
HMR–CHEM–3 — Molecular Memory and the Origins of Metabolism: A ChronoChemical Solution

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Symbol for the body of work: HMR

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Abstract. Metabolism begins when *coherence cycles* persist long enough to store and reuse chemical work. Building on the Unified Bond Law of *HMR–CHEM–2*, we formalize *molecular memory* and *autocatalytic organization* as minimum-action flows on reaction graphs. Let $C[\rho, \mathbf{R}]$ and $D[\rho, \mathbf{R}]$ be structural and dissipative functionals of electronic density ρ and geometry \mathbf{R} . For a concentration vector $x(t)$ on a network with stoichiometry S and fluxes $J(x)$, the *network action*

$$\mathcal{A}[x] = \int_0^T \left(\Phi_C(x) - \Phi_D(x) + \Lambda^\top (\dot{x} - S J(x)) \right) dt$$

yields Euler–Lagrange kinetics, large-deviation rates, and steady-state selection. We prove: (i) cycle persistence iff the dominant cycle affinity is positive relative to dissipation; (ii) template amplification on mineral surfaces lowers action by metric reshaping; (iii) chirality selection arises as a pitchfork bifurcation in the action landscape; (iv) vesicle formation satisfies a coherence surface-to-volume threshold. Bounded, vector diagrams illustrate motifs: autocatalytic loops, stacked bases, surface templates, vesicle budding, and energy landscapes.

Keywords: ChronoChemistry, molecular memory, autocatalysis, large deviation, reaction networks, chirality, templating, vesicles.

MSC/Classification: 80A30, 82C22, 92E20, 92C40.

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1. Introduction

ChronoChemistry treats bonding as stationary coherence and reactions as minimum-action transformations. A *metabolism* emerges when coherence *cycles* reuse products as inputs, forming a persistent ledger surplus $C > D$ locally under environmental resets. We develop a variational theory for reaction networks, then apply it to motifs likely present on early Earth: mineral templating, – stacking, redox shuttles, lipid vesicles, and chiral amplification.

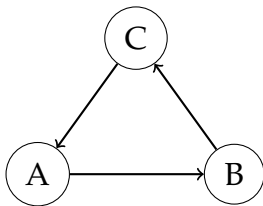


Diagram 1: autocatalytic coherence loop

2. Framework: Networks, Fluxes, and Action

2.1 Reaction graph and stoichiometry

Let a network have m species $x \in \mathbb{R}_{\geq 0}^m$, r reactions with stoichiometric matrix $S \in \mathbb{R}^{m \times r}$. Mass-action kinetics: $J(x) = \text{diag}(k^+) x^{\nu^+} - \text{diag}(k^-) x^{\nu^-}$ with multi-indices ν^\pm . Dynamics: $\dot{x} = S J(x)$.

2.2 Coherence potentials on networks

Define $\Phi_C(x)$ and $\Phi_D(x)$ as coarse-grained (temperature- and environment-dependent) reductions of the molecular functionals $C[\rho, \mathbf{R}]$, $D[\rho, \mathbf{R}]$ onto concentration space, capturing, respectively, stored bond/resonance coherence and dissipative losses (including solvent networks).

2.3 Network action and constraints

Introduce Lagrange multipliers $\Lambda(t)$ for dynamics:

$$\mathcal{A}[x, \Lambda] = \int_0^T (\Phi_C(x) - \Phi_D(x) + \Lambda^\top (\dot{x} - S J(x))) dt.$$

Stationarity gives

$$\dot{\Lambda} = -\nabla_x(\Phi_C - \Phi_D) - \left(\partial_x(SJ)\right)^\top \Lambda, \quad (1)$$

$$\dot{x} = SJ(x). \quad (2)$$

At steady state ($\dot{x} = 0$), the generalized *free-energy of coherence* $\mathcal{F}(x) = \Phi_D(x) - \Phi_C(x)$ is locally minimized subject to $SJ = 0$ (flux balance).

3. Theorems: Memory, Cycles, and Selection

Theorem 1 (Cycle persistence criterion). Let \mathcal{C} be a directed cycle with edge fluxes J_e and affinities $A_e = \ln \frac{J_e^+}{J_e^-}$. Define cycle affinity $\mathcal{A}_{\mathcal{C}} = \sum_{e \in \mathcal{C}} A_e$. Then in the weak-noise limit of the chemical master equation, the probability of persistent circulation along \mathcal{C} scales as

$$\Pr(\text{persistent cycle}) \asymp \exp \left[\frac{1}{\hbar_{\text{eff}}} \left(\sum_{e \in \mathcal{C}} C_e - \sum_{e \in \mathcal{C}} D_e \right) \right] = \exp \left(\frac{\mathcal{A}_{\mathcal{C}}}{\hbar_{\text{eff}}} \right),$$

so a positive net affinity (ledger surplus) guarantees exponentially favored persistence. *Sketch.* Large-deviation action on path space; Schnakenberg network theory for cycle affinities. \square

