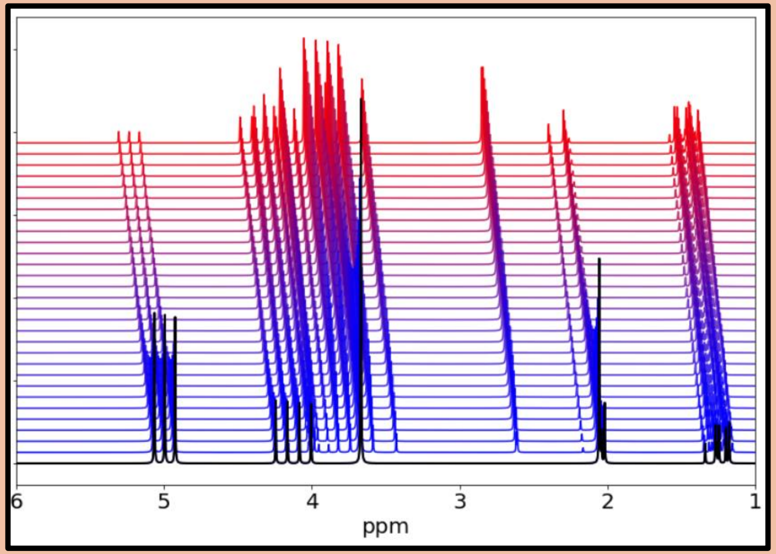


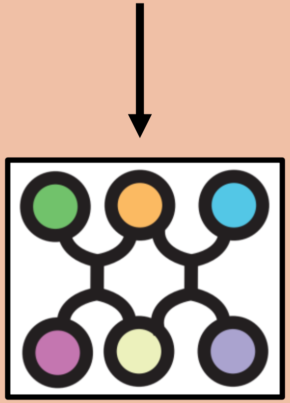
Guess who?

Exponentially narrow down the options

Measurable indices

CRN	d	d^+	$d^\wedge$	I^x
	2	3	3	0
	2	3	4	1
	2	4	4	0
	2	4	4	1
	2	4	4	2
	2	4	5	1
	2	4	5	2
	2	4	6	3



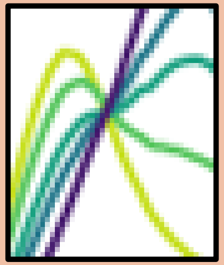


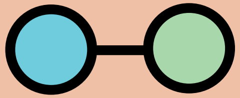
Guess who?

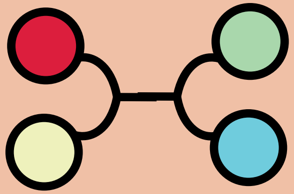
Exponentially narrow down the options

An example of an index, data dimension d

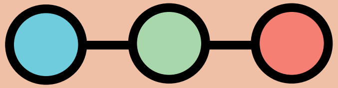
d=1
(isosbestic point*)

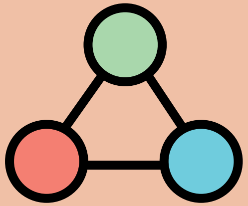


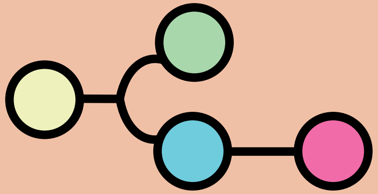




d=2
(Isosbestic line*)



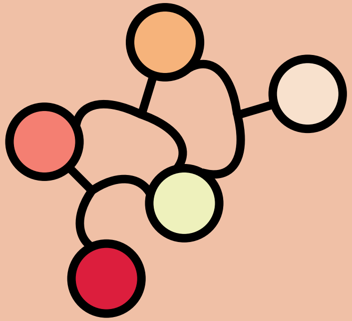




$d = v - \ell$ “# variables - # constraints”

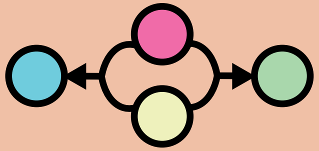
Rank estimation of mean-subtracted data

d=3



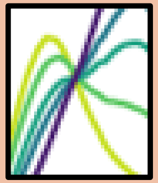
Many chemical phenomena lower data dimension

