match no. 8 pp. 341 - 352 1980

THE MULTIPLEX

A CLASSIFICATION OF FINITE ORDERED POINT SETS IN ORIENTED d-DIMENSIONAL SPACES

André S. Dreiding and Karl Wirth

Organisch-chemisches Institut
der Universität Zürich
Winterthurerstr. 190, 8057 Zürich

(received: February 1980)

In this paper we classify d-dimensional point arrangements. Section A is meant to inform the reader of the background of the multiplex idea [1]. Section B contains a mathematical definition of the multiplex and in section C some implications are mentioned. The multiplex concept poses a number of attractive problems which have hitherto resisted solution.

A. BACKGROUND AND IDEA

Objects are frequently represented by mobile or rigid spatial arrangements of labeled or unlabeled points in our intuitive physical space. Examples are molecules, where the relative position of the atoms are correlated with physical and chemical properties. For most chemical correlations, a molecule is not considered to be fixed in space and some of its atoms are often viewed as mobile with respect to each other.

It is, therefore, not surprising that modern stereochemistry has evolved a number of concepts which may be generalized to mobile point arrangements [2]. One such concept is the factorization of a molecule into chirality elements [3], an idea found most useful since the asymmetric carbon atom was postulated by van't Hoff [4] and Le Bel [5].

A chirality element is a chemically feasible subarrangement of atoms which can exist in a left- and a right-handed form. Each chirality element doubles the number of potential stereoisomers, except when there is special symmetry. The smallest conceivable chirality element consists of a non-planar arrangement of 4 atoms which are different or have different environments. We shall call such a smallest chirality element a chiron. Might it be useful to follow a self-consistent approach which considers the orientation[1]) of all chirons in a molecule? Evidently, not all of the chirons are independent of each other in this respect. In the chiral methane derivative of Fig. 1, for example, the orientations of the 5 chirons are interdependent, as long as it is chemically not feasible to place the carbon atom outside the tetrahedron spanned by the other 4 atoms.

---

[1]) What we call orientation of a chirality element is sometimes also referred to as sense of chirality [3].

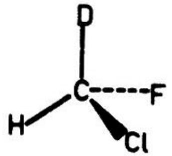

Fig. 1

With the intention of gaining an insight into the problems connected with this approach we generalize the concept of chirality element by considering the atoms of molecules as points and by dropping the restriction of chemical feasibility. This leads to mobile[2]) point arrangements.

In order to define a 3-dimensional mobile point arrangement we factorize it into subarrangements of 4 points. A subarrangement is subjected to a mobility restriction by not allowing each of its points to pass through the planes spanned by 3 other points. When these 4 points are differentiated, as in Fig. 2 and 3, the subarrangement is chiral since our intuitive physical space is orientable[3]). When the points are labeled

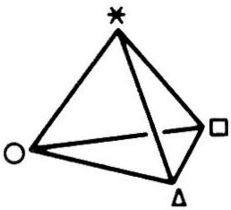

Fig. 2

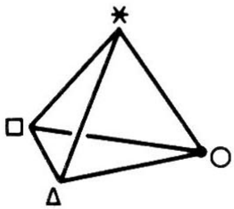

Fig. 3

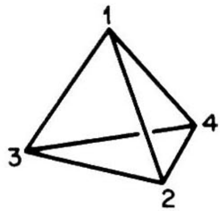

Fig. 4

---

[2]) Note that we use the term mobile in the sense of movable in space and deformable.

[3]) We use the terms chiral [6] for figures and orientable [7] for spaces. Orientation, on the other hand is taken to be an attribute to both figures and spaces [7]. See also [1]).

with ordered symbols, such as symbols of natural numbers, as in Fig. 4, its orientation can be specified. In line with our generalization, we use the term chiron for a mobility restricted, numbered 4-point-subarrangement. A chiron may be considered to be the vertices of a mobile oriented simplex, which retains its orientation. A mobile point arrangement consisting of chirons only will be called a multiplex.