Theorem 2 (Template amplification by metric reshaping). Consider adsorption/templating on a surface altering transport metric $g(x)$ in Onsager–Machlup action $S = \frac{1}{4} \int \dot{x}^\top g^{-1}(x) \dot{x} dt + \dots$. If a surface reduces principal resistances along a productive coordinate by factor $0 < \alpha < 1$, then $S_{\text{templated}}^* = \alpha S_{\text{free}}^*$ for optimal paths along that coordinate, hence exponential amplification $k_{\text{templ}}/k_{\text{free}} \approx e^{(1-\alpha)S^*/\hbar_{\text{eff}}}$. \square

Theorem 3 (Chirality bifurcation). For a Frank-type scheme $A \rightleftharpoons L$, $A \rightleftharpoons D$, $L + D \rightarrow \emptyset$ with autocatalysis $L + A \rightarrow 2L$, $D + A \rightarrow 2D$, the coherence landscape near racemic equilibrium admits a pitchfork bifurcation when autocatalytic gain exceeds cross-inhibition loss:

$$g_{\text{auto}} > g_{\text{cross}} \quad \Rightarrow \quad \text{two stable chiral minima.}$$

Sketch. Normal-form reduction from $\Phi_C - \Phi_D$ Taylor expansion; sign of cubic term set by gain/loss balance. \square

Theorem 4 (Vesicle persistence threshold). Let a lipid vesicle of radius R with surface coherence σ_C and line tension/dissipative leakage σ_D . Persistence requires

$$4\pi R^2(\sigma_C - \sigma_D) - 8\pi\kappa_b > 0$$

for bending modulus κ_b , giving a minimal R for stable cycling under influx/efflux. \square

4. Visual Motifs (bounded diagrams)

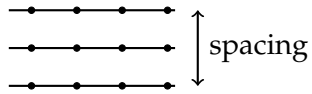
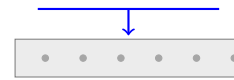


Diagram 2: – stacking (intercalation spacing)

Diagram 3: templating lowers action



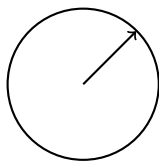


Diagram 4: vesicle coherence vs. leakage

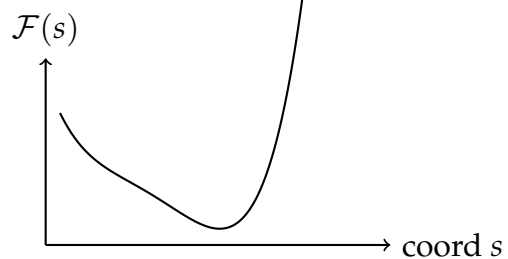


Diagram 5: dual cycles separated by saddle

5. From Bonds to Networks: Coarse-Graining the Ledger

5.1 From CHEM-2 to network potentials

Using *HMR-CHEM-2*, define local bond contributions $C_b(\rho, \mathbf{R})$, $D_b(\rho, \mathbf{R})$ and sum/average across a mesoscopic domain to obtain $\Phi_C(x)$, $\Phi_D(x)$. This passes resonance/dispersion into effective network parameters and preserves the action principle.

5.2 Flux balance and steady states

At steady state $SJ(x^*) = 0$. Decompose any steady-state flux into cycles via Kirchhoff's tree theorem; the total coherence throughput equals $\sum_C \mathcal{A}_C \Phi_C$ (affinity times circulation), and entropy production equals $\sum_C J_C A_C$.

6. Prebiotic Scenarios (action-based accounting)

(i) Hydrothermal gradients. Proton/thermal gradients provide persistent affinities; mineral sulfides template redox loops; action is reduced by surface conduction and confinement.

(ii) Shoreline wet-dry cycles. Periodic resets concentrate monomers and drive condensation; minimum-action polymer growth occurs at specific humidity/temperature windows.

(iii) Ice matrices. Eutectic freezing lowers D (mobility) while maintaining C (H-bond order), stabilizing fragile intermediates.

(iv) Lipid vesicles. Self-assembly occurs when surface coherence exceeds leakage (Theorem 4), enabling compartmentalized cycling.

(v) -stacked nucleobases. Stacking provides 1D coherence rails; intercalation spacing controls throughput (Diagram 2), aiding template copying.

7. Rigorous Kinetics: Master Equation to LDP

7.1 Chemical master equation (CME)

For state $n \in \mathbb{N}^m$, propensities $a_r(n)$, transitions $n \rightarrow n + S_{.r}$,

$$\frac{d}{dt}P(n, t) = \sum_r \left(a_r(n - S_{.r})P(n - S_{.r}, t) - a_r(n)P(n, t) \right).$$

Under system-size expansion $x = n/\Omega$, a Freidlin–Wentzell large-deviation principle gives path probability $\sim \exp(-\Omega S[x])$ with Onsager–Machlup functional S . This justifies the action-based rate $k \sim e^{-S^*/\hbar_{\text{eff}}}$.