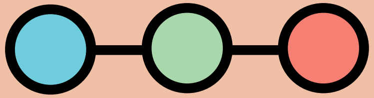
d



$C \leftarrow A + B \longrightarrow D$
$l_s = 2, l_{irr} = 1$

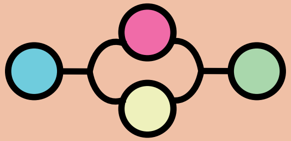
1





$A \rightleftarrows B \rightleftarrows C$
$l_s = 1$

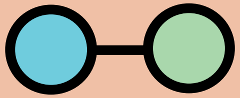
2



$C \rightleftarrows A + B \rightleftarrows D$
$l_s = 2, \mathrm{d} = 2$

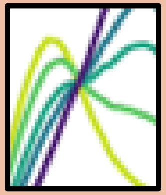
2

fast



$A \rightleftarrows B \rightleftarrows C$
$l_s = 1, \; l_{iso-eq} = 1$

1

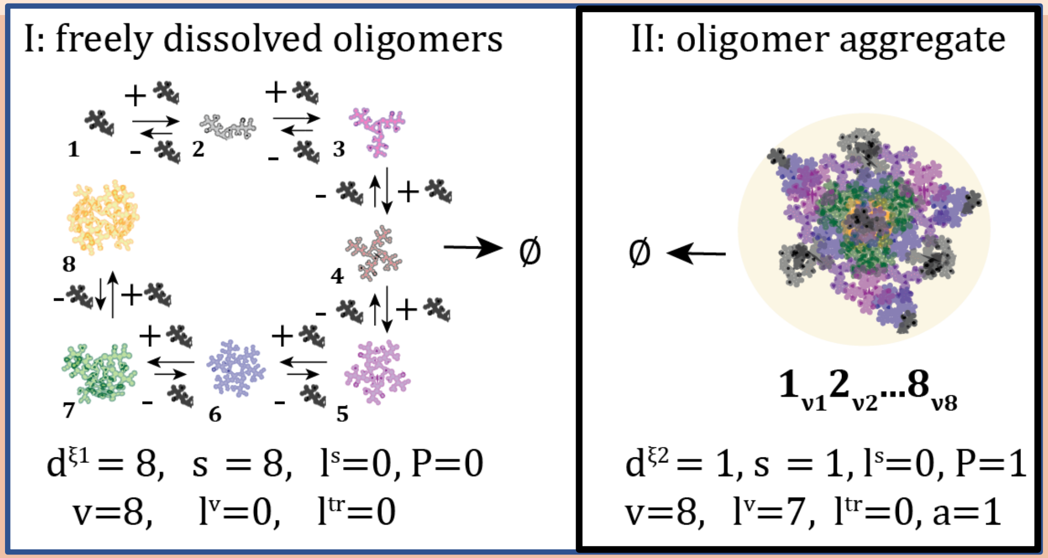


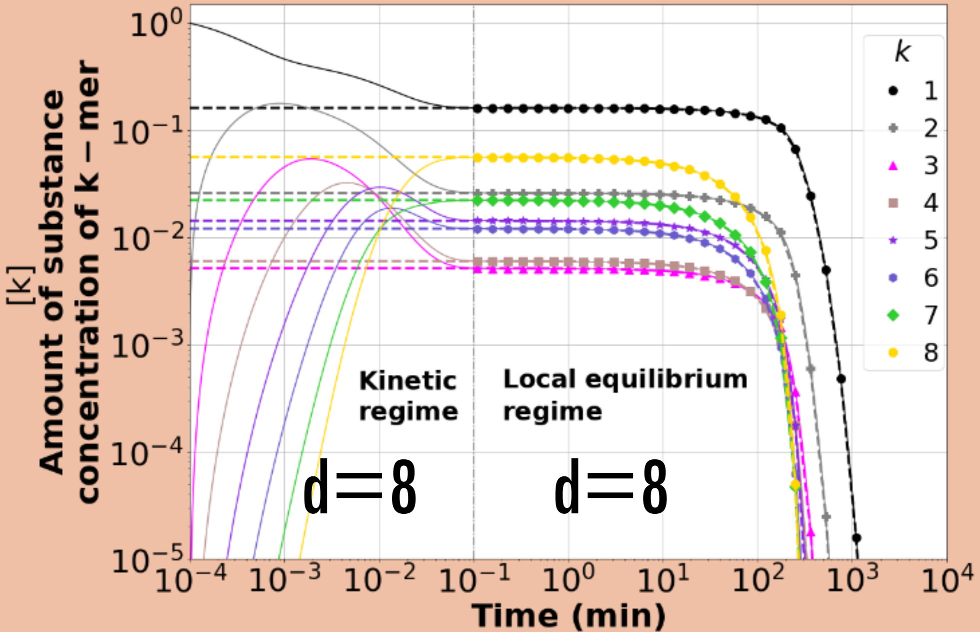
(effectively) irreversible collinear reactions

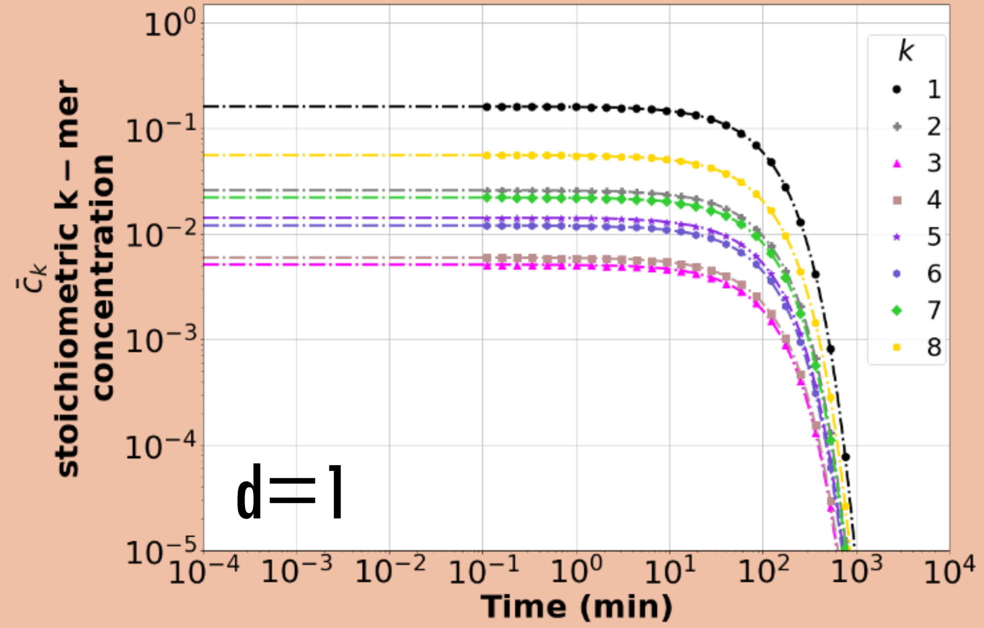
Local isomer equilibria

Fast equilibria + chemostats
(e.g. due to phase separation)