The notion of a chiron and thus of a multiplex can be generalized to any dimension: A d-chiron consists of d+1 numbered points in a d-dimensional space ($d \geq 1$), so that no point is allowed to pass through the hyperplanes spanned by d other points, and a d-dimensional multiplex is a "mobile" point arrangement consisting of d-chirons. A 1-dimensional multiplex corresponds to an ordered arrangement of numbered points on a straight line, sometimes called permutation [8]. In this sense the multiplex notion may be interpreted to be a generalization of the concept of order to higher dimensions and the chiron may be regarded as something like a quantum of order.

B. THE CHARACTERIZATION OF MULTIPLEXES

In the following, $\mathbb{R}^d$ denotes the oriented d-dimensional Euclidean space[4].

Definition: A n-tuple $f = (P_1, P_2, \ldots, P_n)$ is called a (n,d)-figure, if $P_1, P_2, \ldots, P_n$ are points of $\mathbb{R}^d$ ($n > d \geq 1$) in general position. General position means that no d+1 points belong to a hyperplane of $\mathbb{R}^d$.

---

[4]) The orientation of $\mathbb{R}^d$ determines for d=1 the positive sense of a line, for d=2 the positive sense of a circle and for d=3 the positive sense of a helix.

As example we consider f_1, f_2 and f_3:

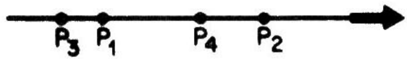

Fig. 5

Fig. 5 visualizes the (4,1)-figure $f_1 = (P_1, P_2, P_3, P_4)$; $\mathbb{R}^1$ is represented by the line with the arrow and the direction of the arrow shows the positive sense of the line.

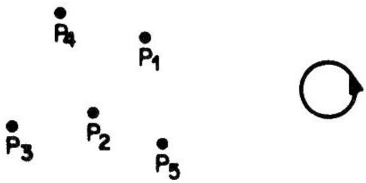

Fig. 6

Fig. 6 visualizes the (5,2)-figure $f_2 = (P_1, P_2, P_3, P_4, P_5)$. The plane of the paper with the arrowed circle represents $\mathbb{R}^2$ and the direction of the arrow shows the positive sense of the circle.

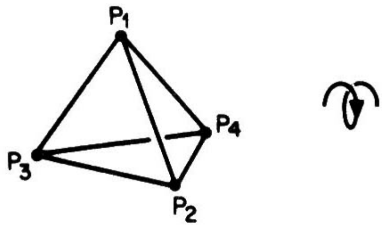

Fig. 7

Fig. 7 visualizes the (4,3)-figure $f_3 = (P_1, P_2, P_3, P_4)$; the lines between the points are only intended to give a 3-dimensional impression. $\mathbb{R}^3$ is represented perspectively in the plane of the paper and the perspective view of the helix shows its positive sense[5]).

---

[5]) Notice that the arrow in Fig. 7 is not needed to show the positive sense of the helix.

The d+1 points $P_{i_1}, P_{i_2}, \ldots, P_{i_{d+1}}$ with $i_1 < i_2 < \ldots < i_{d+1}$ of the (n,d)-figure $f = (P_1, P_2, \ldots, P_n)$ determine a (d+1,d)-figure $(P_{i_1}, P_{i_2}, \ldots, P_{i_{d+1}})$, which is called a simplex-figure of f. All simplex figures of f can be arranged in lexicographic order of their index-sequences. Thus a $\binom{n}{d+1}$-tuple A(f) of simplex-figures corresponds to f. In our examples:

$A(f_1) = ((P_1,P_2),(P_1,P_3),(P_1,P_4),(P_2,P_3),(P_2,P_4),(P_3,P_4));$

$A(f_2) = ((P_1,P_2,P_3),(P_1,P_2,P_4),(P_1,P_2,P_5),(P_1,P_3,P_4),(P_1,P_3,P_5),$
$(P_1,P_4,P_5),(P_2,P_3,P_4),(P_2,P_3,P_5),(P_2,P_4,P_5),(P_3,P_4,P_5));$

