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Matrix Representation of Stereoisomers and New Polygonal Stereoisograms

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Abstract

A new method to find the complete set of stereoisomers of chiral molecules is presented herein. This method consists in the use of binary alphabet (**0**, **1**) instead of the binary code (***R***, ***S***), which was originally coined by Cahn-Ingold-Prelog for characterizing to tetrahedral stereogenic centers. With this change, each one of the stereoisomers of a given molecule

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containing *n* stereogenic centers can be written as a *n*-bit binary string and the full set of stereosiomers can be represented as a *m-by-n* matrix (where *m* is the maximum number of stereoisomers possible, $m \leq 2^n$). In turn, the *n*-bit binary strings can be easily developed by a combinatorial technique starting from an all-zeros string *(u*) until ending in an all-ones string (*f*); in the middle there are subsets of strings with *one*, *two*…, *n-1* substituted 0's by 1's, which are labeled as a_i, b_j, c_k …, etc. Moreover, the numbers of strings in each subset are coincident with those ones in *n*-level of Pascal's Triangle and used as coefficients of a mathematical expression that describes to the total number of stereoisomers of a molecule containing *n* stereogenic centers.

Finally, the full set of stereoisomers represented by the labels mentioned above, was arranged in a polygonal stereoisogram, in such way that any pair of enantiomers occupies antipodal positions and the diastereomers the remaining ones.

1. Introduction

The substituents around a tetrahedral atom can be arranged in space only in two different ways. If those substituents are different each other, then both arrangements can be defined or characterized with the aid of Cahn-Ingold-Prelog (CIP) sequence rules as ***R*** (Rectus = right) and ***S*** (Sinister = left) (Figure 1) [1-3].

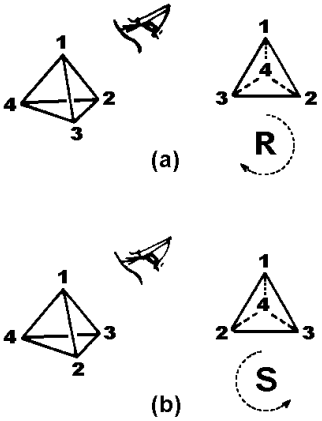


Figure 1 Chiral descriptors ***R*** and ***S***, as used in Stereochemistry to characterize the spatial orientations of substituents around a *Tetrahedral Stereogenic Center* (***R*** = rectus (right) = clockwise and ***S*** = sinister (left) = counter-clockwise orientations). The substituents are prioritized as 1 > 2 > 3 > 4 according to CIP sequence rules and the viewer must be located opposed to the minor priority substituent, 4 [3].

Due to each *Tetrahedral Stereogenic Center (TSC)* generates two possible orientations, this means, two stereoisomers, a molecule with *n* tetrahedral stereogenic centers possesses a maximum number of 2^n stereoisomers[†]. For example, there are four ($2^2 = 4$) stereoisomers in 2,3-dihydroxibutanoic acid, named as: (2*R*, 3*R*)-, (2*S*, 3*S*)-, (2*R*, 3*S*)- and (2*S*, 3*R*)-2,3-dihydroxibutanoic acids. Fischer's projections for these stereoisomers are schematized in Figure 2 and their stereoisomeric relationships are indicated by using the arrows coined by Fujita [4-5]:

Enantiomeric relationships are indicated with red arrows (horizontal lines) while the diastereomeric ones are with blue arrows (vertical and intertwined lines). Thus, the graphic symbols at the center of those double head arrows are concerned with full *RS*-permutations (a mirror plane reflection) and partial *RS*-permutations, respectively.

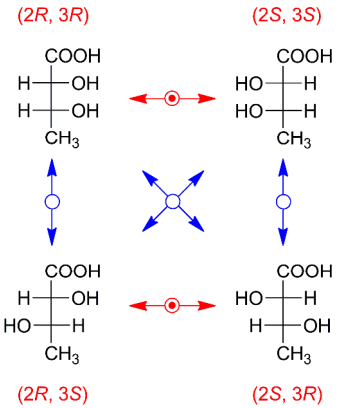


Figure 2 Stereoisogram showing the four possible stereoisomers of 2,3-dihydroxibutanoic acid, which obey the rule of $2^n = 2^2 = 4$ (where *n* = number of tetrahedral stereogenic centers, *NTSCs*). Enantiomeric and diastereomeric relationships are indicated respectively, with red and blue arrows (See in the body text the meaning of this kind of symbols).

