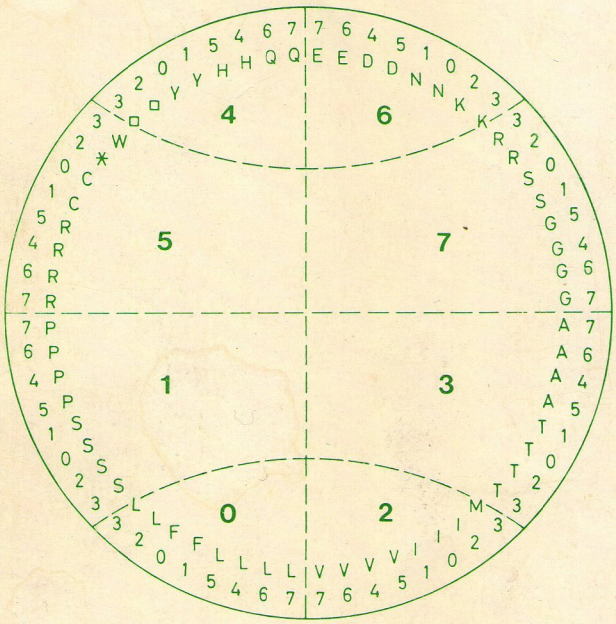
Miloje M. Rakočević

The LOGIC of the GENETIC CODE



Naučna knjiga

NEW NEW NEW

On this way we want to regard the new study of prof. dr M. Rakočević which will be published next year on the English language

The LOGIC of the GENETIC CODE

This study will be continuance of the book Gens, Molecules and Language which was published in 1988 and has been sold out for a few months. As it is known, in the study *Gens, Molecules and Language* author discovered the periodic law and the periodic system of the genetic code.
The result of the new research is absolutely a new theory. In this new theory we see that genetic code has a specially logic unknown in science.
In this study author presents us seriously axioms and laws of the genetic code origin and the way of the life evolution on our planet. The book contents many graphics and tables. This new study contents fundaments science theory and known experimental facts.
Those experimental facts are accordance with mathematics, chemistry, molecular biology, information theory and system theory.
We believe that this study will be interesting for many people and therefore we give you a work of dr M. Rakočević presented on *6th Congress of the Federation of European Societes of Plant physiology* (FESPP) in Split 4-10. Sept. This work was presented on the Congress in poster form but now, on the base of Poster discussion, we give you in the form of the scientific work.
We ask you to subscribe for this study because it is likely it will be sold out very quickly.

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THE OPTIMAL MODEL FOR THE AMINO ACID CODE

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Abstract

This research has led to the discovery of the periodic law of the amino acid code. The amino acid code can be developed into the periodic system (and the table), in which each of 20 natural amino acids has an exactly established place. On the basis of the periodic system, it is possible to construct amino acid ring in which amino acids are distributed according to the criteria of similarity - difference. The results of the research show that the periodic system and the amino acid ring can be shown in two ways. The first way is according to the criteria: the type of bond between first and second base in the codon triplet (P_yP_y; PuP_y, ie. Pupu; P_ypu); and the second way, according the criteria: middle base (P_y or Pu).

Out of the codon matrix, which actually represents a genetic code matrix - a matrix of the distance between the amino acid pairs - can also be drawn. In this matrix which represents also a optimal law of the amino acid code, there is a order made up of number one, by the diagonal (noughts), representing minimum - unit distance between amino acids.

The observation of all these relations which are the outcome of the periodic law (actually, of the law of binary coding) can be of great importance for decoding of conformational forms and stereochemical structures of proteins. Discovery of the periodic law and periodic system of the amino acid code can also throw a new light on the question of the beginning of life and its evolution.

The main results

The three-dimensional topological model - cube with an inscribed sphere - is the source of all the relations within the genetic code: eight cognate codons, disposed on the corners, make up the main cube; then, according to the superposition principle and binary logic, these eight cubes make up a bigger (common) cube containing all the 64 codons (Fig. 1& tab 2). The topological relation between the cube and the sphere inscribed in this cube is expressed by Euler's theorem of homeomorphic translation.

The amino acid code can be developed into the periodic system and two tables (tab. 1 & 2), in which each of 20 natural amino acids has an exactly established place, the new genetic code table, proposed here (table 1), reflects the periodic law in cycles 0-7: the first base - with two (A, U) on three (G, C) bonds, the third base *U, C, A, G,* repeatidly. Positions 0-7 are obtained by the application of the principle of minimization of binary function and form to the binary record of codons on a gray code model.

On the basis of the periodic system, it is possible to construct amino acid ring (Fig. 2) in which amino acids are optimal distributed, according to the criteria of similarity - difference (optimal order: matrix - table 3).

The first significant idea on the steric configuration of the genetic code, i.e. three-dimenisonal genetic code, was suggested by Eigen and Schuster (Fig. 3), the three edges of the cube represent the three positions in a codon.

