# SimSoup: Molecules Designed for Switchable Autocatalytic Memory

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**Abstract**

A memory system based on an artificial chemistry is presented. This is relevant for metabolism based Origin of Life theories, and in the field of biological and chemical computing. Each memory unit can be switched between three alternative active states. A unit maintains itself in a particular state using an autocatalytic reaction process. Switching between states occurs when an external stimulus triggers the autocatalytic process for the new state, along with an associated process that inhibits autocatalytic activity for the old state. Artificial molecular species with structures designed to support the autocatalytic and inhibiting processes are presented. The SimSoup artificial chemistry simulator is used to show that the structures do indeed produce the memory system behaviour. With the advent of engineering at the molecular level, it may be possible to transfer the concepts from an *in silico* environment to a chemical environment.

## Introduction

### Background And Motivation

**Inheritance at the Origin of Life.** Contemporary organisms and viruses use DNA or RNA template molecules to provide the memory needed for inheritance and evolution. Origin of Life research suggests that template molecules and the associated enzymes needed for their accurate replication are too complex to be plausible in a prebiotic environment. Some Origin of Life theories envisage *metabolism based* inheritance in which protocells or lipid enclosed droplets without template molecules reproduced by growth and division. Variations in the metabolisms of different individuals would have led to differences in fitness that would drive evolution. For this to be workable, successful variations in metabolism would have to be 'remembered' and passed on to offspring.

The SimSoup project is investigating memory in chemical networks that could have supported metabolism based inheritance in early organisms.

**Biological and Chemical Computing.** A key challenge for the newer field of biological and chemical computing is the development of memory systems using components that can be readily constructed and manipulated. Such systems may be used for various purposes, including the provision of an inheritance mechanism for the evolution of artificial systems. The simple memory mechanisms being investigated by SimSoup are also relevant in this field.

### Conceptual Background

The SimSoup project takes inspiration from:

- Metabolism based Origin of Life theories including those of Aleksandr Oparin (Oparin, 1957), Stuart Kauffman (Kauffman, 1993), Freeman Dyson (Dyson, 1999), and the Lipid World theory and GARD model of Doron Lancet's group (Segré et al., 1998, 2001a,b)
- Günter Wächtershäuser's chemo-autotrophic Iron-Sulphur World (Wächtershäuser, 2006)
- Walter Fontana's Algorithmic Chemistry (Fontana, 1992)
- Graham Cairns-Smith's clay crystal and genetic takeover theory (Cairns-Smith, 1982)
- Tibor Gánti's principles of life and chemoton theory (Gánti, 2003)
- Network theory, particularly the work of Sanjay Jain and Sandeep Krishna (Krishna, 2003)
- The Chemical Organisation Theory of Peter Dittrich and Pietro Speroni di Fenizio (Dittrich and di Fenizio, 2007)
- Linus Pauling's chemical bond theory (Pauling, 1960).

### The SimSoup Artificial Chemistry Model

The main features of the model are outlined below. A detailed description is available elsewhere (Gordon-Smith, 2013). The program code is also available (SimSoup, 2013).

SimSoup *Molecules* are two dimensional rigid structures built from *Atoms* bonded together such that they occupy fixed positions on a square 'Board' (similar to a chess board). Each square contains at most one Atom. Bond angles are always either 90° or 180°, and bond lengths are all equal. Atoms bond together in a way broadly consistent with valence bond theory. Each distinct molecular structure (or species) is a *Molecule Type*.

Molecules can join or split to form Molecules of different types. Joining must respect the 'one Atom per square' rule, and can take place with the Molecules in any of their eight possible relative orientations. Splitting occurs by breaking the weakest set of bonds that hold the Molecule into a single unit. When two Molecules join (eg $\mathrm{A} + \mathrm{B} \rightarrow \mathrm{C}$), a *Construction Interaction* takes place. A splitting interaction (eg $\mathrm{D} \rightarrow \mathrm{E} + \mathrm{F}$) is called a *Fission Interaction*.

Bond strengths are usually fixed according to the types of Atom at each end of the bond. However, some bonds are *Perturbable*; they can be weakened or strengthened by nearby Atoms that do not themselves participate in the bond.

Construction and Fission Interactions take place in a well-mixed *Reactor*. This is the physical environment in which the Molecules exist. Interaction rates are determined by rate constants that are calculated using parameters analogous to the Arrenhius parameters used by chemists. Fissions typically proceed more quickly for Molecule Types with weak bonds. The rates of Constructions are proportional to the product of the concentrations of the reactants.

### Previous Work: A Non-Switchable Memory Bank

A previous work (Gordon-Smith, 2011), described an artificial chemistry providing a 'memory bank'. The motivation was to provide a proof of concept demonstrating that a chemical network could have a large number of alternative states, as would be needed for metabolism based inheritance.

Each memory unit in the previous work is an *Autocatalytic Sub-Network* within the overall network, and has two states: active and inactive. Interactions occurring in the active state produce Molecules needed for further activity. Each unit corresponds to a particular monomer Molecule Type. Units are arranged in series in the network, and the shapes of their Molecule Types depend on series and position in series.