The difficulty of finding the complete set of stereoisomers increases with increasing the number of stereogenic centers; for example, there are 512 stereoisomers for amphidinolide-H,

[†] The number of stereoisomers in a *meso*-compound is less than 2^n, usually 2^n-1.

a molecule which possesses n = 9 stereogenic centers and exhibits activity in the picomolar range against human epidermoid cancer cells [6].

This fact led us to develop a systematic approach to simplify this task, giving rise to an elegant combinatorial process whose results can be correlated with Pascal's Triangle. This finding could be included in the emerging area of Mathematical Stereochemistry, being one of its aims to reduce or overcome the imprecisions in stereochemistry [7]. Although this method is valid for any value of *n*, it is illustrated here in the range of n = 1 to 4.

2. Matrix representation of stereoisomers of molecules containing *n* = 1 - 4 tetrahedral stereogenic centers

In the systematic nomenclature, the stereochemistry of a tetrahedral stereogenic center is indicated by means of a locator number accompanied with the uppercase italic letter ***R*** or ***S***, corresponding to its chirality (See Figure 1). In order to organize and mathematize the full set of stereoisomers of a given compound, in this proposal:

2.1. The binary code (***R, S***) is switched to binary number system (**0, 1**); this means, assigning the values R = 0 and S = 1 and separating them from their chiral carbon's locators.

2.2. With this change, the stereochemistry of a molecule containing n stereogenic centers can be written as a n-bit binary string and its full set of stereoisomers as a matrix composed by m-rows and n-columns (where m is the maximum number of stereoisomers possible, $m \leq 2^n$) (Table 1).

2.3. The initial (u) and final (f) rows of that matrix are all-zero and all-ones strings, respectively. Then, if 0's are *mono-*, *di-*, *tri-*…, *(n-1)*-substituted by 1's in a combinatorial way from right-to-left, middle rows can be easily developed taking into account their increasing decimal value (This process is named "Hales numbering" in reference [8]). For example, the full set of strings of 2,3,4-trihydroxipentanoic acid (n = 3; $2^3 = 8$) is (Table 2):

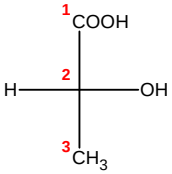
(0 0 0); (0 0 1) < (0 1 0) < (1 0 0); (0 1 1) < (1 0 1) < (1 1 0) and (1 1 1).

2.4. Those strings are label following the increasing degree of substitution as: u, a_i, b_j, c_k …, f. In fact, they could be considered as a new kind of ***Stereoisomer Descriptor***, ***SD***.

2.5. Note in the previous and in the following examples that the numbers of strings in each subset occur in a symmetrical way (Tables 2 and 3); this means, one unsubstituted string, three monosusbstituted, three disubstituted and one full-substituted string: 1*u*, 3a_i, 3b_j, 1*f*. These coefficients are coincident with the ones in the *3rd*-level of Pascal's Triangle and they can be used as coefficients of symmetrical mathematical expressions that describe to the total number of stereoisomers of a molecule containing *n* stereogenic centers (See section 4).

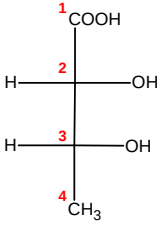
Table 1 Matrix representation of stereoisomers of four chiral hydroxy carboxylic acids: a) 2-hydroxipropanoic; b) 2,3-dihydroxibutanoic; c) 2,3,4-trihydroxipentanoic and d) 2,3,4,5-tetrahydroxihexanoic. Labels C_x above the columns indicate the chiral carbons to be represented by means of the binary alphabet [0, 1] = [*R*, *S*]

(a)



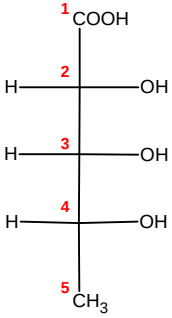
C_2
0
1

(b)



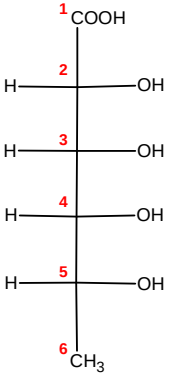
C_2	C_3
0	0
0	1
1	0
1	1

(c)



C_2	C_3	C_4
0	0	0
0	0	1
0	1	0
1	0	0
0	1	1
1	0	1
1	1	0
1	1	1

(d)



C_2	C_3	C_4	C_5
0	0	0	0
0	0	0	1
0	0	1	0
0	1	0	0
1	0	0	0
0	0	1	1
0	1	0	1
0	1	1	0
1	0	0	1
1	0	1	0
1	1	0	0
0	1	1	1
1	0	1	1
1	1	0	1
1	1	1	0
1	1	1	1

Taking into account the mentioned above, the full set of stereoisomers of the hydroxicarboxylic acids containing 1-4 stereogenic centers are arranged as matrices in Table 1: a) 2-hydroxipropanoic; b) 2,3-dihydroxibutanoic); c) 2,3,4-trihydroxipentanoic and d) 2,3,4,5-tetrahydroxihexanoic.