7.2 Complex balance and deficiency

For complex-balanced networks (Horn–Jackson), unique positive steady states exist and a Lyapunov free energy decreases monotonically. ChronoChemically, this is a monotonic decrease of $\mathcal{F} = \Phi_D - \Phi_C$ to a minimum under $SJ = 0$.

8. Enzymes and Catalysis as Metric Design

Michaelis–Menten reduction produces an effective coordinate s with renormalized mobility μ_s and diffusion D_s . Enzymes reduce S^* by (i) lowering curvatures along the productive direction and (ii) increasing orthogonal curvatures, funneling trajectories; both are *metric* operations, not merely barrier drops.

9. Mineral Surfaces and Cooperative Templating

Layered silicates, iron–sulfur clusters, and carbonaceous surfaces contribute (i) adsorption geometry (reducing path length), (ii) local field alignment (phase matching), and (iii) diffusion corridors (lower friction), all of which multiply to reduce S^* (Theorem 2).

10. Consequences and Predictions

- **C1. Cycle discovery by action mapping.** Rank experimental network motifs by estimated S^* using umbrella sampling/NEB on $\mathcal{F}(x)$.

- **C2. Chirality windows.** Predict critical feed concentrations and temperatures where the pitchfork appears; test via flow reactors.
- **C3. Vesicle coherence threshold.** Measure minimal R at which encapsulated cycles persist; compare to $\sigma_C, \sigma_D, \kappa_b$ estimates.
- **C4. Template amplification factors.** Quantify $k_{\text{templ}}/k_{\text{free}}$ as $e^{(1-\alpha)S^*/\hbar_{\text{eff}}}$ by varying mineral surfaces.
- **C5. -stack spacing control.** Tune stacking distance and ionic strength to maximize throughput in template copying assays.

11. Discussion

Metabolism is *minimum-action coherence cycling*. Autocatalysis, templating, chirality selection, vesicles, and stacking all reduce S^* or increase cycle affinity. ChronoChemistry unifies these mechanisms with the same calculus that governs bonding (CHEM-2) and kinetics (PHYS-4/5 analogues). The diagrams here—loops, stacks, templates, vesicles—are the alphabet of molecular memory.

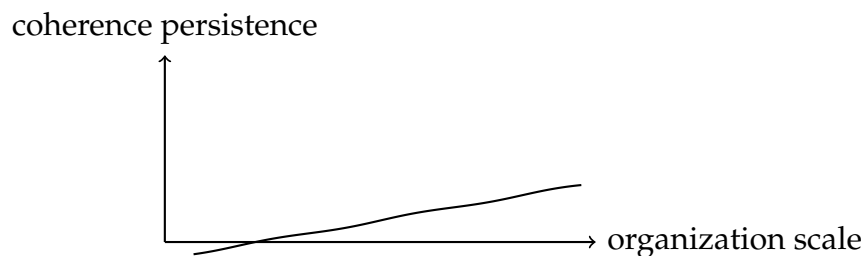


Diagram 6: thresholds—stacking, templating, vesicles

12. References

- Horn, F.; Jackson, R. (1972). *General mass action kinetics*. Arch. Rational Mech. Anal.
- Schnakenberg, J. (1976). *Network theory of nonequilibrium*. Rev. Mod. Phys.
- Freidlin, M.; Wentzell, A. (1998). *Random Perturbations of Dynamical Systems*.
- Eyring, H. (1935). *The activated complex*. Chem. Rev.
- Kramers, H. A. (1940). *Brownian motion in a field of force*. Physica.
- Marcus, R. (1964). *Chemical and electrochemical electron-transfer*. Annu. Rev. Phys. Chem.

- Nitschke, J. R. (2009). *Self-assembly in chemistry*. Acc. Chem. Res.
- Luisi, P. L. (2016). *The Emergence of Life*. Cambridge.

13. Conclusion

We have given a rigorous, visual calculus for the onset of metabolism:

$$\boxed{\min \mathcal{A}[x] \text{ over } \dot{x} = SJ(x) \iff \text{persistent cycles, memory, and organization}}$$

Autocatalytic loops persist when their net affinity overcomes dissipation; surfaces, stacks, and vesicles reduce action to make this possible. *HMR-CHEM-4* will quantify specific prebiotic motifs (mineral-redox cycles, lipid growth-division, nucleotide condensation) with parameterized actions and testable thresholds, completing the bridge to Chronobiology.

Keywords: molecular memory, autocatalysis, templating, vesicles, large deviation, ChronoChemistry.

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