Swanson (1984) started from the same idea and she drew up a "codon path cube" (fig. 4) but not as an element of a complex topological system.

An obvious expression of the minimization principle is the binary tree (Fig. 5) with eight rosettes - each of them bearing eight three-bit codon records. In the genetic code rosettes are "packed" according to the principle of superposition and the optimal law: codons are arranged first, in the 7 6 4 5 1 0 2 3 sequence (Fig. 6) and then the rosettes, in the sequence which corresponds with the path linking the corners of the cube with unit dimensions in three-dimensional space.

Introduction

In recent years, there have been several attempts at bringing the characteristics of the genetic code into relation with the chemistry of the protein amino acids. In this respect, the papers of R. Swanson (1984) and R. Doolitle (1985) are particularly significant. R. Swanson has demonstrated that the genetic code can be reduced and interpreted to a "Gray code" model, by way of the binary logic, and that a search for a unifying concept of the amino acid code makes sense. On the other hand, R. Doolittle has demonstrated that the main factors influencing the encoding process in the genetic code, are: polarity and molecular size of amino acids. However, in spite of such specification, the impossibility of amino acid classification into four groups, according to the four codon groups in the genetic code table (with U, C, A or G as the middle bases), has not been explained so far. This paper is trying to answer the question, and to point at the correlation between the chemistry of the amino acids and the cybernetics of the genetic code.

Preliminary considerations of the problem

The investigations of the correlations and interdependence between the genetic code and physico-chemical characteristics of the amino acids opened new questions and new problems, rather than answered the preliminary hypotheses. The most significant "new" issues certainly include the following questions:
1) Is it possible to arrange the amino acids in the topological area of physico-chemical characteristics in the one and only optimal way, i.e. is it possible arrange them in such a way that the distance from one to another remains the same? 2) Did the evolutionary process of the life on Earth, perhaps, begin with a two-letter (A,T), instead of the four-letter (A,T,G,C) alphabet? 3) Was the codon triplet

preceded by a "doublet"? 4) Did the evolution of the organic matter start with less than 20 amino acids, and 5) Has the evolution of the genetic code stopped "halfway", since there are "only" 20 amino acids, and 64 codons?

The answer to the first question was given in our last study (Rakočević, 1988), while this article is trying to answer the remaining four questions. Namely, it was established (Rakočević, 1988), that the genetic code functions according to a firmly established periodic law, followed by axiomatic conclusions and attitudes, considered here to be established facts, the most significant of them being:

I. The genetic code is based on a specific binary logic: "having purine quality" (1), and "having pyrimidine quality" (0), in the following order: in the position of the middle base in the triplet, then in the position of the first and last bases and, finally, in the position of the third (variable) base, through which synonymy is made possible;

II. The model of the genetic code (in topological terms) is a cube with a sphere inscribed in. The optimal arrangement of both codons and amino acids is brought about through this model, in such a way that any two neighbours are always at the same distance (at a distance of one bit, if the binary record of codons is put together for each pair of neighbouring codons, after the module 2).

III. The genetic code obtained out of the "Gray code" model, can be developed into a periodic system with codon (and amino acid) groups of similar properties. From this fact, it can be concluded that codons and amino acids, in the topological area of physico-chemical characteristics, can be arranged in at least two ways: 1) after a "Gray code" model, which represents our spatial variant, with the distance of one bit between neighbouring units, following the shortest path linking the cube angles - 7 6 4 5 1 0 2 3 , and 2) after the periodic system model, with the distance of one bit between neighbouring groups (classes, following the usual numerical order - 0 1 2 3. 4 5 6 7.

IV. The optimal law of the genetic code, besides its following the shortest path, is also expressed in the maximum representation of the minimization principle of binary function and form. So, despite the fact that a binary

record of a codon requires long word, as necessary a binary six-bit the periodic law is fully expressed by only one half of the binary word (last three digits).

V. The complementarity principle must be conceived far more broadly and more completely than the complementarity expressed by AT and GC pairs. Both codons (Blalock, 1986) and amino acids (Rakočević, 1988, p. 201), are complementary among themselves.

Research methodology

In the investigations of connections between and interdependence of, the chemistry of amino acids and the genetic code characteristics, the usual methodology, used in the information theory and system theory was applied. The array of 20 protein amino acids, their physico-chemical properties and interrelations, were considered to be a system, as conceived by Bertalamffy (1949) and Mesarović (1964, 1968). The central part of this systemic analysis was taken by a relational approach which made it possible to reduce the complicated amino acid interactions to binary relations; at the same time, the sub-clusters were observed as partial clusters within a universal cluster, and the partitive cluster as the reflection of all the observes sub-clusters, interactions.