Table 2 Binary strings length-three, subset classification depending on the substitution degree of 0's by 1's and labels for *Stereoisomer Descriptors* (*SD's*) of 2,3,4-trihydroxipentanoic acid. Note in each subset, the arrangement of strings from their minor to major decimal values ("Hales numbering process" [8]).

Binary strings length-3 in alphabets *R/S* and *0/1*	**Subset classification**	**Labels for *SD's***
(*R R R*) = (0 0 0)	*un*-substituted	*u*
(*R R S*) = (0 0 1)	*mono*-substituted	a_1
(*R S R*) = (0 1 0)		a_2
(*S R R*) = (1 0 0)		a_3
(*R S S*) = (0 1 1)	*di*-substituted	b_1
(*S R S*) = (1 0 1)		b_2
(*S S R*) = (1 1 0)		b_3
(*S S S*) = (1 1 1)	*full*-substituted	*f*

3. Outstanding features of *m*-by-*n* matrix that represents a full set of stereoisomers of a molecule containing *n* stereogenic centers

The rectangular matrices formed with *n*-bit binary strings coming from combinatory replacement of 0´s by 1's possess interesting mathematical features (See Tables 3-6). For example:

3.1. At any column, the count of 1's is equal to $2^n/2$ or 2^{n-1} (Equation 1). This is because each stereogenic center contributes only in a half of the rows with its value of 1.

$\sum_{k=1}^{m} e_{kj} = 2^n/2 = 2^{n-1}$ (where e_{kj} are the matrix elements of *j-th* column) (1)

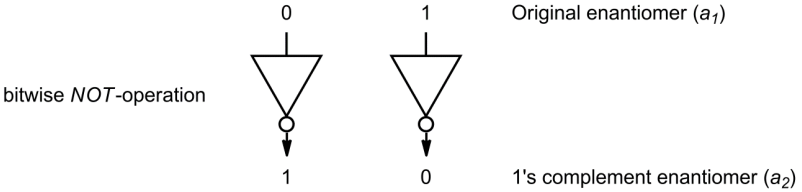
3.2. At any row, the count of 1's takes a value ranged from 0 to "*n*" (Equation 2).

$0 \geq \sum_{k=1}^{n} e_{ik} \leq n$ (where e_{ik} are the matrix elements of *i-th* row) (2)

3.3. If the substitution of 0's by 1's are carried out following "Hales numbering process" [8]; this means, taking into account their increasing decimal value, then:

a) The strings corresponding to enantiomer couples are located symmetrically nested (See Tables 3-6 and Figure 3) and they can be recognized because their *element*-by-*element* values are inverted, 0/1; this is a bitwise operation known as "*NOT*". For example (Equation 3):

NOT (0, 1) = (1, 0) (3)



b) According to the above, a couple of enantiomers complement each other, meaning that their sum is an all 1's string. In our example:

$a_1 + a_2$ = (0 1) + (1 0) = ((0+1) (1+0)) = (1 1) (4)

c) In general, the count of 1's of any couple of enantiomers is equal to "*n*":

$e_{ik} + NOT\ (e_{ik}) = (1 \cdots 1) = n$ (5)

d) Thus, for the example mentioned in equation 4 (n = 2):

$a_1 + a_2$ = (1 1) = 2 (6)

Moreover, the sums of count of 1's in rows and columns take the same values (1, 4, 12, 32) and constitute another set of numbers given by $n*2^{(n-1)}$ [9]:

$$\sum_{k=1}^{m} e_{kj} = \sum_{k=1}^{n} e_{ik} = n * 2^{(n-1)} \quad (7)$$

In practice, this fact should be used as a tool to verify if the *n*-bit strings were correctly developed.

