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ON THE ORIGIN OF SELF-REPLICATING INFORMATION-CONTAINING POLYMERS FROM OLIGOMERIC MIXTURES

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ON THE ORIGIN OF SELF-REPLICATING INFORMATION-CONTAINING POLYMERS FROM OLIGOMERIC MIXTURES

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The process which leads from inanimate matter to life has several crucial steps, one of which is undoubtly the growth of the first information-containing polymers (DNA, RNA, proteins, or their precursors) from relatively simple molecules[1,2]. Our initial state then is the primitive organic soup containing suitable concentrations of molecules such as purines, pyrimidines, phosphate ions, etc. The final state of this key step is a polymer capable of self-replication through a complementary template. Starting with small fragments (monomers, dimers, etc.) how could one account for the growth of a polymer with a biologically promising sequence of oligomers? We propose that the process occurs through condensation reactions which are catalysed by fragments complementary to the original ones. By focusing on the transient chemical bonds of the activated complex formed by these complementary fragments, this step in the transition between inanimate and living matter can be thought at as a critical phenomenon. As such it is in principle manageable within the renormalisation group framework[3] which has proved its power in related problems[4].

We will assume a model in which the biologically meaningful polymer is a linear macromolecule with an appropriate sequence of oligomers. For the sake of simplicity let us consider the sequence ABABAB..., where the residues A and B represent oligomers such as the purine and pyrimidine deoxy-nucleotides in DNA. We consider the dimer AB (smallest non-trivial fragment which already presents the sequence we intend to construct) and analyse how could it grow into, let us say, the tetramer ABAB (or BABA). We assume that residues A and B can form complementary pairs $\binom{A}{B}$ and that the growth is catalysed by complementary oligomers such as ABA:

$$(AB) + (AB) + (ABA) \rightleftarrows \begin{matrix}(AB)\\ |\\ (ABA)\end{matrix} + (AB) \rightleftarrows$$

$$\begin{matrix}(AB)\,(AB)\\ |\quad\;|\;|\\ (A\quad BA)\end{matrix} \rightleftarrows \begin{matrix}(ABAB)\\ |\;|\;|\\ (ABA)\end{matrix} \rightleftarrows (ABAB) + (ABA) \qquad (1)$$

Clearly, if this process continues, it will eventually form a polymer with a codified sequence of residues and which will be self-duplicating through a complementary template.

The bonds between the complementary fragments (indicated by the vertical lines in the above diagram) play a crucial role in our description of the process. At this stage there is no need to speculate on their nature; they could be hydrogen bonds, for example. We denote by K ($K \geq 0$) the associated equilibrium constants (fugacities).

In real space renormalisation group (RG) formalism, the growth of a large system is discussed through the configurational analysis of the aggregation of small parts of it. In Table I we have listed, for a dimer AB and a trimer ABA, all the possible growth path ways, subject to the following constraints: (i) the bonds between complementary fragments are assumed independent; (ii) the catalysing fragment cannot be longer than twice the growing fragment (we want to retain only the most probable mechanisms); (iii) the number of non-connected residues of the catalysing fragment cannot exceed the number of its residues which are actually connected to the growing fragment (otherwise they are to be associated with other growing fragments and not with the one under consideration), and if they are equal a weight 1/2 is introduced to avoid double counting; (iv) multiple catalysing processes (involving more than one catalysing fragment) are neglected because of a pre-

sumably low probability of occurrence. It is clear that the above conditions have a certain degree of arbitrariness, however it is hoped that any other "reasonable" set of rules would provide results that would not essentially differ from those presented in what follows.

The effective fugacities associated with the growth of the dimer and the trimer are respectively given (see Table I) by

$$R_2(K) = K + 4K^2 \tag{2}$$

$$R_3(K) = K + 3K^2 + 8K^3 \tag{3}$$

The RG recursive relation is given by $R_2(K')=R_3(K)$, hence

$$K' = \frac{1}{8}[\sqrt{1+16R_3(K)}-1] \tag{4}$$

This recursion admits two trivial (stable) fixed points, namely K=0 (corresponding to lack of growth) and K=∞ (corresponding to infinite growth), as well as a critical (unstable) one at K*=1/8. The RG flow provided by Eq. (4) is indicated in Fig. 1 (a). The *existence* of an unstable (therefore *critical*) fixed point such as that appearing in Fig. 1 (a) can be considered as a relevant result of the present work: it is worthy to insist on the fact that the RG flow could in principle have been of the undesirable types indicated in Fig. 1 (b) (indefinite growth *independently of the strength* of the catalysing bond) or in Fig. 1 (c) (lack of growth under *any* circumstances). The actual numerical value 1/8 obtained, within the present approximation, for the critical point K* should not be given a particular importance: considera

tion of larger oligomers and more complex (multiple) processes should be necessary to achieve numerical reliability. The same remark holds for the critical exponent ν defined through $\xi \propto (K^*-K)^{-\nu}$, where ξ is the mean length of the growing polymer: within the present RG approach ν is given by $\ell n(3/2)/\ell n(dK'/dK)_{K^*} \simeq 6.7$, which quite probably is too high. Furthermore mechanisms tending to stop the growth once the convenient length is attained should be included to make the model more realistic. Anderson[5] has recently proposed a numerical simulation program for a similar model which contains more detailed mechanisms than those included in the present schematic approach. In this context, it is significative that Anderson has concluded that the concept of complementarity is "essential in getting life started". Hopefully the implementation of Anderson's program could confirm the criticality we have pointed out.

