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THE NOMENCLATURE OF CHROMATOGRAPHY

III. GENERAL RULES FOR FUTURE REVISIONS

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CONTENTS

1. INTRODUCTION

In the discussion of the nomenclatures of gas and liquid chromatography in Parts I and II[1,2] of this series, we have already pointed out the problems which exist with the present nomenclatures and proposed modifications and corrections to be considered for future revisions. There is no reason to repeat these here. However, this series could not be finished without drawing attention to the general rules proposed in a major IUPAC publication[3], to certain rules followed by the major nomenclatures in the selection of lower-case and capital letters used as symbols and subscripts and, finally, to some basic considerations in the proper naming of certain important terms.

2. IUPAC MANUAL OF SYMBOLS

A major IUPAC publication issued in 1970 by the Division of Physical Chemistry[3] discusses in detail the rules to be followed in setting up nomenclatures for physical and physico-chemical methods, and the general symbols to be used for the major physical and physico-chemical quantities and units. Table 1 lists those which are also used in chromatography. These recommendations have important consequences. For example, the table clearly defines that *time* is t and not T while *temperature* (always in degrees Kelvin) is T; that *weight* is always W and not w while *width* should be w, etc. This distinction between lower-case and capital letters is very important to avoid confusion. These rules are often violated, not only due to simple sloppiness but also due to the use of lettering sets in the preparation of figures or to the recent fad of preparing tables and graphs by computers which can only print capital letters*. Not only should this habit be discouraged but journal editors shall

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* The use of capital letters only also creates confusion with various units. For example, one often finds in graphs MV for millivolts although the correct symbol is mV; MV means megavolts.

TABLE 1

GENERAL SYMBOLS RECOMMENDED BY IUPAC FOR PHYSICAL AND PHYSICO-CHEMICAL QUANTITIES AND UNITS[3]

Quantity, unit or term	*Symbol*
Area	A
Density	ϱ
Diameter	d
Diffusion coefficient	D
Equilibrium constant	K
Length	l
Pressure	p or P
Radius	r
Rate constant	k
Temperature (degrees Kelvin)	T
Time	t
Velocity	u
Viscosity	η
Volume	V
Weight	W

not accept such material. Authors who do this violate the elementary rules set up by the highest international body in chemistry.

There is one symbol where deviation from the IUPAC recommendations[3] is proposed: the use of L instead of l for "length". The reason for this is the easy interchangeability in a printed, and particularly typed, text of the letter l with the numeral "one".

3. GENERAL RULES

Obviously, only the most important quantities and units are listed in the IUPAC Manual of Symbols and therefore further differentiation is necessary. This differentiation should be done by using subscripts and superscripts and not composite symbols. Thus, symbols such as *tm*, *ts* and *tms* are not only against the words but also against the spirit of the official, carefully compiled nomenclatures*. Naturally, acronyms (*e.g.*, HETP and GC) may be used, but these should be capitalized and there is no need to use full stops after each letter.

Superscripts are generally used only for the various retention times and volumes, such as t'_R and V'_R for the adjusted retention time and volume, and t°_R and V°_R for the corrected retention time and volume (see ref. 1). Thus, practically all the differentiation is done by subscripts. Through their proper use one can use the same main symbol and still express quite different terms, such as $r_{i,s}$ representing relative retention and r_c the (inside) column radius.

The major nomenclatures[4-9] generally follow distinct rules in the selection of the proper subscripts. These rules are summarized below.

(a) In general, subscripts referring to the physical conditions or the phase should be capitalized. In gas chromatography, G refers to "gas" or the gas phase and

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* In fact, most of the compound symbols found in the literature are due to typing errors (not typing the subscript half-way down) and sloppy copy-editing.

L to "liquid" or the liquid phase; in generalized usage, M refers to the mobile phase and S to the stationary phase. Thus, *e.g.*, the diffusion coefficient in a gas is D_G and not D_g, the liquid diffusion coefficient is D_L and not D_l and, in general, the diffusion coefficient in the mobile phase is D_M and not D_m. Similarly, the mobile phase hold-up time (volume) is $t_M(V_M)$ and not $t_m(V_m)$. In subscripts, S should always refer to "stationary phase" and never to "support".

(b) In addition to those mentioned above, a few capitalized subscripts are used to describe specific terms, such as R in t_R and V_R for "retention", N in V_N to express "net retention" and I in V_I for "interstitial". In general, however, other capitalized subscripts should be avoided except those used to identify peaks, such as A or B.

(c) Subscript o generally refers to the outlet of the column such as in u_o or P_o. Thus it should not be used for "zero" because printers usually do not distinguish between o (lower case letter) and 0 (zero) in small characters. This is the reason why hold-up time (volume) is $t_M(V_M)$ and not $t_o(V_o)$ or t_0 (V_0). As discussed in connection with exclusion chromatography, an exception may be made there.

(d) Similarly to the rule against compound symbols, one should also avoid compound subscripts. Compound subscripts should only be used to identify individual peaks, *e.g.*, $r_{i,s}$, t_{R2} or $t_{R(z+1)}$. Sometimes, however, abbrevations have to be used as subscripts, such as V_{ext} for the external volume or n_{req} for the number of theoretical plates required for a given separation.

(e) Individual peaks may be characterized either by arabic numerals (1, 2, ...) or capital letters (A, B, ...) used as subscripts. It should always be assumed that the smallest numeral or the earlier letter refers to the peak which emerges first; in other words, by definition, $t_{R2} > t_{R1}$, $t_{R(B)} > t_{R(A)}$, etc.