The presence or absence of monomers of particular types in the Reactor corresponds to stored information. Memory capacity depends on the number of monomer series, and on the number of monomer types in each series.

This previous memory bank has the drawback that the memory units are not easily switchable; once a unit has been activated it cannot be readily de-activated. It can be argued that such switchability may not be essential in some Origin of Life contexts[1]. However, it would be required in many chemical computing scenarios.

## A Switchable Memory Unit

This section presents an *in silico* chemical memory unit that can be readily switched between states. Multiple memory units can co-exist within the same physical environment (Reactor) without interfering with one another; this is due to specific features of the molecular structures.

[1] Although it may affect capacity for co-evolution.

### Concept For Switchability: Rock-Paper-Scissors

The design for switchable memory units is based on the game 'Rock-Paper-Scissors'. The ability of a unit to 'remember' is due to the operation of its three Autocatalytic Sub-Networks. In order to make the memory unit switchable, a mechanism is introduced that enables activity in one Autocatalytic Sub-Network to cause activity in another to be inhibited.

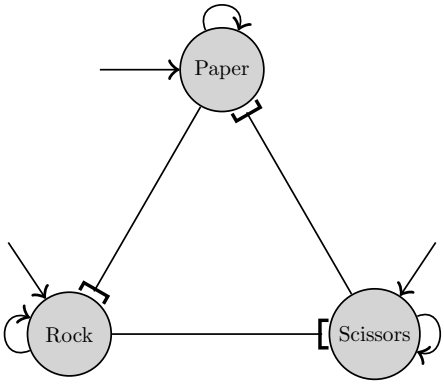


Figure 1: Rock-Paper-Scissors concept for switchable memory units

The overall concept is illustrated in Figure 1. The diagram as a whole represents a switchable memory unit with three active states.[2] Each circle corresponds to an Autocatalytic Sub-Network maintaining one of the states. The 'loopback' arrows denote the (autocatalytic) positive feedback mechanisms by which they maintain themselves. The straight arrows terminating at each circle denote external stimuli that can activate the Autocatalytic Sub-Networks. The lines between circles terminated with '[' symbols signify that Molecules produced by autocatalytic activity maintaining one state can inhibit activity for another state. For example, the 'Scissors' Autocatalytic Sub-Network inhibits the Paper Autocatalytic Sub-Network.

Except during state transitions, only one state can remain active during any period; if two are active simultaneously then one inhibits and 'kills' the other. If all three were active, then all three would also be inhibited, leading to an unstable state with no clear overall 'winner'.

In order for the memory unit to be switched, an external stimulus must be provided to activate the new state. For example, if Rock is currently active, then switching occurs when an external stimulus is provided to activate the Paper state. The system then goes through a transition in which the Rock Autocatalytic Sub-Network is inhibited by a process using Molecules produced by the growing autocatalyic activity for the Paper state. The Paper state itself *is subject*

[2] In the inactive or 'dead' state, none of the three Autocatalytic Sub-Networks would be active.

*to no such inhibiting constraint*. If the unit is to be switched to Scissors, then two separate switching actions must take place, first to Paper and then to Scissors.[3]

## Overview Of Memory Unit Design

Figure 2 illustrates the design for a memory unit. It shows both the structure of the (artificial) chemical network, and a 'thumbnail' structure diagram for each Molecule Type involved in maintaining and inhibiting the unit's 'Rock' state. The arcs between lines joining Molecule Types identify Constructions and Fissions. Specific details of the molecular structures and bonds, and the way they support the operation of the memory unit are given later, along with naming conventions for Molecule Types.

Each co-existing memory unit has its own set of characteristic 'Rock-Paper-Scissors' Molecule Types and states. For example, memory unit $n$ has possible active states, $\mathrm{Rock_n}$, $\mathrm{Paper_n}$, and $\mathrm{Scissors_n}$, and uses Molecule Types such as $\mathrm{R_n}$ and $\mathrm{R_{n_{pre}}}$. Each memory unit state has an Autocatalytic Sub-Network, and an *Inhibiting Sub-Network* for the inhibition mechanism.