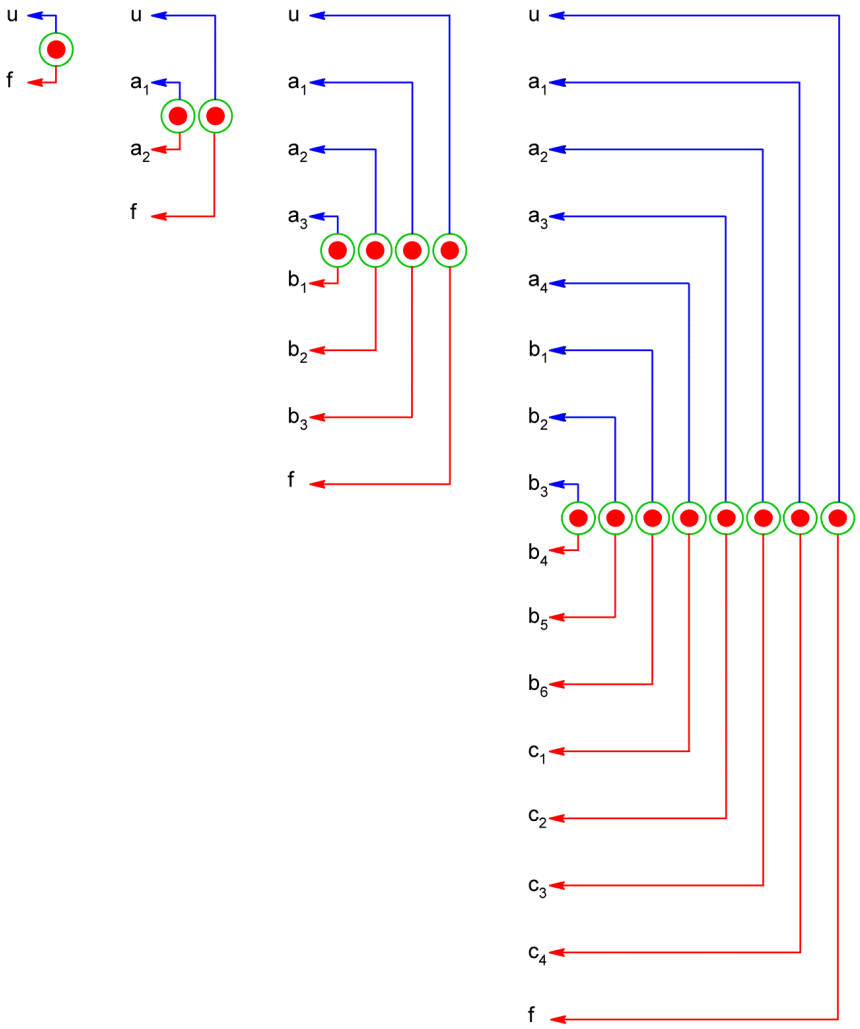


Figure 3 Enantiomeric couples of molecules a-d. The labels u, a_i, b_j, c_k…, f are assigned to strings coming from the combinatorial replacement of 0's by 1's, being u and f respectively, an all 0's and all 1's strings (Tables 3-6).

Table 3 Mathematical array (middle of second column) used to describe the stereoisomers of 2-hydroxipropanoic acid (molecule a); labels used to design the substitution degree of numbers 0 by 1 (fourth column) and the equation generated for describing its total number of stereoisomers, *TNS* (right bottom).

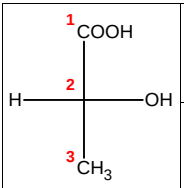
	**NTSCs** **(C_2)**	**Count of 1's in rows**	**SD's**
	0	0	u
	1	1	f
Count of 1's in columns	1	1	$TNS_a = 1u + 1f = 2$

Table 4 Mathematical array (middle of second column) used to describe the stereoisomers of 2,3-dihydroxibutanoic acid (molecule b); labels used to design the substitution degree of numbers 0 by 1 (fourth column) and the equation generated for describing its total number of stereoisomers, *TNS* (right bottom).

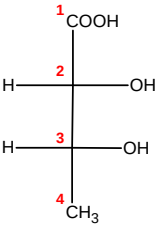
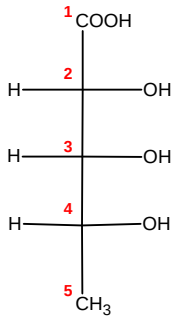
	**NTSCs** **(C_2** **C_3)**		**Count of 1's in rows**	**SD's**
	0	**0**	0	u
	0	**1**	1	a_1
	1	**0**	1	a_2
	1	**1**	2	f
Count of 1's in columns	2	2	4	$TNS_b = 1u + 2a_i + 1f = 4$

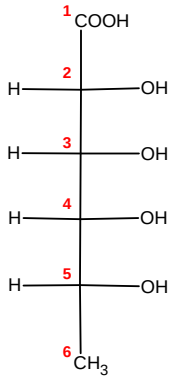
Table 5 Mathematical array (middle of second column) used to describe the stereoisomers of 2,3,4-trihydroxipentanoic acid (molecule c); labels used to design the substitution degree of numbers 0 by 1 (fourth column) and the equation generated for describing its total number of stereoisomers, *TNS* (right bottom).