A proposal for a new gentic code table

The classic table of the genetic code (Crick, 1966) does not reflect its essential characteristics. The new table proposed here (Table 1), reflects the periodic law in cycles 0-7, after the following criterium: the first base in the triplets *U* or *A* (two hydrogen bonds), the third base *U*, *C*, *A*, *G*, repeatid by. Positions 0-7 are obtained by the application of the principle of minimization of binary function and form to the binary record of codons on a Gray code model, put forward by R. Swanson (1984), according to this, rather simple, relation:

A + AB = A

Here two cases can be distinguished:

I. The elements of the set *A* are "all the purine or pyrimidine bases taking part in the building of nucleic acids". The elements of the set *B* include "all the bases taking part in the building of nucleic molecules acids, with two hydrogen bonds each".

II. The elements of set *A* include "all the purine or pyrimidine bases taking part in the building of nucleic acids". The elements of set *B* include all the bases taking part in the building of nucleic acids, with three hydrogen bonds each".

An obvious expression of the minimization principle is the binary three (Fig. 5) with eight rosettes - each of them bearing eight codons, recorded by way of three-bit records. In the genetic code, which can be presented only as a cube with an inscribed sphere (Fig. 1), codons and rosettes are "packed" according to the principle of superposition and the optimal law: codons are arranged first, in the 7 6 4 5 1 0 2 3 sequence, and then the rosettes, in the sequence which corresponds to the path linking the corners of the cube with unit dimensions in three-dimensional space. However the optimal law is also reflected in this: the biggest distance between the codons in a rosette makes three bits; although it is possible to link the rosettes by engaging just one more bit. The four groups (or eight subgroups) of codons in the new table of the genetic code are separated one from another by a distance of four bits.

The new table of the genetic code makes it possible to determine the final, optimal, sequence (and ring!) of the 20 protein amino acids (Fig. 2), which has been searched for by numerous authors (Dayhoff, 1978; Argyle, 1980; French and Robson, 1983; McLachlan, 1984; Doolittle, 1985). The optimal amino acid sequence (F L I M V T A P S G N K D E R C W Y H Q), enables to construct a matrix in which each pair of the neighbouring amino acids always differs for one unit (distance of one bit, Table 3).

The positional hyerarchy

In order to make the periodic law and the optimal principle of the genetic code (hence, consequently, of the amino acids code) more comprehensible, it is necessary to observe that the "course of change" in the "area" of physicochemical properties of purine and pyrimidine bases follows the binary logic (Fig. 1). What is even more, the principle of the positional hyerarchy of the binary numbering system is completely applicable to the genetic code:

2^0 - third position (z)	$2^2\ 2^1\ 2^0$	
	4 2 1	U = 0
2^1 - second position (y)	U U C = 1	C = 1
	U C U = 2	A = 2
2^2 - First positon (x)	C U U = 4	G = 3
	U U A = 2	
	A C G = 13	

Binary numerical values of each of the triplets* represent, in fact, their distance from the starting (zero) point (UUU) (Table 2).

From the aforesaid, and from the figures and tables, follows the axiomatic conclusion:

1. The genetic code could not start its evolution as a two-letter alphabet (A,T); 2. A "doublet" is not possible; 3. Codons, 64 of them, can encode 21 different situations, which is maximum (20 amino acids and a "stop" command); 4. The genetic code evolution has not ended halg - way.

Binary values of the amino acids, calculated as mean values of the codons encoding them, are shown together with the values for hydropathy (Doolittle, 1982) and polarity (Woese, 1966) (Table 4).

The relational approach (instead of the functional one) of the analysis of the relationship between amino acids provides a very good agreement of binary values,

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* Since we are concerned with a spatial arrangement, the sequence T-A is not fully confirmed.

hydropathy and polarity. For instance, the relation closer further shows that the zero-point (U U U) is further from the amino acids encoded by codons having *A* and *G* in the position of the first base in a triplet (the first, and strongest position!). Conversely, amino acids encoded by the codons *U* and *C* in the position of the third base, are nearer to the zero point. The values for hydropathy and polarity are in good accordance with this pattern. It is interesting that, in groups having *A* and *G* as the middle bases, the values of amino acids Y, W, C differ drastically from values of other amino acids in the group - both in their values and in hydropathy and polarity. It was only to be expected, if the genetic code follows the principle of the positional hyerarchy in the binary numerical system: all the three cases have *U* in the position of the first base, which can have nought value in the first (strongest) position, too. Moreover, cysteine C is considerably more positive than *W*, because its third positions are also occupied by small values (U,C). Taking into consideration the small-value position, *H* should come next, which is confirmed by its values for hydropathy and polarity (Table 4).

One can get the impression that glycine cannot be included in this discussion, because of its highest binary value, and the lowest (absolute) hydropathic value?! However, the genetic code model is a sphere (a spatial, three-dimensional Gray code model) so that there comes a moment when an amino acid placed "further" in its group, draws closer to another group. This is the case with glycine, which is placed at the very border between "opposite" amino acids.

The analysis of the relation "to be at the border line" also confirms the *position theory* of the genetic code. The amino acid at the border must have characteristics of both groups. This is possible only when the codons with approximate values in the first and second positions (I and II base), are conducted across the border, so that a lower-value base is placed in a higher position, and vice versa.