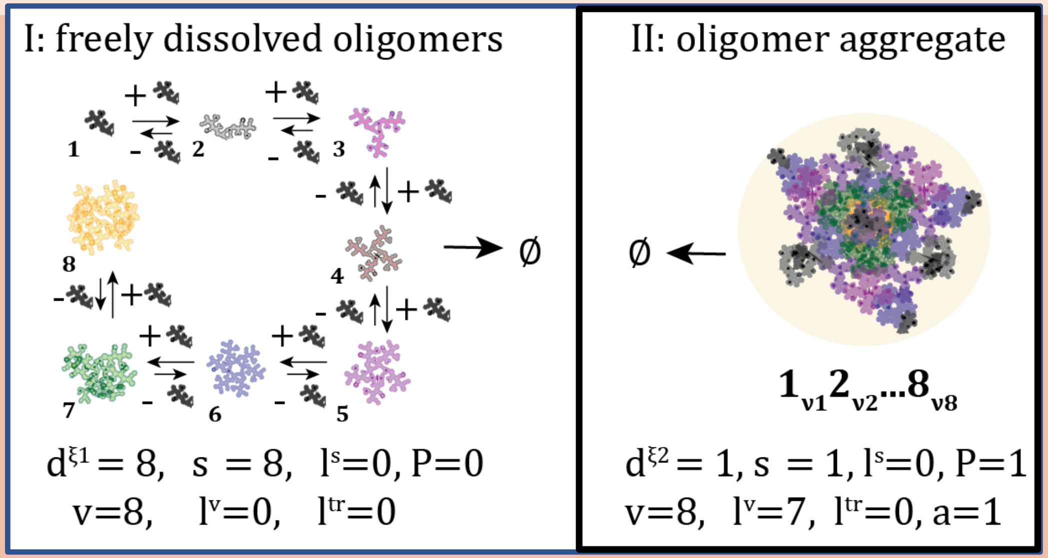
Dramatic dimension reduction with nanoscopic phase separation