	**NTSCs** (**C_2** **C_3** **C_4**)			**Count of 1's in rows**	**SD's**
	0	**0**	**0**	0	u
	0	**0**	**1**	1	a_1
	0	**1**	**0**	1	a_2
	1	**0**	**0**	1	a_3
	0	**1**	**1**	2	b_1
	1	**0**	**1**	2	b_2
	1	**1**	**0**	2	b_3
	1	**1**	**1**	3	f
Count of 1's in columns	4	4	4	12	$TNS_c = 1u + 3a_i + 3b_j + 1f = 8$

4. On the use of Pascal's Triangle for developing a mathematical expression to describe a full set of stereoisomers

In order to describe the mathematical properties of matrices of compounds a-d (sections 2 and 3; Table 1), they have converted below in Tables 3-6. Note that "Hales numbering process" allows to group their strings in subsets whose quantity of elements corresponds with those numbers in the (*n+1*)-row of Pascal's Triangle (Figure 4). Consequently, by using these numbers is possible to write an expression for the "Total Number of Stereoisomers", m (m = TNS = 2^n), which contains *n+1* summands (Figure 4). For example, for molecules *a-d* possessing *n* = 1, 2, 3 and 4 stereogenic centers:

Table 6 Mathematical array (middle of second column) used to describe the stereoisomers of 2,3,4,5-tetrahydroxihexanoic acid (molecule d); labels used to design the substitution degree of numbers 0 by 1 (fourth column) and the equation generated for describing its total number of stereoisomers, *TNS* (right bottom).

	**NTSCs**				**Count of 1's in rows**	**SD's**
	(C_2	**C_3**	**C_4**	**C_5)**		
	0	**0**	**0**	**0**	0	u
	0	**0**	**0**	**1**	1	a_1
	0	**0**	**1**	**0**	1	a_2
	0	**1**	**0**	**0**	1	a_3
	1	**0**	**0**	**0**	1	a_4
	0	**0**	**1**	**1**	2	b_1
	0	**1**	**0**	**1**	2	b_2
	0	**1**	**1**	**0**	2	b_3
	1	**0**	**0**	**1**	2	b_4
	1	**0**	**1**	**0**	2	b_5
	1	**1**	**0**	**0**	2	b_6
	0	**1**	**1**	**1**	3	c_1
	1	**0**	**1**	**1**	3	c_2
	1	**1**	**0**	**1**	3	c_3
	1	**1**	**1**	**0**	3	c_4
	1	**1**	**1**	**1**	4	f
Count of 1's in columns	8	8	8	8	32	$TNS_d = 1u + 4a_i + 6b_j + 4c_k + 1f = 16$

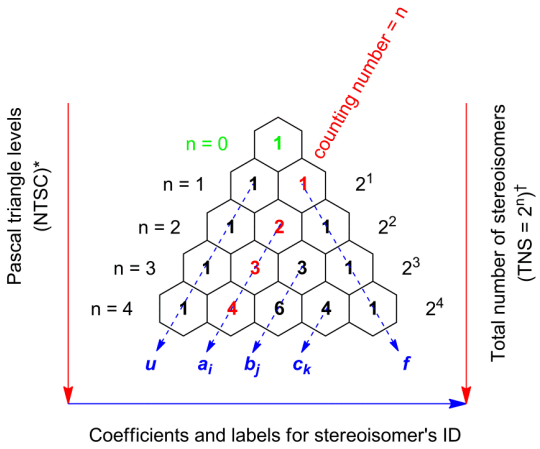


Figure 4 Pascal's triangle (up to n = 4) as a tool for developing mathematical expressions for the "Total Number of Stereoisomers, †TNS or m" of a given compound. Note that numbers at the right diagonal are the powers of two; thus, if n = 4 then TNS = 16 stereoisomers (2^4) = $1u + 4a_i + 6b_j + 4c_k + 1f$. The labels u, a_i, b_j, c_k and f indicate the substitution degree of 0's by 1's and the coefficients are taken from 4*th* level. *NTSC = Number of Tetrahedral Stereogenic Centers (numbers in left diagonal, n).