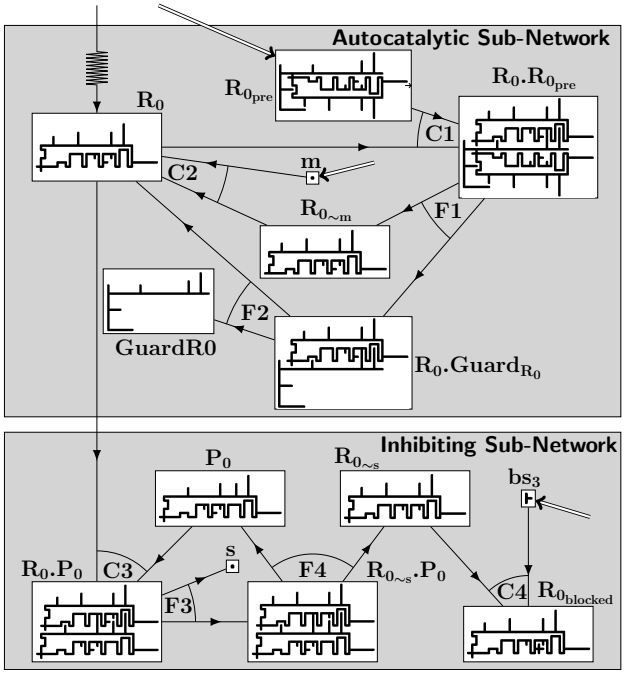


Figure 2: Overview of Network and Molecular Structures for the '$\mathrm{Rock_0}$' State. The top section shows Molecule Types and Interaction Types for the $\mathrm{Rock_0}$ Autocatalytic Sub-Network. The lower section shows the Inhibiting Sub-Network for $\mathrm{Rock_0}$. The zig-zag arrow indicates an external stimulus. Double arrows indicate a constant supply. Labelled arcs indicate Constructions and Fissions.

[3]The need for two stage switching is a drawback, but a consequence of the simple design in which the same input is used both for activating one sub-network and inhibiting another.

**The Autocatalytic Sub-Network.** The zig-zag arrow terminating at $\mathrm{R_0}$ indicates that an external stimulus consisting of a few $\mathrm{R_0}$ Molecules can be provided to the memory unit. The double arrows terminating at $\mathrm{R_{0_{pre}}}$ and m (Metal) indicate that a constant supply of each is provided.

The autocatalytic reaction process begins when $\mathrm{R_{0_{pre}}}$ and $\mathrm{R_0}$ combine under Construction C1 to form $\mathrm{R_0.R_{0_{pre}}}$. Each $\mathrm{R_0.R_{0_{pre}}}$ Molecule then breaks up in two successive Fissions, F1 and F2. F1 produces one Molecule of $\mathrm{R_{0_{\sim m}}}$ and one of $\mathrm{R_0.Guard_{R_0}}$. The $\mathrm{R_{0_{\sim m}}}$ Molecule goes on to combine with an 'm' Atom (Metal) in Construction C2 to return an $\mathrm{R_0}$ Molecule. F2 splits the $\mathrm{R_0.Guard_{R_0}}$ Molecule into one Molecule of $\mathrm{Guard_{R_0}}$, and a second (excess) $\mathrm{R_0}$ Molecule. The overall reaction process is:

$$\mathrm{R_{0_{pre}} + m} \xrightarrow{\mathrm{R_0}} \mathrm{R_0 + Guard_{R_0}}.$$[4]

The process can only start if an initial input of $\mathrm{R_0}$ is provided as a catalyst. Once started, the process produces an excess of $\mathrm{R_0}$, and no further external input of $\mathrm{R_0}$ is needed.

**The Inhibiting Sub-Network.** The Inhibiting Sub-Network impedes activity of the Autocatalytic Sub-Network by converting $\mathrm{R_0}$ Molecules to $\mathrm{R_{0_{blocked}}}$ Molecules that cannot participate in the autocatalytic reaction process. The conversion starts with Construction C3, which produces $\mathrm{R_0.P_0}$ from $\mathrm{R_0}$ and $\mathrm{P_0}$. Each $\mathrm{R_0.P_0}$ Molecule then splits (Fission F3) to produce an Atom of s (Stoppite) and an $\mathrm{R_{0_{\sim s}}.P_0}$ Molecule. Each $\mathrm{R_{0_{\sim s}}.P_0}$ Molecule splits (Fission F4) to produce a Molecule of $\mathrm{R_{0_{\sim s}}}$ and a Molecule of $\mathrm{P_0}$, returning the one required for Construction C3. Finally, the $\mathrm{R_{0_{blocked}}}$ Molecule is produced by combining the $\mathrm{R_{0_{\sim s}}}$ Molecule with a $\mathrm{bs_3}$ Molecule (Construction C4).

The overall reaction process for the Inhibiting Sub-Network is:

$$\mathrm{R_0 + bs_3} \xrightarrow{\mathrm{P_0}} \mathrm{R_{0_{blocked}} + s}.$$

The process can only proceed in the presence of $\mathrm{P_0}$ as a catalyst. The Autocatalytic Sub-Network for the $\mathrm{Paper_0}$ state produces $\mathrm{P_0}$, and this is the basis by which the $\mathrm{Paper_0}$ inhibits the $\mathrm{Rock_0}$ state.

## Molecular Structures and Bonds

This section details the molecular structures used by the memory unit, and the way they support its operation. The structures are constructed from (artificial) Atoms that bond in particular ways, and so the Atom Types and Bond Types are described first.