Consequently, codons - "candidates" for the border begin with:

the border*			the neighbours	
UC	0 + 2;	2 - 0 = 2	CC	4 + 2; 4 - 2 = 2
AG	8 + 6;	8 - 6 = 2	GG	12 + 6; 12 - 6 = 6
CG	4 + 6;	6 - 4 = 2	AA	8 + 4; 8 - 4 = 4
UG	0 + 6;	6 - 0 = 6		
UA	0 + 4;	4 - 0 = 4		
CA	4 + 4;	4 - 4 = 0		

It is now quite conceivable that *S* and *R* should be at the border-line; the distance between binary values of bases in the first and second positions (I and II base) is shortest with their codons. As far as the neighbours are concerned, some of them are closer and some further from the border glycine as an exception has already been discussed. The distance of *CA* (H and Q) equals nought. Only in one more case there is such a distance: *UU*. It is therefore understandable that the amino acid ring closes when the bond between F and Q is established.

The gradualness of changes on the "path of change" for the whole amino acid ring, is shown on Fig. 2. It is interesting that the distance between complementary amino acids is, in the majority of cases, 4 binary units. The distance between border-line amino acids S-R equals nought (zero); the same applies to T-C,W, which is the only possible place for the division for the "sphere" model into two symmetrical parts, if we take into account the distinction between the subrosettes 7 6 4 5 and 3 2 0 1. The distinction A-R equals 8 binary units, and the largest distance is V-H, which is in accordance with both model and values for polarity and hydropathy (Table 4).

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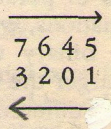
* It is interesting that codons carry out the "path of change" through the border, with mutual distance of only three instead of four bits, which is the difference between different groups. Consequently, they are not separated in the genetic code, but linked. The mankind could draw a lesson from it!

Chemical basis of the cybernetic topological model

Besides its following the positional hyerarchy in the binary numerical system, the genetic code is also in keeping with the spherical model with one-way and (in space) opposite direction in the arrangement of the numbers of codons with two sub-rosettes in the fields of two hemispheres:



What is more, the genetic code is also in full accordance with the cube model: by drawing the line 7 6 4 5 1 0 2 3 along the cube edges, some of the edges will stay out of the "path of change" (broken lines in Fig. 1). Amino acids on the rosettes whose binary numbers are at the ends of "full" edges of the model, (Fig. 1) form a homogenous group - both with hydropathic and polar values; conversely, amino acids from the rosettes whose binary numbers are at the ends of "empty" edges of the model, do not form a homogenous group.

All the cases of relative homogeneity, from the standpoint of physico-chemical characteristics, which are also compatible with the course of the "path of change" on the cybernetic topological "sphere-cube" model, are shown in Tables 4.

The compatibility of the physico-chemical parameters of protein amino acids with the cybernetic model of the amino acid (genetic) code can also be observed by the following analysis. There are three possible ways of "arranging" the codons according to the criterium of the first, the second, or the third base. It has proved justified to classify the codons into 4 groups, giving priority to the second (middle) base. In each of the four groups formed in this way, there is a triplet made up of three equal bases, their encoding capacity being - just one amino acid: UUU/F/; CCC/P/; AAA/K/; GGG/glycine/. The encoding capacity of the two bases can be pursued through all the four groups:

1. UC - F L S P
2. UA - L I Y N
3. UG - L V C W
4. CA - P T M Q N
5. CG - P A R G
6. AG - R G K E

If we compare the values of parameters given in Table 4 for all the six different situations, we shall see the following relation: the higher the binary values of bases in the combinations (A,G), the larger the encoding capacity, from the standpoint of degree of difference.

This regularity is even more evident if we look at the values of hydropathic parameters, polarity and binary values for amino acids *C*, *W*, and *Y* (Table 4). Their drastically low values, as compared with other "members" in the group, are the result of uracile presence in the first position (0×4=0) of the binary numbering system.

A more complex investigation of the cybernetic topological genetic code model shows, however, that its periodicity is in full accordance with the logic and pattern, not only of the binary but also of the tetrade, octal and hexadecimal numbering systems (Fig. 5). In this way, maximum possible optimization is brought about, using the maximum possible number in minimization.

For the definitions of particular types of periodicity, we shall state the necessary and the sufficient conditions:

I Binary periodicity

0 - first base: any purine or pyrimidine; third base: with two hydrogen bonds
1 - first base: any purine or pyrimidine; third base: with three hydrogen bonds

II Tetrade periodicity

0 - first base: any purine or pyrimidine; third base: *U*
1 - first base, any purine or pyrimidine; third base, *C*
2 - first base, any purine or pyrimidine; third base, *A*
3 - first base: any purine or pyrimidine; third base, *G*

III Octal periodicity

0 - first base, with two hydrogen bonds (*U* or *A*), third base *U*

1,2,3 - first base, with two hydrogen bonds (*U* or *A*); third base *C*, *A*, *G*, respectively.

4,5,6,7 - first base, with three hydrogen bonds (C or G), and third base, U,C,A,G, respectively.