$A(f_3) = ((P_1,P_2,P_3,P_4)).$

Now we consider the orientation of the simplex-figures of f and put 1 for positive and 0 for negative orientation[6]). Thus we get a $\binom{n}{d+1}$-tuple $\alpha(f)$ of numbers 1 and 0. In our examples: $\alpha(f_1) = (1,0,1,0,0,1)$; $\alpha(f_2) = (0,0,1,0,1,1,0,1,0,0)$; $\alpha(f_3) = (1)$. $\alpha(f)$ can be considered as a dyadic representation of a non-negative integer, which we call the signature of f and designate it as $\sigma(f)$. In our examples: $\sigma(f_1) = 41$; $\sigma(f_2) = 180$; $\sigma(f_3) = 1$. We now define an equivalence relation on the set of all (n,d)-figures as follows:

Definition: Two (n,d)-figures f and f' are equivalent if $\sigma(f) = \sigma(f')$. An equivalence class [f] is called an (n,d)-multiplex. The common signature of all the representative (n,d)-figures is the signature of the (n,d)-multiplex. A (d+1,d)-multiplex is said to be a d-chiron.

---

[6]) The orientation of the simplex figure $(P_{i_1}, P_{i_2}, \ldots, P_{i_{d+1}})$ is positive or negative according to the sign of the determinant $\det(\overrightarrow{P_{i_1}P_{i_2}}, \overrightarrow{P_{i_1}P_{i_3}}, \ldots, \overrightarrow{P_{i_1}P_{i_{d+1}}})$. This orientation can also be derived by following the points in the order of their indices and determining whether for d=1, 2 or 3 the sense of the line, circle or helix, respectively, is positive or negative.

The signatures of (n,d)-multiplexes belong to the set $I(n,d) = \{\nu \in \mathbb{Z} \,/\, 0 \leq \nu < 2^{\binom{n}{d+1}}\}$. But not every integer $\nu \in I(n,d)$ is the signature of a (n,d)-multiplex. There is, for instance, no (4,2)-multiplex with the signature 5, because there is no (4,2)-figure $f = (P_1,P_2,P_3,P_4,P_5)$ with $\sigma(f) = 5$. If it would exist, it would have $A(f) = ((P_1,P_2,P_3),(P_1,P_2,P_4),(P_1,P_3,P_4),(P_2,P_3,P_4))$ and $\alpha(f) = (0,1,0,1)$. As can be seen in Fig. 8, P_4 would then have to lie in the intersection of the three shaded half-planes, which, however, is empty.

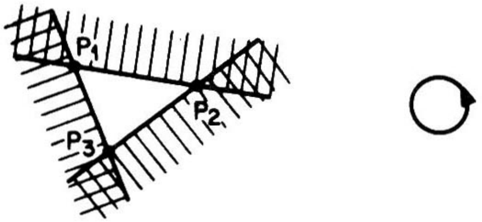

Fig. 8

We denote the set of integers which occur as signatures of (n,d)-multiplexes as M(n,d). For some of the simplest cases we get:

M(2,1) = {0,1}
M(3,1) = {0,1,3,4,6,7}
M(4,1) = {0,1,3,4,6,7,11,15,20,22,30,31,32,33,41,43,48,52,56, 57,59,60,62,63}
M(5,1) = {0,1,3,4,6,7,11,15,20,22,30,31,32,33,41,43,48,52,56, 57,59,60,62,63,75,79,95,107,123,127,148,150,158,180, 188,190,222,223,254,255,288,289,297,304,312,313,361, 363,377,379,432,436,440,444,504,505,507,508,510,511, 512,513,515,516,518,519,579,583,587,591,644,646,660, 662,710,711,719,726,734,735,768,769,800,801,833,835, 843,865,873,875,896,900,916,928,944,948,960,961,963, 964,966,967,971,975,980,982,990,991,992,993,1001, 1003,1008,1012,1016,1017,1019,1020,1022,1023}