### Atom Types

The memory unit uses Atom Types with properties designed to support the Interaction Types that are needed for its operation. Table 1 shows these Atom Types. The 'Bonds' col-

[4]$Guard_{R_0}$ produces further 'waste' products (not shown).

umn indicates the number of bonds that each Atom Type can form. All the Atom Types have mass 10.

| Name/Symbol | Bonds | Usage / Capability |
|---|---|---|
| Assemblite ● | 2 | Used to build framework of molecular structures |
| Blockite b | 4 | Used to build $bs_3$ 'Blocker' |
| Hookite h | 4 | Used to provide a 'hook' bonding site |
| Junctium j | 3 | Used to provide a 3 way junction in a structure |
| Loosium-1 w | 2 | Provides a weak (loose) bonding site for Loosium-2 |
| Loosium-2 x | 2 | Provides a weak (loose) bonding site for Loosium-1 |
| Metal m | 1 | Can perturb nearby Perturbium bonds, even though not bonded to Perturbium |
| Perturbium p | 3 | Produces bonds that can be weakened or strengthened by nearby Metal atoms |
| Stoppite s | 1 | Stops further growth of the Molecule at a site |

Table 1: Atom Types used for the switchable memory units

## Bond Types

Table 2 shows the Bond Types that can exist between the various Atom Types. The meanings of the cell entries are as follows:

- Blank: Atom of these types do not bond
- x: Atoms bond with Enthalpy (strength) 100
- w: Atoms bond weakly, with Enthalpy 10
- p: Perturbable Bond

| | **a** | **h** | **j** | **b** | **m** | **p** | **s** | **w** | **x** |
|---|---|---|---|---|---|---|---|---|---|
| **a** | x | | | | | | | | |
| **h** | x | | | | | | | | |
| **j** | x | x | x | | | | | | |
| **b** | | | | | | | | | |
| **m** | x | x | x | | | | | | |
| **p** | x | p | x | x | | | | | |
| **s** | x | x | x | x | | p | x | | |
| **w** | x | | x | | | | | | |
| **x** | x | | x | | | | | w | |

Table 2: Bond Types: Each cell shows the characteristics of a bond between a top row Atom and a left column Atom.

A *Perturbable Bond* is one whose strength can be affected by the presence of a nearby Atom of a specific type, even though that Atom is not bonded to either of the Atoms participating in the bond. For the work described in this paper, the normal Enthalpy of the Perturbable Bonds shown in the table is 100, but reduces to 5 in the presence of a nearby Metal Atom, making the bond more likely to break quickly.

## Molecule Types

This section shows details of the Molecule Types for the memory unit, and describes the way they support its operation. Conventions for naming Molecule Types are described where they are first used.

**Core Molecule Types: $\mathbf{R_n}$, $\mathbf{P_n}$, $\mathbf{S_n}$.** Figure 3 shows the *Core Molecule Types* for the three Autocatalytic Sub-Networks of the n=0 memory unit. $R_0$ is produced by the $Rock_0$ Autocatalytic Sub-Network. Similarly $P_0$ and $S_0$ are produced by the $Paper_0$ and $Scissors_0$ Autocatalytic Sub-Networks respectively.

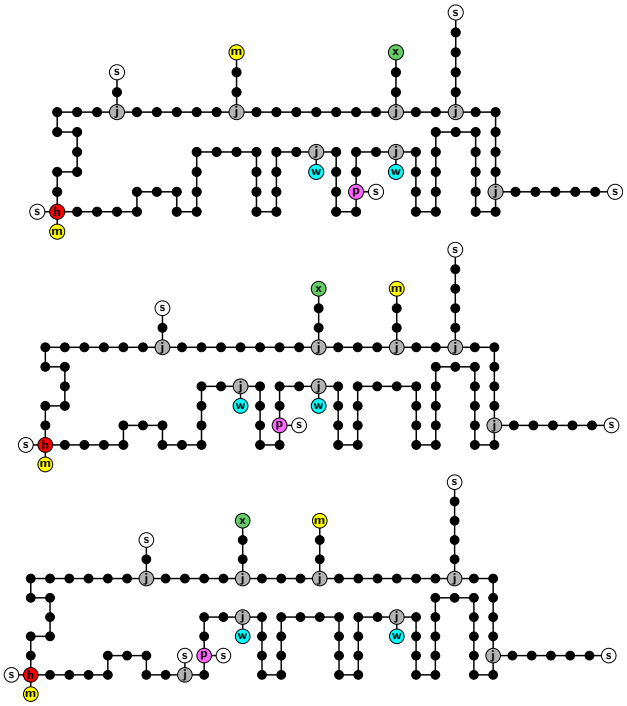

Figure 3: $R_0$ (top), $P_0$ (centre) and $S_0$ (lower): The Core Molecule Types for the $Rock_0$, $Paper_0$ and $Scissors_0$ Autocatalytic Sub-Networks.