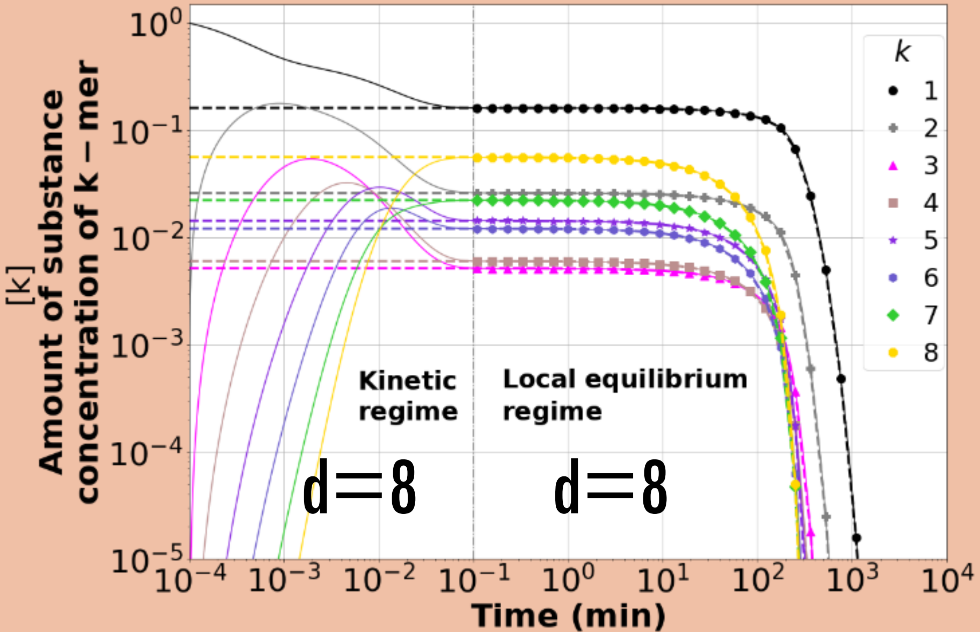


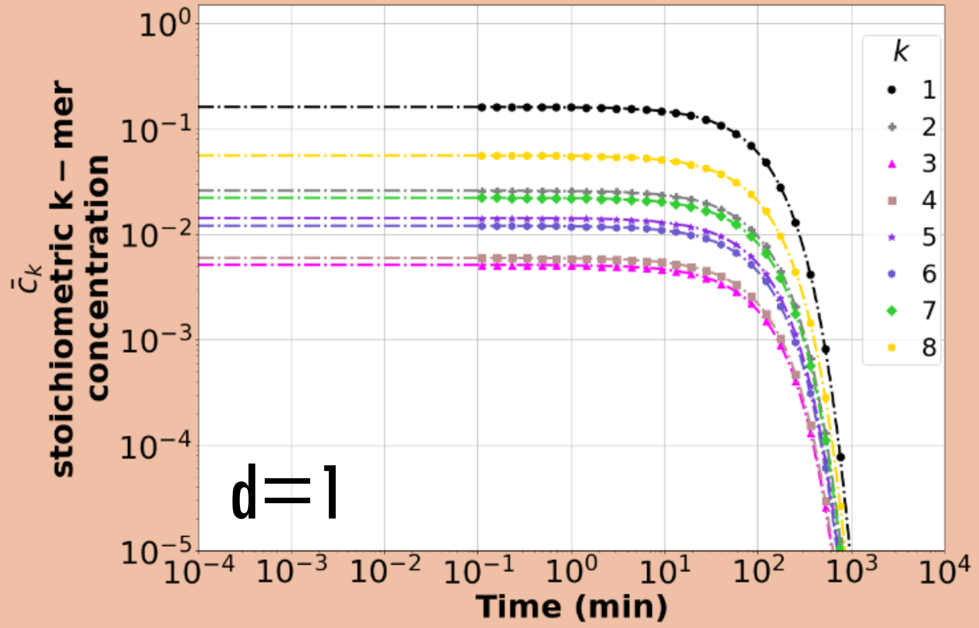


Dramatic dimension reduction with nanoscopic phase separation



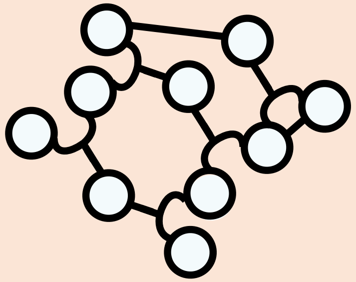
In dynamic combinatorial chemistry, one oftentimes observes very low-dimensional data (d=1,2) in spite of there being many species that can be isolated (e.g. by HPLC-MS)

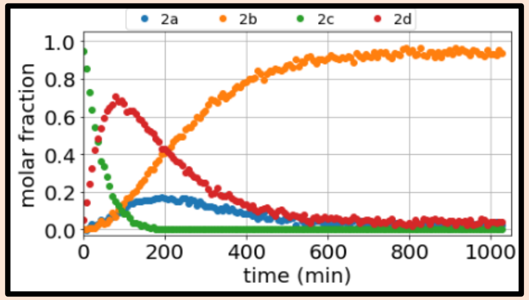


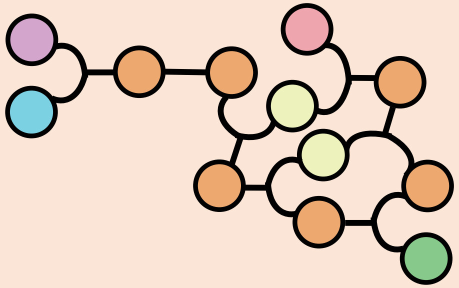


Chemical reaction networks, two problems

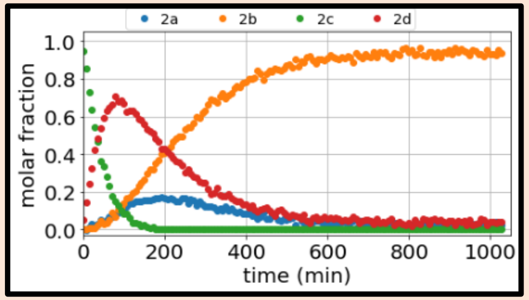
I) How does the structure of a CRN relate to what it can and cannot do?

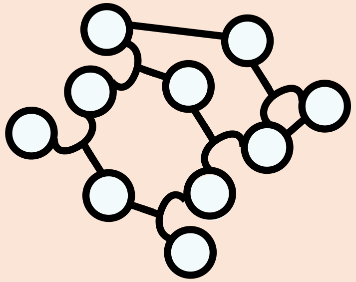






II) How do I know what CRN I'm looking at*?





Thank you

Ottolab

Martijn van Kuppeveld

Hermanslab

oLife

Robert Pollice

Daan van de Weem