$$TNS_a = (u) + (f) = \mathbf{1}u + \mathbf{1}f \quad (8)$$

$$TNS_b = (u) + (a_1 + a_2) + (f) = \mathbf{1}u + \mathbf{2}a_i + \mathbf{1}f \quad (9)$$

$$TNS_c = (u) + (a_1 + a_2 + a_3) + (b_1 + b_2 + b_3) + (f) = \mathbf{1}u + \mathbf{3}a_i + \mathbf{3}b_j + \mathbf{1}f \quad (10)$$

$$TNS_d = (u) + (a_1 + a_2 + a_3 + a_4) + (b_1 + b_2 + b_3 + b_4 + b_5 + b_6) + (c_1 + c_2 + c_3 + c_4) + (f)$$

$$= \mathbf{1}u + \mathbf{4}a_i + \mathbf{6}b_j + \mathbf{4}c_k + \mathbf{1}f \quad (11)$$

These expressions appear at the right bottom of tables 3-6.

Note that both, the subsets of n-bit strings built earlier and the coefficients into expressions 8-11 can be computed by hand or using different programming languages. In fact, when a = 1 and b = 1 the classic binomial sum (equation (12)) affords "Binomial Coefficients" (equation 13):

$$(a + b)^n = \sum_{k=0}^{n} \binom{n}{k} a^{n-k} b^k \quad (12)$$

$$(1+1)^n = 2^n = \sum_{k=0}^{n}\binom{n}{k} = \frac{n!}{k!(n-k)!} \quad (13)$$

For example, the coefficients for $n = 4$ are:

$$\binom{4}{0}\ \binom{4}{1}\ \binom{4}{2}\ \binom{4}{3}\ \binom{4}{4} = \left(\frac{4!}{0!(4-0)!}\right)\ \left(\frac{4!}{1!(4-1)!}\right)\ \left(\frac{4!}{2!(4-2)!}\right)\ \left(\frac{4!}{3!(4-3)!}\right)\ \left(\frac{4!}{4!(4-4)!}\right)$$

$$= \left(\frac{4!}{1*(4)!}\right)\ \left(\frac{4*(3!)}{1*(3)!}\right)\ \left(\frac{4*3*(2!)}{2*1*(2)!}\right)\ \left(\frac{4*(3!)}{3!(1)!}\right)\ \left(\frac{4!}{4!(0)!}\right) = \mathbf{1\ 4\ 6\ 4\ 1} \quad (14)$$

5. A new polygonal stereoisograms for stereoisomers of chiral molecules carrying *n* = 1 to 4 stereogenic centers

5.1 Enantiomeric relationship

Because the representation of enantiomeric couples in Figure 3 results impractical for n > 2 [10], we propose a new geometric representation for it: It is based in the definition of *geometric progression* as it is the sequence of numbers generated by powers of two, 2^n = 2, 4, 8, 16, etc. (where *n* is a natural number). Thus, if the enantiomeric couples are placed as points on opposite sides of a circumference, they generate respectively, a line and 4-, 8- and 16-sided polygons for n = 1, 2, 3 and 4 (Figure 5). Obviously, the definition of a polygon is not accomplished in the case of *n* = 1 because there are only two points (2^1 = 2 stereoisomers). From another point of view, the circumferences are divided into halves, quarters, eights and sixteenths; this means the ratio of this new progression is ½.

Once the line and polygons are sketched inside the circumferences, the couple of enantiomers are joined by means of two headed straight arrows proposed by Fujita in 2006 [10]. Note that the symbol at the centre of red arrows (Figure 5) really works as a "*chirality inversion center*" producing the bitwise "*NOT*" or "complement operation" (eq. 3-4) or a "*full R/S permutation*" as it was claimed by Fujita.

5.2 Diastereomeric relationship

The recognition of enantiomers is commonly made visually through a computational model, by comparing 2D projections or, at best, with the aid of 3D-models. After this physical or computational comparison, the stereoisomeric relationship is determined as follows:

"Enantiomers are mirror plane images that cannot be superimposed" [11]. In addition: "Diastereomers are stereoisomers that are not mirror plane images".