The following features can be noted:

- Each Molecule Type has various recesses and protuberances. These are positioned to prevent Constructions that would produce Molecule Types that interfere with the operation of the memory unit
- $S_0$ is one unit wider than $P_0$, which is one unit wider than $S_0$. This is also to prevent the production of interfering Molecule Types
- The three central recesses along the bottom of each of $R_0$, $P_0$ and $S_0$ are key to the mechanisms for both autocatalysis and inhibition. The recess that includes both a Loosium-1 (w) Atom and a Stoppite (s) Atom is called the

*Owner Recess*. The recess that includes just a Loosium-1 (w) Atom is called the *Successor Recess*, and the 'empty' recess is called the *Predecessor Recess*

- The recesses are arranged cyclically, so that the Successor Recess for one Molecule Type lines up with the Owner Recess for the Molecule Type that 'beats' (or succeeds) it
- Above each Owner Recess there is a protuberance (the *Owner Protuberance*) that terminates with a Loosium-2 Atom. Above each Predecessor Recess there is a *Predecessor Protuberance* that terminates with a Metal Atom.

The roles of these protuberances and recesses in the operation of the memory unit are described later in this section.

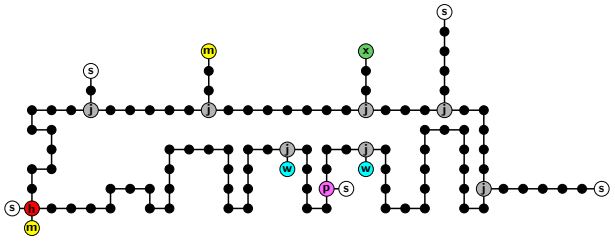

Figure 4: $\mathrm{R}_1$, the Core Molecule Type for $\mathrm{Rock}_1$.

Figure 4 shows $\mathrm{R}_1$, the Core Molecule Type for the $\mathrm{Rock}_1$ Autocatalytic Sub-Network. It is identical to $\mathrm{R}_0$, except that there is an additional space to the right of the Owner Recess. $\mathrm{P}_1$ and $\mathrm{S}_1$ have similar additional space by comparison with their n=0 counterparts. Core Molecule Types for larger n values have correspondingly larger spaces. The spacing ensures that corresponding Molecules (eg $\mathrm{R}_0, \mathrm{R}_1$) for different co-existing memory units do not interfere.

**'Missing Atom' Variants of Core Molecules.** Variants of the Core Molecule Types with a 'missing' Metal or Stoppite Atoms occur in the Autocatalytic and Inhibiting Sub-Networks. If the Stoppite Atom in the Owner Recess of the $\mathrm{R}_0$ Molecule shown at the top of Figure 3 is removed, the result is called $\mathrm{R}_{0_{\sim \mathrm{s}}}$. Similarly, if the Metal Atom at the bottom left of the Molecule is removed, the result is $\mathrm{R}_{0_{\sim \mathrm{m}}}$.

**Core Molecule Type Precursors and Guards.** The Autocatalytic Sub-Network for a memory unit is provided with a constant supply of *Precursors* for its Core Molecule Types.

Figure 5 shows $\mathrm{R}_{0_{\mathrm{pre}}}$, the Precursor for $\mathrm{R}_0$. This consists of $\mathrm{R}_{0_{\sim \mathrm{m}}}$ ($\mathrm{R}_0$ less a Metal Atom) with an adjoined *Guard*. The Guard covers the Owner, Successor and Predecessor Recesses for the Core Molecule Type, making them inaccessible to protuberances. Figure 6 shows $\mathrm{Guard}_{\mathrm{R}_0}$, the Guard for $\mathrm{R}_0$.

**Role Of The Precursor.** A type $n$ memory unit is provided with a supply of $\mathrm{R}_{\mathrm{n}_{\mathrm{pre}}}$, $\mathrm{P}_{\mathrm{n}_{\mathrm{pre}}}$ and $\mathrm{S}_{\mathrm{n}_{\mathrm{pre}}}$, the Precursors

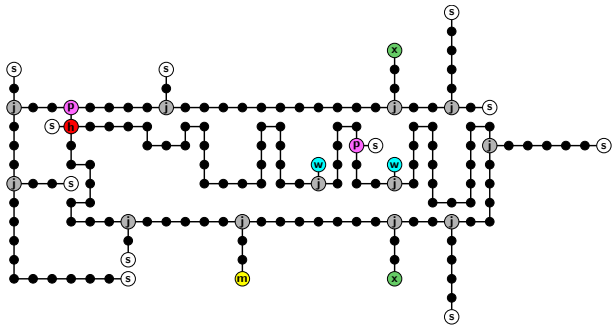

Figure 5: $\mathrm{R}_{0_{\mathrm{pre}}}$, the Precursor for $\mathrm{R}_0$.

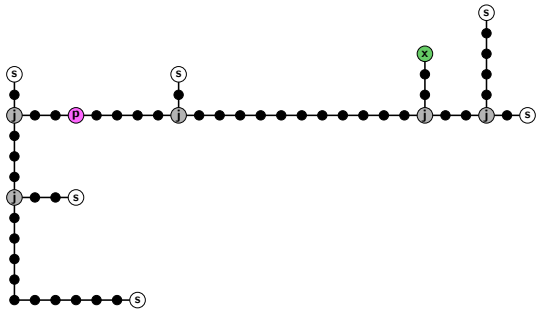

Figure 6: $\mathrm{Guard}_{\mathrm{R}_0}$, the Guard for $\mathrm{R}_0$.

for its Core Molecule Types $\mathrm{R}_0$, $\mathrm{P}_0$ and $\mathrm{S}_0$. The Precursor can be split as described shortly by the Autocatalytic Sub-Network to release a Core Molecule. The steady supply of Precursor Molecules therefore provides the 'food' that enables a memory unit to maintain its active state.

