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SELF REPLICATION AND CHEMICAL SELECTION IN PRIMORDIAL MUTUALLY CATALYTIC SETS

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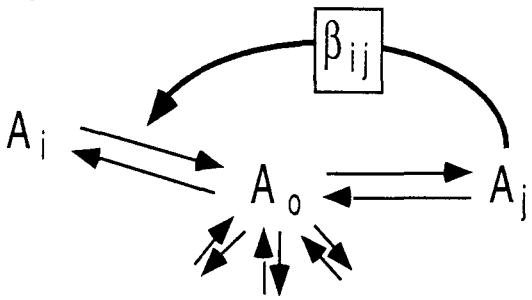
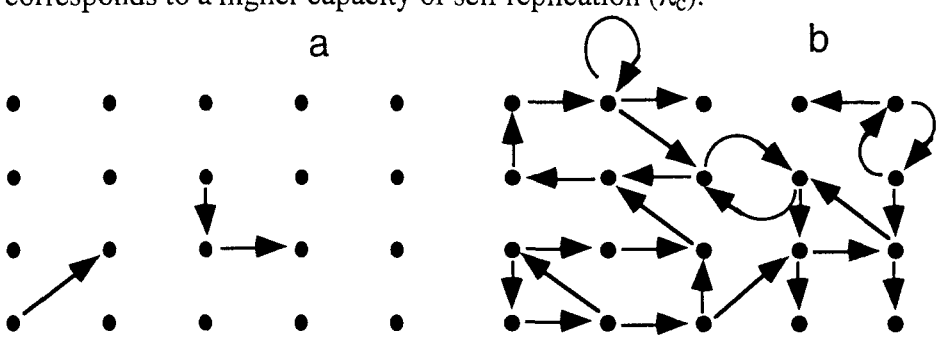
Template-mediated replication of individual molecules has been pursued as the basis for primordial chemical evolution. In parallel, it has been suggested that sets of mutually catalytic molecules could undergo replication, even if none of their individual components is autocatalytic, thus constituting a primitive metabolism without a genome (1). In support of the latter concept, we describe here an explicit kinetic model for a Graded Autocatalysis Replication Domain (GARD), in which mutual catalysis in a set of N types of molecules (A_i) derived from a common precursor (A_0), can sustain self-replication of the entire ensemble. The components of GARD may be *any* organic molecules, endowed with sufficient complexity to allow for structural diversity and mutual complementarity. The mutual catalytic rate enhancement exerted on the species A_i by the species A_j is denoted by a matrix element β_{ij}. For GARD simulations we use a formalism that allows one to assign likelihood values for any degree of catalysis between two randomly chosen species A_i and A_j. This is described in the form of a probability distribution $\phi(\beta_{ij})$ (2), analogous to our previously developed Receptor Affinity Distribution (RAD) model (3). We further assume that the system is subjected to a constant dilution effect, (e.g. due to expansion of its vesicle enclosed volume). The time-dependent concentrations of the species A_i then obey the differential equations (i=1,N)



$$\frac{dA_i}{dt} = k_i A_0 - k_{-i} A_i + \sum_{j=1}^{N} k_i \beta_{ij} A_0 A_j - \sum_{j=1}^{N} k_{-i} \beta_{ij} A_i A_j - \lambda A_i$$

where k_i and k_{-i} are the uncatalysed rate constants of the reaction of formation and degradation of A_i and λ describes the system's exponential expansion rate, according to $V(t)=V(0) \cdot Exp(\lambda t)$.

The main question addressed by the GARD model is whether a chemical system, connected through random catalytic interactions, and governed by a RAD-like model, can propagate its own chemical composition with no absolute requirement for autocatalysis for any of its individual components. For this, we define a graded quantitative measure for GARD's self replication through a critical rate of dilution (λ_c), that is shown to increase with the extent and connectivity of mutual catalysis. We then envisage an evolutionary process, where the content of GARD is subjected to random compositional fluctuations, which affect the prevailing network of catalytic interactions. We analyze this process by stochastic computer simulation, where compositional "mutants" with an augmented capacity of self replication may spontaneously appear, which may take over the prevailing GARD. The beginning and the end of a typical simulation are presented in the figure below. In each of the plots the catalytic network of GARD with N=20 is presented, where each species is represented by a dot. A directed arrow between two species denotes a value of β_{ij} higher then a pre-defined threshold. At the beginning of the simulation (a) a sparse network with low connectivity and catalytic values occurs. At the end of the simulation (b) a well-connected metabolism-like network of catalysis is obtained, which corresponds to a higher capacity of self replication (λ_c).



The GARD model demonstrates quantitatively how self replication may be a property of a molecular ensemble, without any specific constraints on the structure of the components. No individual molecule needs to be endowed with the specialized chemical properties currently associated with replicating macromolecules such as DNA and RNA. Our analysis also allows to compute the probability for a primordial spontaneous emergence of a GARD-like entity based on first chemical principles. GARD may thus be considered as a feasible paradigm for understanding the early emergence of chemical self-replication and chemical selection.

1. Kaufmann, The origins of order, Oxford Univ. Press, Oxford (1993).
2. Lancet et al, Ber. Bunsenges. Phys. Chem. 98, 1166-69 (1994) No.9.
3. Lancet et al, Proc. Natl. Acad. Sci. 90, 3715-18 (1993).