IV Hexadecimal periodicity

0, 1, 2, 3 - first base U, third base U, C, A, G, respectively;

4, 5, 6, 7 - first base C, third base U, C, A, G, respectively;

8, 9, 10, 11 - first base A, third base U, C, A, G, respectively;

12, 13, 14, 15 - first base G, third base U, C, A, G, respectively.

One can notice easily that the central place is taken by the octal periodic system (Fig. 5 and Table 1) which was confirmated by experimental results.

J.E. Blalock et al (1986) have recently shown that codons from both the codogenous and non-codogenous DNA (from the standpoint of hydropathy) are complementary. Their main conclusion, however, was wrong: starting from the classic table of the genetic code, they concluded that amino acids are - anticomplementary. But, if their results are compared with the new table of the genetic code, proposed here, (Table 1), we can achieve full agreement, correcting the errors along the way. Namely, amino acids are also complementary (Table 4)!

Complementarity of codons and amino acids is a proof that the genetic code functions as a specific optimal cybernetic topological model, arising from the periodic law based on the positional hyerarchy of the binary numbering system. Its binarity and periodicity, on the other hand, arise directly from the "distribution" of physico-chemical characteristics of the purine and pyrimidine bases themselves, as well as of protein amino acids.

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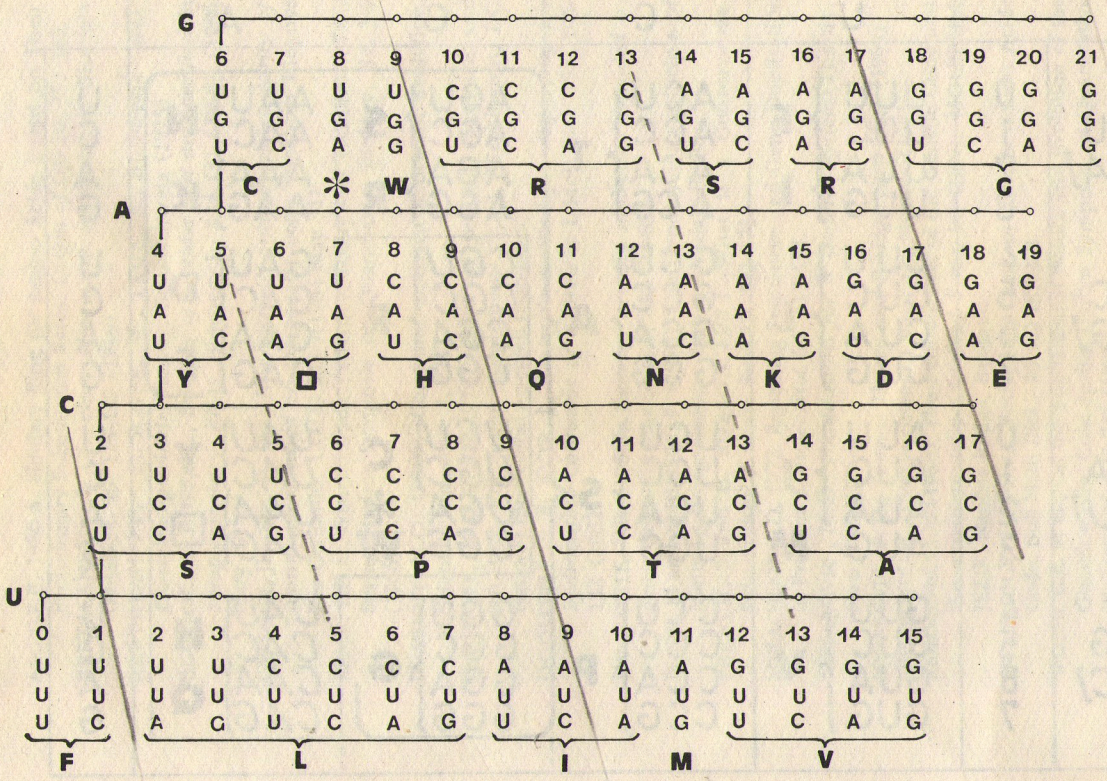
Table 1 The new table of the genetic code

		U	C	G	A	
U [A]	0	UUU } F	ACU } T	AGU } S	AAU } N	U
	1	UUC } F	ACC } T	AGC } S	AAC } N	C
	2	UUA } L	ACA } T	AGA } R	AAA } K	A
	3	UUG } L	ACG } T	AGG } R	AAG } K	G
C [G]	4	CUU } L	GCU } A	CGU } R	GAU } D	U
	5	CUC } L	GCC } A	CGC } R	GAC } D	C
	6	CUA } L	GCA } A	CGA } R	GAA } E	A
	7	CUG } L	GCG } A	CGG } R	GAG } E	G
A [U]	0	AUU } I	UCU } S	UGU } C	UAU } Y	U
	1	AUC } I	UCC } S	UGC } C	UAC } Y	C
	2	AUA } I	UCA } S	UGA *	UAA □	A
	3	AUG M	UCG } S	UGG W	UAG □	G
G [C]	4	GUU } V	CCU } P	GGU } G	CAU } H	U
	5	GUC } V	CCC } P	GGC } G	CAC } H	C
	6	GUA } V	CCA } P	GGA } G	CAA } Q	A
	7	GUG } V	CCG } P	GGG } G	CAG } Q	G