**Role Of The Guard.** The Guard part of a Precursor Molecule Type has two roles:

- It has a Protuberance terminated with a Loosium-2 (x) Atom that bonds weakly to the Loosium-1 (w) Atom in the corresponding Core Molecule Type to form a Precursor Splitter Complex
- It prevents Precursors from combining with successor Core Molecules to produce Precursor.Core Complexes instead of Core.Core Complexes that are essential for the Inhibiting Sub-Network.

**The Precursor Splitter Complex.** A Core Molecule Type can join with its Precursor to produce a *Precursor Splitter Complex*. Figure 7 shows the Precursor Splitter Complex, $\mathrm{R}_0.\mathrm{R}_{0_{\mathrm{pre}}}$, for the $\mathrm{Rock}_0$ Autocatalytic Sub-Network.

The two Molecules join at the Loosium-1 to Loosium-2 (w-x) bond in the Core Molecule's Owner Recess (see Construction C1 in Figure 2). The Metal Atom at the bottom left of the Core Molecule is placed just above (but not bonded to) the Perturbium-Hookite bond at the top left of the Precursor.

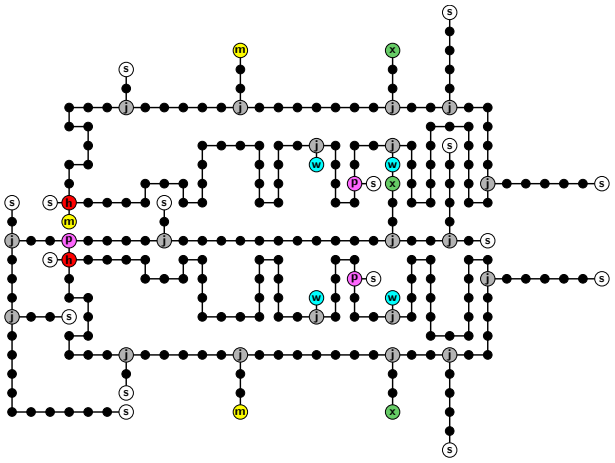

Figure 7: $\mathrm{R}_0.\mathrm{R}_{0_{\mathrm{pre}}}$: The Precursor Splitter Complex for the $\mathrm{Rock}_0$ Autocatalytic Sub-Network

This weakens the bond, which soon splits (Fission F1) releasing a 'missing Metal' variant of the Core Molecule and a Reverse Guard Complex (see next section).

The 'missing Metal' Core variant combines with freely available Metal to form a Core Molecule. This replaces the Core Molecule that combined with the Precursor.

**The Reverse Guard Complex.** When a Precursor Splitter Complex splits, one of the products is a *Reverse Guard Complex*. This is a Core Molecule with a Guard in a 'reverse' configuration. Figure 8 shows the Reverse Guard Complex, $\mathrm{R0.Guard}_{\mathrm{R}_0}$, for the $\mathrm{Rock}_0$ Autocatalytic Sub-Network.

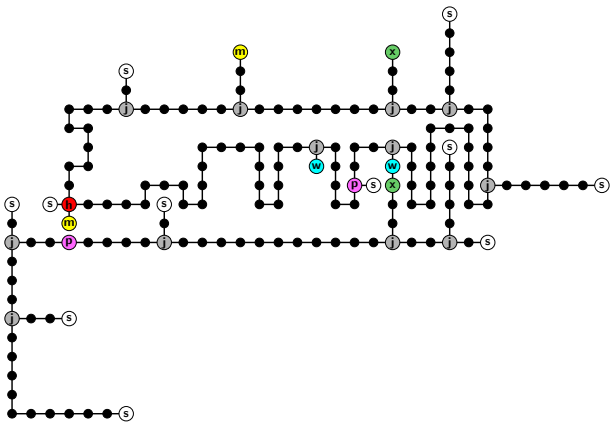

Figure 8: $\mathrm{R}_0.\mathrm{Guard}_{\mathrm{R}_0}$, the Reverse Guard Complex for the $\mathrm{Rock}_0$ Autocatalytic Sub-Network

The Reverse Guard Complex is held together by the Loosium-1 to Loosium-2 (w-x) bond that was formed when the Core Molecule joined with a Precursor in Construction C1. This is a weak bond (see Table 2), and soon breaks (Fission F2), releasing a Core Molecule and an (un-needed) Guard. The Core Molecule released here is the one that previously combined with the Precursor. A Core Molecule was also produced by Fission F1, and so there is an excess.