Our main conclusion, then, is that the transition from inanimate matter to life can be seen as a critical phenomenon intimately related to the probability of occurrence of chemical bonds responsible for complementary connections. The existence of *large and self-duplicating* molecules, essential to life, appears as a natural consequence of our model (like "two faces of a single coin"). We also note that the need of complementary structures for growth could have a bearing on the problem of whether DNA or proteins are the more primitive biomolecules.

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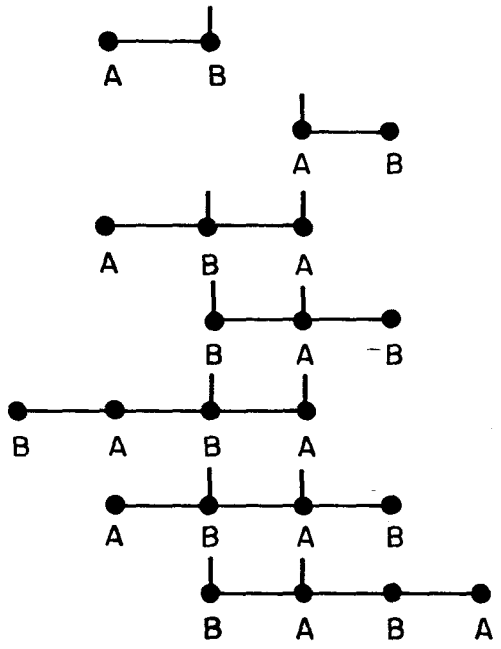
CAPTION FOR TABLE AND FIGURE

Table I - Configurational analysis of the growths of the dimer AB (a) and the trimer ABA (b), respectively leading to Eqs. (2) and (3) through the performance of $\sum$(weight x fugacity).

Fig. 1 - Renormalization group of the fugacity K: (a) present theory (from Eq. (4); out of scale; K* denotes the critical point); (b) indefinite growth; (c) lack of growth.

(a) A B (GROWING FRAGMENT)	WEIGHT	FUGACITY
	1/2	K
	1/2	K
	1	K^2
	1	K^2
	1/2	K^2
	1	K^2
	1/2	K^2

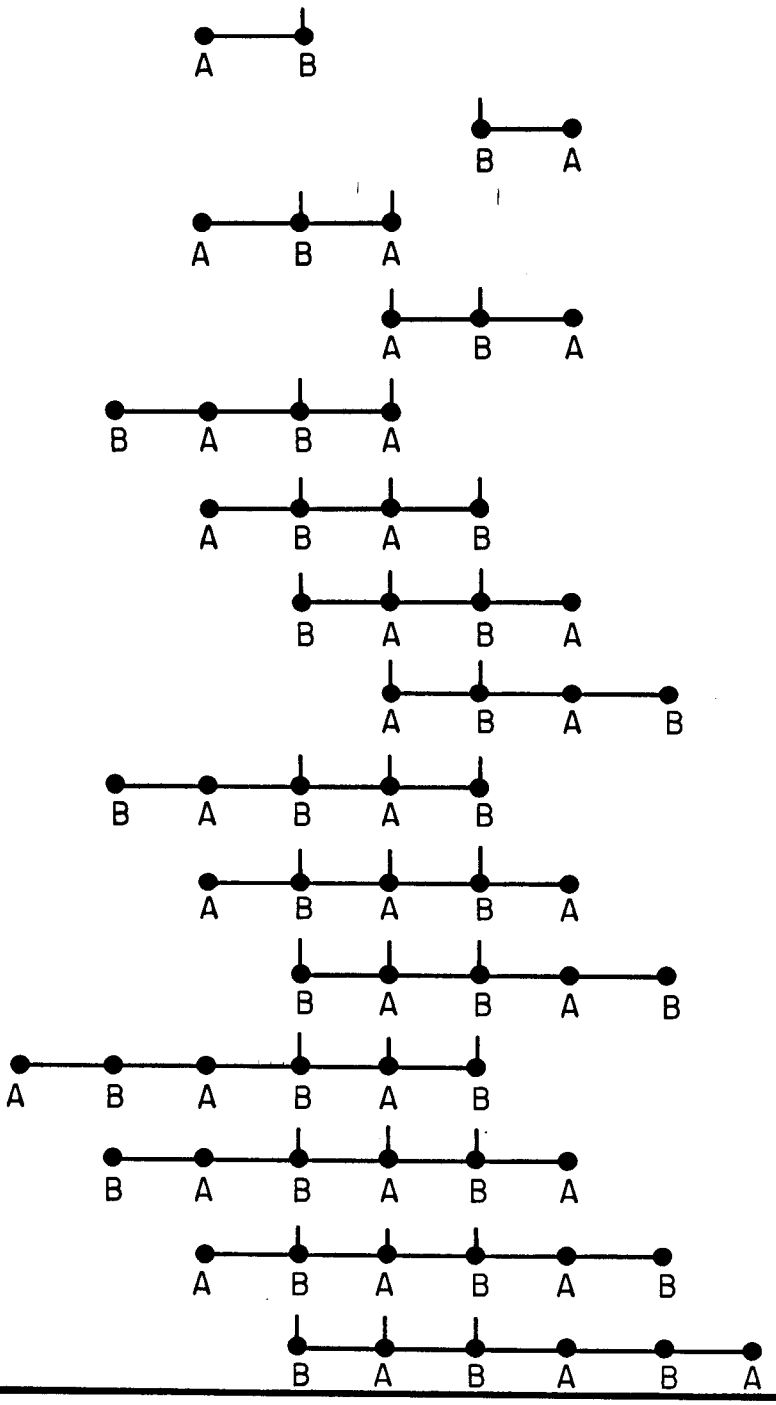
(b) A B A (GROWING FRAGMENT)	WEIGHT	FUGACITY
		