Table 2 64 codons for 20 amino acids and 1 „Stop“ command



Tab. 3 The optimal distance matrix for 20 protein amino acids

	F	L	I	M	V	T	A	P	S	G	N	K	D	E	R	C	W	Y	H	Q
F	0	**1**	1	1	1	2	2	1	1	3	2	2	2	2	2	2	2	1	1	1
L	1	0	**1**	1	1	2	2	1	1	3	2	2	2	2	2	2	2	1	1	1
I	1	1	0	**1**	1	1	1	2	2	2	1	1	1	1	2	3	3	2	2	2
M	1	1	1	0	**1**	1	1	2	2	2	1	1	1	1	2	3	3	2	2	2
V	1	1	1	1	0	**1**	1	2	2	2	1	1	1	1	2	3	3	2	2	2
T	2	2	1	1	1	0	**1**	1	1	1	2	2	2	2	1	2	2	3	3	3
A	2	2	1	1	1	1	0	**1**	1	1	2	2	2	2	1	2	2	3	3	3
P	1	1	2	2	2	1	1	0	**1**	2	3	3	3	3	1	1	1	2	2	2
S	1	1	2	2	2	1	1	1	0	**1**	1	1	1	1	1	1	1	2	2	2
G	3	3	2	2	2	1	1	2	1	0	**1**	1	1	1	1	1	1	2	2	2
N	2	2	1	1	1	2	2	3	1	1	0	**1**	1	1	1	2	2	1	1	1
K	2	2	1	1	1	2	2	3	1	1	1	0	**1**	1	1	2	2	1	1	1
D	2	2	1	1	1	2	2	3	1	1	1	1	0	**1**	1	2	2	1	1	1
E	2	2	1	1	1	2	2	3	1	1	1	1	1	0	**1**	2	2	1	1	1
R	2	2	2	2	2	1	1	1	1	1	1	1	1	1	0	**1**	1	1	1	1
C	2	2	3	3	3	2	2	1	1	1	2	2	2	2	1	0	**1**	1	1	1
W	2	2	3	3	3	2	2	1	1	1	2	2	2	2	1	1	0	**1**	1	1
Y	1	1	2	2	2	3	3	2	2	2	1	1	1	1	1	1	1	0	**1**	1
H	1	1	2	2	2	3	3	2	2	2	1	1	1	1	1	1	1	1	0	**1**
Q	1	1	2	2	2	3	3	2	2	2	1	1	1	1	1	1	1	1	1	0

Tab. 4 Complementarity of the amino acids

Hydropathy	Polarity	Binary value	Hidropathy	Polarity	Binary value
F + 2,8	5,0	0,5	K - 3,9	10,1	14,5
L + 3,8	4,9	4,5	N - 3,5 E - 3,5 D - 3,5	10,0 12,5 13,0	12,5 18,5 16,5
I + 4,5 M + 1,9	4,9 5,3	9,0 11,0	Y - 1,3 Y - 1,3	5,4 5,4	4,5 4,5
V + 4,2	5,6	13,5	H - 3,2 Q - 3,5	8,4 8,6	8,5 10,5
T - 0,7	6,6	11,5	W - 0,9 C + 2,5	5,2 4,8	9,0 6,5
A + 1,8 S - 0,8	7,0 7,5	15,5 7,2	R - 4,5	9,1	13,2
P - 1,6	6,6	7,5	G - 0,4	7,9	19,5