**The Core.Core Complex.** Two Core Molecule Types for different states of the same memory unit can join to form a *Core.Core Complex* that plays a key role in the Inhibiting Sub-Network. Figure 9 shows the $\mathrm{R}_0.\mathrm{P}_0$ Core.Core Complex.

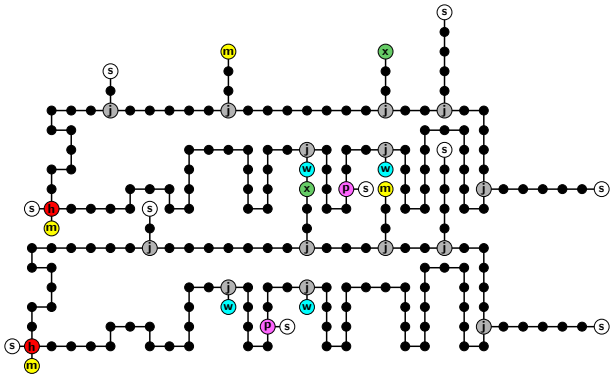

Figure 9: $\mathrm{R}_0.\mathrm{P}_0$: The Core.Core Complex for the $\mathrm{Rock}_0$ Inhibiting Sub-Network

The two Core Molecules are joined at the weak Loosium-1 to Loosium-2 (w-x) bond in the top Molecule's Successor Recess, and will soon break apart again (Fission F4). However, while the complex persists, a Metal Atom from the lower (Successor) Molecule is held next to the Perturbium to Stoppite bond in the top Molecule's Owner Recess. This bond is weakened, and the Stoppite Atom soon splits off (Fission F3). This makes available a bonding site that will be used to block autocatalysis.

**Blocked Core Molecule Types and bs3 Blockers.** The Inhibiting Sub-Network converts Core Molecules to *Blocked Core Molecules* that cannot participate in the autocatalytic reaction process.

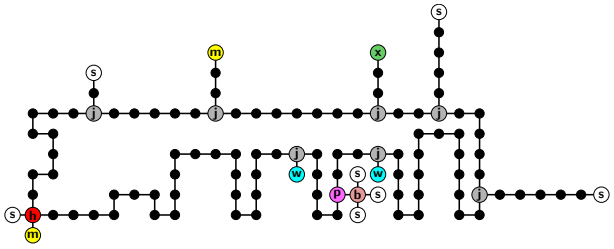

Figure 10: $\mathrm{R}_{0_{\mathrm{blocked}}}$: the Blocked Core Molecule for the $Rock_0$ Inhibiting Sub-Network

The blocking is achieved by incorporating a small *Blocker* Molecule, $\mathrm{bs}_3$, into the Core Molecule's Owner Recess.

This is done by removing a Stoppite Atom from a Core Molecule to produce a 'missing Stoppite' variant (Fissions F3 and F4), and attaching a freely available Blocker at the bonding site that this creates (Construction C4).

Figure 10 shows $\mathrm{R}_{0_{\mathrm{blocked}}}$, the Blocked Core Molecule Type for $\mathrm{R}_0$. The small $\mathrm{bs}_3$ Blocker can be seen in the Owner Recess.

## Results

Figure 11 shows the operation of a 9-state memory system comprising two 3-state memory units co-existing in the same Reactor. The scenario was as follows:

- Atom Types and Bond Types as described earlier
- A constant supply of Precursors for the $n = 0$ memory unit ($\mathrm{R}_{0_{\mathrm{pre}}}$, $\mathrm{P}_{0_{\mathrm{pre}}}$ and $\mathrm{S}_{0_{\mathrm{pre}}}$) is provided, 400 of each every 10 timesteps
- A similar supply of $n = 1$ Precursors is setup
- A constant supply of Metal Atoms and $\mathrm{bs}_3$ Blockers is setup, 2000 of each every 10 timesteps
- A small stimulus of 7 $\mathrm{R}_0$ Molecules is input at time 10000, and at subsequent intervals of 60,000 timesteps. Similar series of stimuli are setup for $\mathrm{P}_0$ and $\mathrm{S}_0$, starting at times 30,000 and 50,000 respectively
- Stimuli are setup for the $n = 1$ Core Molecules at times 10,000, 70,000 and 130,000
- Each Molecule has a removal probability at each timestep of 0.005.

The top plot shows that following the $\mathrm{R}_0$ stimulus at time 10,000, the number of $\mathrm{R}_0$ Molecules in the Reactor rises from zero to about 850, and stays at that level. This is due to the operation of the $\mathrm{Rock}_0$ Autocatalytic Sub-Network. At time 30,000 the $\mathrm{P}_0$ stimulus is added. The number of $\mathrm{P}_0$ Molecules rises to about 850 due to the operation of the $\mathrm{Paper}_0$ Autocatalytic Sub-Network, and the number of $\mathrm{R}_0$ Molecules falls to zero due to the operation of the $\mathrm{Rock}_0$ Inhibiting Sub-Network. The rest of the plot shows repeated cyclic switching between states of the $n = 0$ unit.[5]

The middle plot shows the numbers of Core.Core Complex Molecules. These are key to the operation of the Inhibiting Sub-Network during the transition from one state of the memory unit to another. As the plot shows, they are present only during these transitional periods.