M(3,2) = {0,1}
M(4,2) = {0,1,2,3,4,6,7,8,9,11,12,13,14,15}
M(5,2) = {0,1,3,7,8,12,14,15,16,18,19,23,24,28,29,31,48,50,54,
55,56,57,61,63,65,67,70,71,72,73,76,78,97,98,99,102,
105,108,109,110,112,113,114,118,121,125,126,127,128,
129,136,160,164,168,176,180,182,183,184,185,187,191,
193,200,201,209,217,219,240,241,244,246,249,251,254,
255,274,275,279,290,292,294,306,310,311,323,324,326,
327,328,329,331,332,339,343,347,354,355,356,358,361,
363,364,365,384,385,386,401,402,403,416,418,420,465,
467,475,480,482,483,484,491,492,493,495,496,497,499,
500,507,508,510,511,512,513,515,516,523,524,526,527,
528,530,531,532,539,540,541,543,548,556,558,603,605,
607,620,621,622,637,638,639,658,659,660,662,665,667,
668,669,676,680,684,691,692,694,695,696,697,699,700,
712,713,717,729,731,733,744,748,749,768,769,772,774,
777,779,782,783,804,806,814,822,823,830,832,836,838,
839,840,841,843,847,855,859,863,887,894,895,896,897,
898,902,905,909,910,911,913,914,915,918,921,924,925,
926,945,947,950,951,952,953,956,958,960,962,966,967,
968,969,973,975,992,994,995,999,1000,1004,1005,1007,
1008,1009,1011,1015,1016,1020,1022,1023}

Using $\overline{M}(n,d)$ for the complement of M(n,d) with respect to I(n,d), the following can be verified:

1. $M(d+1,d) = \{0,1\}$ and

$$\overline{M}(d+2,d) = \left\{ \frac{2^{d+3}+(-1)^{d}-3}{6} \ , \ \frac{2^{d+4}+(-1)^{d+1}-3}{6} \right\}$$

2. If $n<n'$, then $M(n,1) \subset M(n',1)$

3. If $n<n'$, then $\overline{M}(n,d) \subset \overline{M}(n',d)$

4. If $\nu+\nu' = 2^{\binom{n}{d+1}}-1$, then $\nu \in M(n,d) \Longleftrightarrow \nu' \in M(n,d)$

   Note that, if ν and ν' are signatures of two (n,d)-multiplexes, these multiplexes can be represented by mirror image (n,d)-figures.

The full characterization of M(n,d) turns out to be a difficult problem. Its solution would answer a question which was alluded to in section A, namely how many and which of the $\binom{n}{d+1}$ chirons must be specified in order to fully determine a given (n,d)-multiplex.

Even the simpler task of counting the number $|M(n,d)|$ of (n,d)-multiplexes has not been solved except for d=1, when it is n!. Without proof we mention a lower bound:

$$|M(n,d)| \geq 2 \prod_{k=d+1}^{n-1} r(k,d),$$

where r(k,d) denotes the maximum number of regions into which $\mathbb{R}^d$ may be partitioned by the hyperplanes of a (n,d)-figure, each hyperplane being spanned by d points of that figure. For the calculation of r(k,d), the results of Zaslavsky [9] can be used.

C. REMARKS

For the characterization of a (n,d)-multiplex [f] by an integer, other possibilities exist than the one defined in section B. It is worth considering some of them since they might express certain aspects of particular interest. Thus, for instance, the lexicographic order of the $\binom{n}{d+1}$ simplex-figures of f used for the construction of A(f) could be replaced by another order. Furthermore, $\alpha(f)$ may be considered as some other representation of an integer rather than the dyadic one.