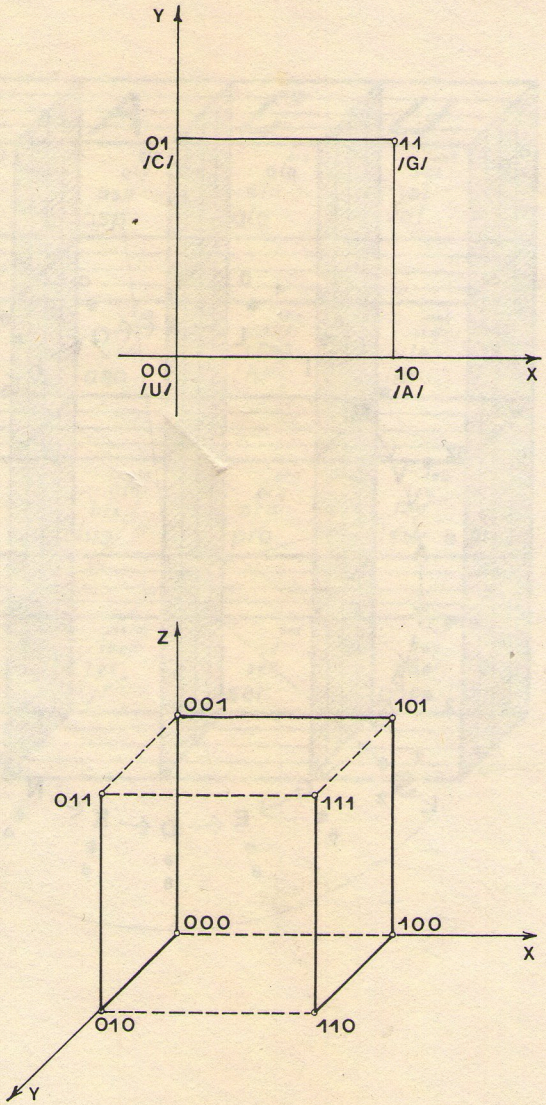


Fig. 1 The codon's cub: Change path and binary logic

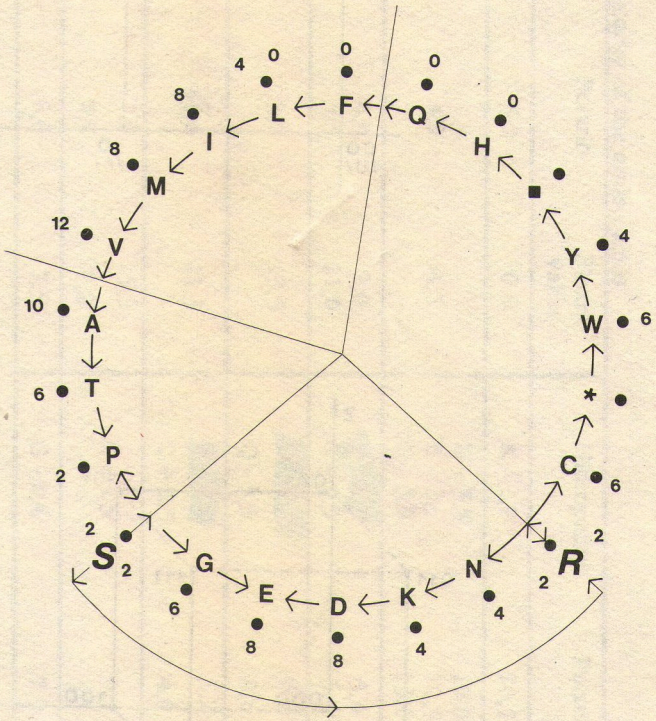


Fig. 2. The optimal amino acid ring

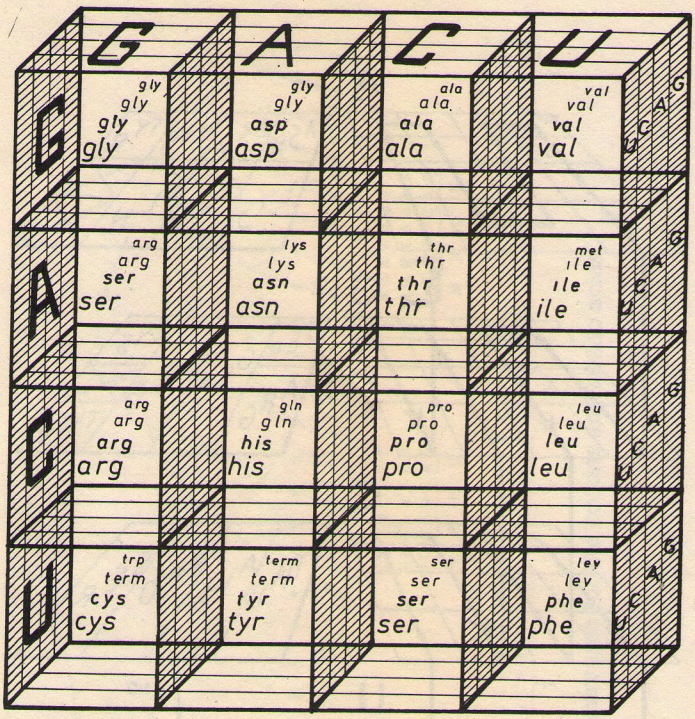


Fig. 3 The three edges of the cubes represent the three positions in a codon (according to: EIGEN, SCHUSTER, 1979