However, these definitions sometimes carry ambiguities and other problems associated with the management of different types of 2D structural formulas such as Fischer's, Newman's and sawhorse projections. Thus, taking advantage of the *n*-bit binary string approach presented above, it is possible to give a mathematical definition of stereoisomers as follows:

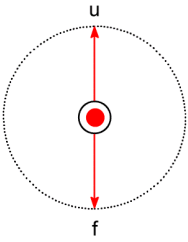
Enantiomers are a couple of n-bit binary strings that complement each other to afford an all 1's-bit string. By the way, it is possible to find easily the 1's complement of a bit string by means of the binary code inverter called ***"bitwise NOT-operation"*** (Equations 3-5). Thus, the sum of 1's of both enantiomers is equal to *n* (equations 5 and 15):

$$\sum_{k=1}^{n}[e_{ik} + NOT(e_{ik})] = n \qquad (15)$$

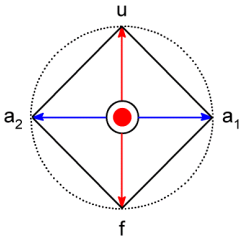
Consequently, ***diastereomers are couples of stereoisomers whose n-bit binary strings do not complement each other*:**

$$\sum_{k=1}^{n}[e_{ik} + e_{lk}] \neq n \qquad \text{(where } e_{ik} \text{ and } e_{lk} \text{ are elements of } i\text{-th and } l\text{-th rows)} \qquad (16)$$

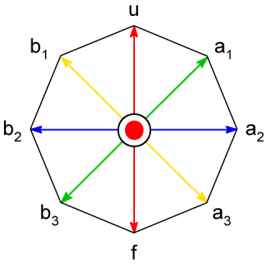
Because the couples of enantiomers are located in antipodal vertices of a polygonal stereoisogram, then any couples of stereoisomers that are not linked by straight lines are called diastereomers. Therefore, in our example possessing three stereogenic centers, the *u*-stereoisomer has six diastereomers: a_1, a_2, a_3, b_3, b_2 and b_1 (Figure 5, bottom); this means that in general, any stereoisomer possesses *n-2* diastereomers.



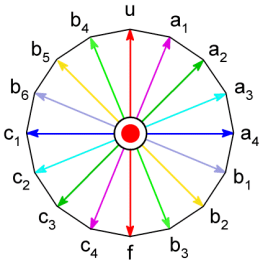
$TNS_{(2^1)} = 1(u) + 1(f) = 2$



$TNS_{(2^2)} = 1(u) + 2(a_i) + 1(f) = 4$



$TNS_{(2^3)} = 1(u) + 3(a_i) + 3(b_j) + 1(f) = 8$



$TNS_{(2^4)} = 1(u) + 4(a_i) + 6(b_j) + 4(c_k) + 1(f) = 16$

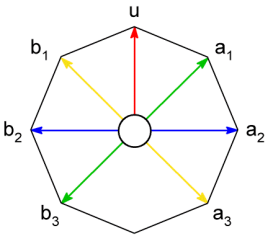


Figure 5 Geometric stereoisograms for molecules *a-d* represented with a circle (Top left), a circle and polygon (Top right) and only polygons (Middle row). Coloured straight double-headed arrows connect enantiomeric couples, whereas at the bottom, for stereoisomer *"u"* of molecule *d*, its antipode *"f"* was removed to evidence the diastereomeric relationship with a_1, a_2, a_3, b_3, b_2 and b_1. The empty circle indicates that there is not chirality inversion center between them.

6. On the application of the MPS method to cyclic molecules (Note added during the revision process)

Matrix Representation of Stereoisomers is a method valid for cyclic molecules too; for example, (-)-menthol or *levo*-menthol, (IUPAC name: (1*R*, 2*S*, 5*R*)-5-methyl-2-(propan-2-yl)cyclohexanol), is a natural anaesthetic fragrant terpenoid present in the peppermint oil that possesses three stereogenic centers and hence $2^3 = 8$ stereosiomers. Taking the triad of chiral descriptors (*R*, *S*, *R*) and switching them by their corresponding binary numbers, the mono-substituted 3-bit binary string labeled a_2 = (0 1 0) is obtained (see table 2).

The structure of the full set of menthol's stereoisomers, their trivial names, chiral descriptors and binary strings are given in figure 6 [12].