(n,d)-Multiplexes can be classified as follows: If π denotes a permutation of the points of the (n,d)-figure $f = (P_1, P_2, \ldots, P_n)$ we write $\pi(f) = (\pi(P_1), \pi(P_2), \ldots, \pi(P_n))$. Two (n,d)-multiplexes [f] and [f'] are now equivalent when there exists a permutation π such that $[\pi(f)] = [f']$ [7]. Accordingly, a class of (n,d)-multiplexes is represented by a set of n points in $\mathbb{R}^d$. For example, each of the two point sets of Fig. 9 and 10 represent a class of (4,2)-multiplexes; the corresponding classes of signatures are {0,3,6,9,12,15} for Fig. 9 and {1,2,4,7,8,11,13,14} for Fig. 10.

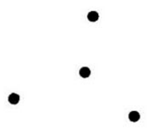

Fig. 9

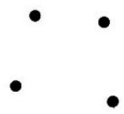

Fig. 10

If a (n,d)-multiplex is considered to be a mobile arrangement of numbered points, a class of (n,d)-multiplexes may be taken to be a mobile arrangement of unnumbered points. The problem of the characterization of (n,d)-multiplex classes for d>1 turns out to be difficult. It may be related to the problem of the axiomatization of a d-dimensional order structure, one aspect of which will be discussed in [12] and another in [13].

In a (n,d)-multiplex [f] the points of f are required to be in general position. If one drops this requirement there may

[7]) A class of equivalent (n,d)-multiplexes corresponds to a realizable (n,d+1)-tournament. (n,d+1)-Tournaments were defined in [10] as generalizations of tournaments, which are oriented complete graphs [11], and those that can be embedded in $\mathbb{R}^d$ were called realizable.

be non-oriented simplex-figures, so that three values should be available to assign to simplex-figures, such as, for instance, 1, 0 and -1. A signature can then be derived by interpreting the $\binom{n}{d+1}$-tuple of values as a triadic or some other representation of an integer.

For our definition of a multiplex the Euclidean space was used because it is close to the physical space; the affine space, however, would be sufficient. Finally, it might be of interest to examine a generalization of the multiplex concept by basing it on orientable d-dimensional manifolds other than $\mathbb{R}^d$.

This work was supported by the Schweizerische Nationalfonds zur Förderung der wissenschaftlichen Forschung and by Sandoz AG, Basel. We thank S. Bilinski, H.R. Haegi and F. Siegerist for informative discussions.

REFERENCES

[1] A.S. Dreiding, Lecture at the Stereochemistry Symposium in Sheffield on December 13, 1968, (report in Chemistry & Industry 1969, 43).

[2] K. Wirth, M. Huber, D. Pazis and A.S. Dreiding, "Structure and Names, I. Describing Method", manuscript in preparation.

[3] R.S. Cahn, C.K. Ingold and V. Prelog, Angew. Chem. 78, 413 (1966).

[4] J.H. van't Hoff, Archives Néerlandaises 9, 445 (1874).

[5] J.-A. Le Bel, Bull.Soc.chim. Paris 22, 337 (1874).

[6] Lord Kelvin, Footnote in "Baltimore Lectures on Molecular Dynamics and the Wave Theory of Light", O.J. Clay & Sons, London, 1904, p. 619.

[7] D. Hilbert and S. Cohn-Vossen, "Anschauliche Geometrie", Julius Springer, 1932, p. 269.

[8] C.L. Liu, "Introduction to Combinatorial Mathematics", McGraw Hill, 1968, p. 2.

[9] Th.K. Zaslawsky, "Facing Up to Arrangements: Face-Count Formulas for Partitions of Space by Hyperplanes", Ph.D. thesis, MIT, 1974, p. 95.

[10] K. Wirth, "Endliche Hyperturniere", Dissertation ETH, 1978, p. 7, p. 10.

[11] F. Harary, "Graph Theory", Addison-Wesley Publishing Co., 1969, p. 205.

[12] A.S. Dreiding, A. Dress and H.R. Haegi, "Chirotopes. A Combinatorial Theory of Orientation", manuscript in preparation.

[13] A. Häussler and K. Wirth, "On Transitive Hypertournaments", manuscript in preparation.