The lower plot shows the numbers of Core Molecules for the co-existing $n = 1$ memory unit. The top and lower plots together show that the system as a whole has 9 states, corresponding to the number of possible states for two independently switchable 3-state units.

[5]The small excess of $\mathrm{P}_0$ at time 100,000 is as yet unexplained.

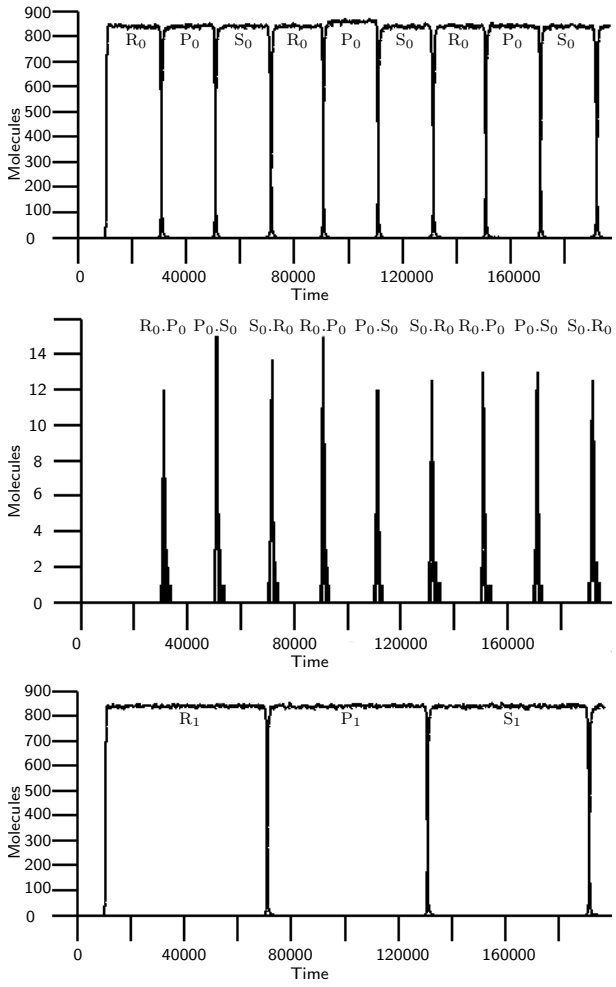


Figure 11: Operation of two co-existing 3 state memory units. Top: The $n = 0$ unit cycling through its three states. Middle: Numbers of Core.Core Complexes present during switching of the $n = 0$ unit. Bottom: The $n = 1$ unit cycling through its three states.

## Conclusions

1. It has been demonstrated that it is possible to produce a switchable memory unit using (artificial) Molecules with structures specifically designed to produce a reaction network with Autocatalytic and Inhibiting Sub-Networks
2. It is possible to combine multiple memory units in the same (well mixed) chemical environment in such a way that they do not interfere with each other's operation. In the results presented here, two 3-state units were combined to produce a memory system with 9 states
3. The design of the Molecules is such that further memory units with higher $n$ values can be produced by new Core Molecule Types with additional spaces to the right of the Owner Recess. The number of states for a system including $m$ memory units is $3^m$, and the number

of Core Molecule Types needed is $3m$. A memory system with 30 Core Molecule Types could therefore support $3^{10} = 59049$ states. The number of states for a system with 60 Core Molecule Types would be almost 3.5 million

4. From an Origin Of Life perspective, a population of protocells can be envisaged, each containing a memory system in a particular state. The memory system would influence other aspects of a larger reaction network affecting behaviour, such that it could support an evolutionary process in which fitter protocells were selected.

   It can be argued that an inheritance mechanism supporting 3.5 million alternative 'phenotypes' provides sufficient scope for such an evolutionary process to get a foothold. This would require a protocell to have a foodset including 60 Core Precursor Molecule Types. This requirement may not be as stringent as appears at first sight; the Core Molecule Types and the Precursors all follow the same basic pattern. It can be envisaged that they could be produced by a systematic process with scope for random variations within the framework of that pattern

5. From the perspective of chemical and biological computing systems, it may be possible, with the advent of engineering at the molecular level, to use the concepts described here as the basis of a similar artificial evolutionary mechanism, or as memory for different applications.

6. The molecular structures shown in this paper are just one way of implementing the memory units. It is likely that there are many alternatives with totally different structures. Molecular structure design could take account of considerations regarding what can be easily engineered

7. There is a trade-off between the chemical complexity involved in a larger number of Core Molecule Types required for co-existing memory units vs physically separate memory units but fewer Core Molecule Types. For droplet (or 'protocell') based artificial evolution, the former is likely to be preferred, as it does not require physical separation of different memory units within the droplet.

## Prospects

The author would like to hear from anyone interested in transferring the concepts described here from an *in silico* environment to a chemical environment.

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