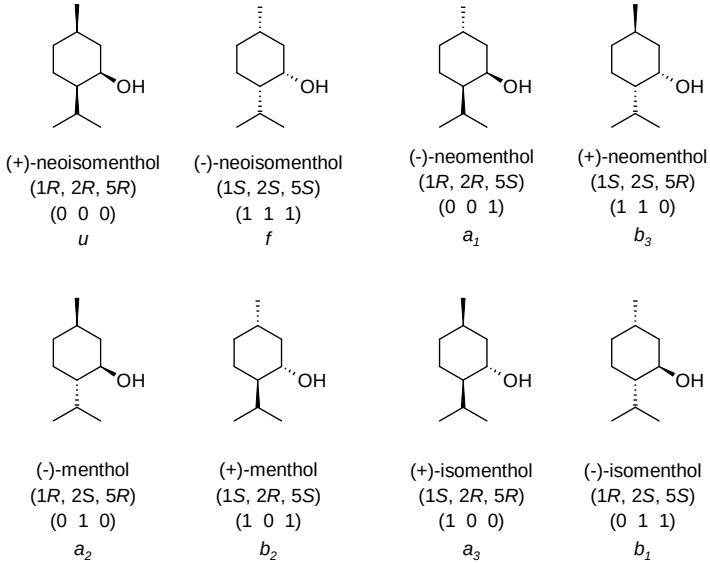


Figure 6 Structural formulas, trivial names and 3-bit binary notation for stereoisomers of 5-methyl-2-(propan-2-yl)cyclohexanol. The stereoisomers are arranged in couple of enantiomers: *u*-*f*, a_1-b_3, a_2-b_2 and a_3-b_1 (See stereoisogram $TNS_{(2^3)}$ at middle row of figure 5).

7. Conclusion

By using the binary alphabet [0, 1] instead of chiral descriptors [*R*, *S*], the stereochemistry of a given compound possessing *n*-stereogenic centers and the full set of their stereoisomers could be represented respectively, as a *n*-bit binary string and an *m*-by-*n* matrix composed only by 0's and 1's. Because "Hales numbering process" was used to develop those matrices, they acquired mathematical properties that can be used both as a tool to verify if the set of stereoisomers was complete and to propose a new mathematical definition for enantiomers and diastereomers. In fact, it was found that enantiomers are nested into the matrix and related each other by the bitwise *NOT*-operation.

Moreover, and in relation with (*n+1*)-row of Pascal's Triangle, the coefficients for an algebraic expression for Total Number of Stereoisomers could be obtained when the strings were group depending on their substitution degree of 0's by 1's. Finally, new polygonal stereoisograms were proposed to illustrate graphically, the stereoisomerical relationships of chiral hydroxy acids containing 1-4 stereogenic centers.

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References

[1] R. S. Cahn, C. K. Ingold, V. Prelog, The specification of asymmetric configuration in organic chemistry, *Experientia* **12** (1956) 81-124.

[2] IUPAC, Commission on Nomenclature of Organic Chemistry. A Guide to IUPAC Nomenclature of Organic Compounds (Recommendations 1993), 1993. Blackwell Scientific publications. R-7.2.1 The R/S convention. <http://www.acdlabs.com/iupac/nomenclature/93/r93_630.htm> [Online; accessed on April 27th, 2018]

[3] D. G. Morris, E. W. Abel, *Stereochemistry*, Cambridge, Royal Soc. Chem., 2001, pp. 26-29.

[4] S. Fujita, Type-itemized enumeration of quadruplets of RS-stereoisomers. I. Cycle indices with chirality fittingness modulated by type-IV quadruplets, *J. Math. Chem.* **54** (2016) 286-309.

[5] S. Fujita, Asymmetry revisited by Fujita's stereoisogram approach. Part 1: Asymmetry under point-group symmetry and under *RS*-permutation-group symmetry, *Tetrahedron Asymmetry* **27** (2016) 675-686.

[6] A. Fürstner, L. C. Bouchez, J. A. Funel, V. Liepins, F. H. Porée, R. Gilmour, F. Beaufils, D. Laurich, M. Tamiya, Total syntheses of amphidinolide H and G, *Angew. Chem. Int. Ed.* **46** (2007) 9265-9270.

[7] S. Fujita, *Mathematical Stereochemistry*, De Gruyter, Berlin, 2015, pp. 28-29.

[8] L. H. Harper, *Global Methods for Combinatorial Isoperimetric Problems*, Cambridge Univ. Press, Cambridge, 2010, pp. 59-59.

[9] N. J. A. Sloane, A001787, The on-line encyclopedia of integer sequences, <http://oeis.org/A001787> [Online; accessed on April 27th, 2018]

[10] S. Fujita, Complete settlement of long-standing confusion on the term 'prochirality' in stereochemistry. Proposal of pro-*RS*-stereogenicity and integrated treatment with prochirality, *Tetrahedron* **62** (2006) 691-705.

[11] D. L. Reger, S. R. Goode, D. W. Ball, *Chemistry: Principles and Practice*, Brooks/Cole, Belmont, 2010, pp. 841-841.

[12] S. K. Talapatra, B. Talapatra, *Chemistry of Plant Natural Products: Stereochemistry, Conformation, Synthesis, Biology, and Medicine*, Springer, Heidelberg, 2015, pp. 391-391.