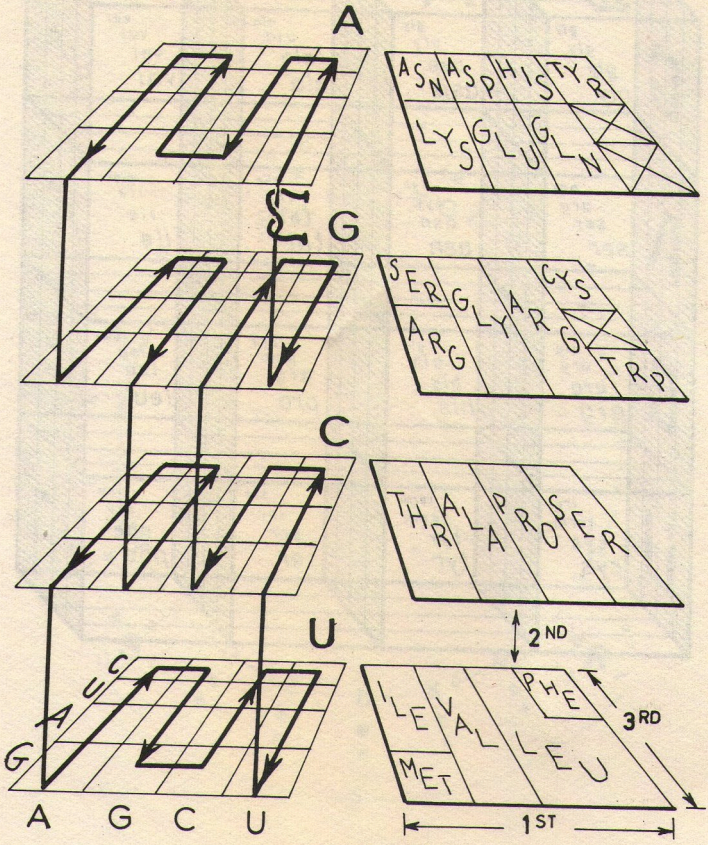


Fig. 4 Codon's path cube (R. SWANSON, 1984.)

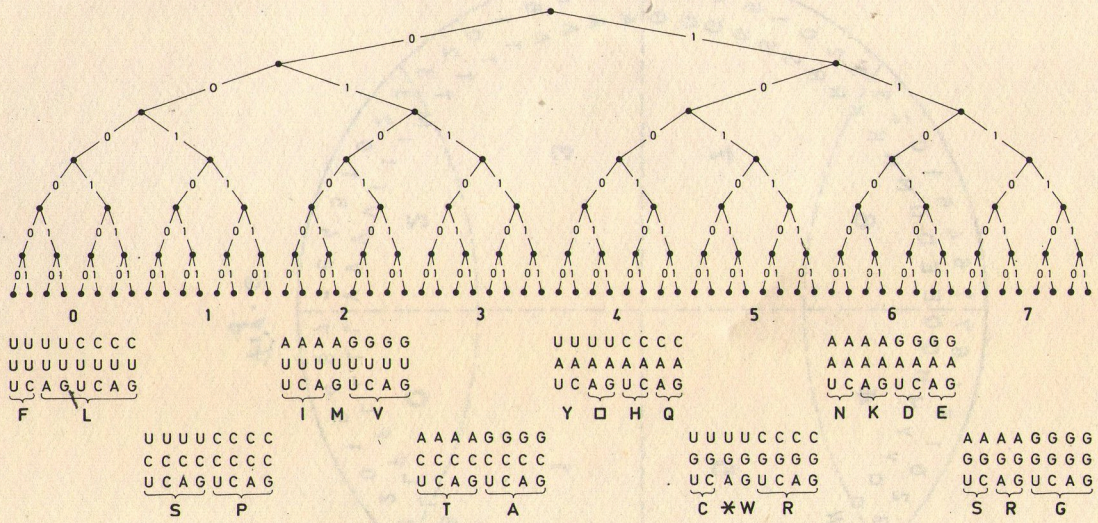


Fig. 5. The binary tree for the codons and amino acids

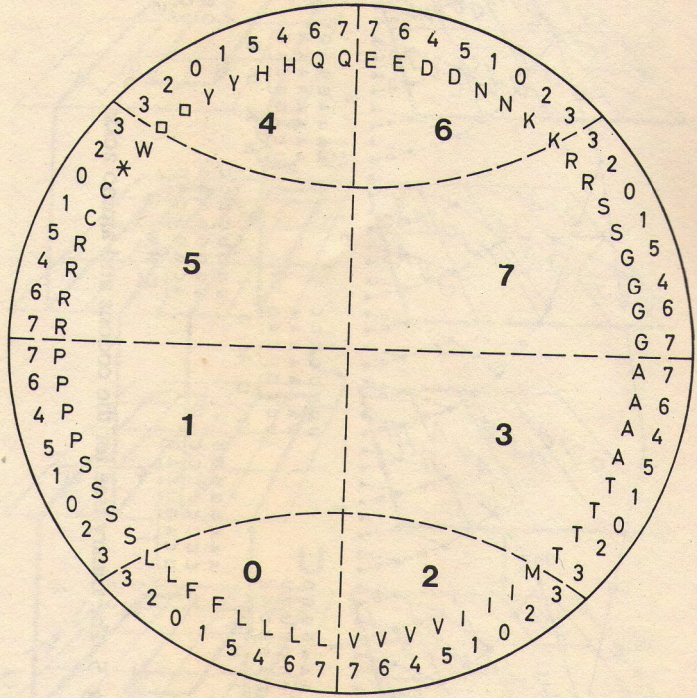


Fig. 6