A B	1/2	K
B A	1/2	K
A B A	1	K^2
A B A	1	K^2
B A B A	1/2	K^2
A B A B	1	K^3
B A B A	1	K^3
A B A B	1/2	K^2
B A B A B	1	K^3
A B A B A	1	K^3
B A B A B	1	K^3
A B A B A B	1/2	K^3
B A B A B A	1	K^3
A B A B A B	1	K^3
B A B A B A	1/2	K^3

TABLE I

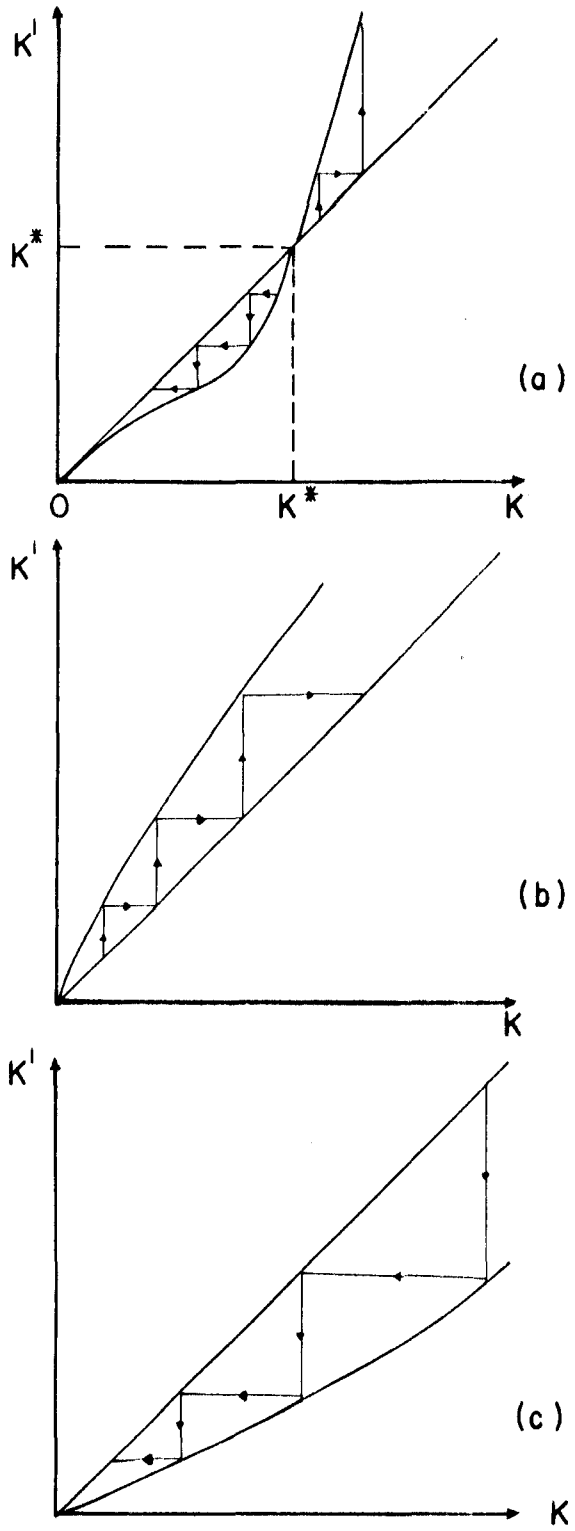


FIG. 1