(f) If a symbol already has a subscript, one should not create a subscript to a subscript; thus, it should be t_{R2} and not t_{R_2}. Simple subscripts indicating a given peak need not be placed in parentheses; however, parentheses are needed if complex subscripts are to be used or there is the possibility of any misunderstanding. For example, it is t_{R2} and not $t_{R(2)}$; on the other hand, the retention time of an *n*-alkane with $z+1$ carbon atoms in the molecule is $t_{R(z+1)}$.

4. MAJOR TERMS

In Parts I and II we discussed in detail the modifications or further clarifications recommended in connection with the major terms, such as:

diffusion coefficients;
distribution (equilibrium) constants;
open tubular columns;
capillary columns;
capacity factor

Hence there is no need to repeat these discussions here. However, one more major term should be mentioned where further revisions of the existing nomenclatures must include clear specifications. This term is the *retention index*.

The retention index system was first introduced in 1958 by Kováts[10] as a more precise expression of relative retention. By definition it gives the carbon number*

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* The number of carbon atoms in the molecule of the compound.

(multiplied by 100) of a hypothetical n-alkane which, under the given conditions and in isothermal operation, would give the same adjusted retention time (volume) as the component of interest. Mathematically, the retention index (I) can be expressed as

$$I_i = 100\left[\frac{\log X_i - \log X_z}{\log X_{(z+1)} - \log X_z} + z\right] \quad (1)$$

where X represents the adjusted retention time or volume, subscript i refers to the compound of interest and z represents the carbon number of the n-alkane emerging just before the compound of interest.

In the 20 years since its introduction the retention index system has become more and more accepted universally, in recognition of its simplicity.

In addition to the retention index system of Kováts, other similar systems have also been described in the literature. At the beginning, very correctly, these similar systems were indicated by different names, such as the *carbon number*[11] and *equivalent chain length*[12], both of which use the methyl esters of straight-chain saturated fatty acids instead of the n-alkanes as the reference series, the *steroid number*[13], where two hydrocarbons with steroidal structure are used as the bracketing reference compounds, the *methylene unit*[14], which is identical with the carbon number of the hypothetical n-alkane (*i.e.*, omitting multiplication by 100) but is determined under programmed-temperature conditions, the *arithmetic index*[15], which is similar to the retention index but calculated without the use of logarithms, and the *physico-chemical index*[16], which is a theoretical retention index value calculated from vapor pressure and molar volume data. Unfortunately, however, more and more authors are describing similar systems by keeping the term "retention index", indicating the difference by an adjective only. Examples are the *standard retention index* of Robinson and Odell[17], the *linear retention index* of Vigdergauz[18,19] and the *molecular retention index* of Evans[20]. Sometimes the difference is not even indicated in the name, such as the retention index calculated for programmed-temperature runs[21], where the logarithm is omitted, the retention index for iodoalkanes[22,23], where the 1-iodoalkanes are used instead of n-alkanes as the reference series, or the retention index system for polynuclear aromatics[24], where a series of polynuclear hydrocarbons are used as the reference compounds.

This uncritical use of the term "retention index" for other expressions starts to create confusion in the proper interpretation of the data published in the literature. For this reason, it is recommended that future revisions of the major nomenclatures clearly define the meaning of the "retention index" and specify that *only data corresponding to Kováts' original definition* can be listed under this name: all other expressions, however similar, must be clearly defined by another name.

5. SUMMARY

General rules of IUPAC concerning symbols for physical and physicochemical units are discussed which should be considered in any future revisions of chromatography nomenclatures. In addition, other important questions related to future nomenclature revisions are also discussed.

REFERENCES

1 L. S. Ettre, *J. Chromatogr.*, 165 (1979) 235–256.
2 L. S. Ettre, *J. Chromatogr.*, 220 (1981) 29–63.
3 *Manual of Symbols and Terminology for Physicochemical Quantities and Units, Pure Appl. Chem.*, 21 (1970) 3–44.
4 *Glossary of Terms to Gas Chromatography, British Standard 3282*, British Standards Institution, London; originally issued 1963; latestst revision 1969.
5 *Recommendations on Nomenclature and Presentation of Data in Gas Chromatography, Pure Appl. Chem.*, 8 (1964) 553–562.
6 *Recommendations on Nomenclature for Chromatography, Pure Appl. Chem.*, 37 (1974) 447–462.
7 *Gas Chromatography Terms and Relationships, ASTM E 355*, American Society for Testing and Materials, Philadelphia, PA; originally published 1968; latest revision 1977.
8 *Liquid Chromatography Terms and Relationships, ASTM E 682*, American Society for Testing and Materials, Philadelphia, PA; originally published 1979.
9 *Recommendations on Ion-Exchange Nomenclature, Pure Appl. Chem.*, 29 (1972) 619–624.
10 E. sz. Kováts, *Helv. Chim. Acta*, 41 (1958) 1915–1932.
11 F. P. Woodford and C. M. van Gent, *J. Lipid. Res.*, 1 (1960) 188–190.
12 T. K. Miwa, K. L. Mikolajczak, F. R. Earle and I. A. Wolff, *Anal. Chem.*, 32 (1960) 1739–1742.
13 W. J. A. VandenHeuvel and E. C. Horning, *Biochim. Biophys. Acta*, 64 (1962) 416–429.
14 W. J. A. VandenHeuvel, W. L. Gardiner and E. C. Horning, *Anal. Chem.*, 36 (1964) 1450–1560.
15 C. L. A. Harbourn, cited by A. G. Douglas, *J. Chromatogr. Sci.*, 7 (1969) 581–583.
16 N. Dimov and D. Shopov, *J. Chromatogr.*, 44 (1969) 170–172.
17 P. G. Robinson and A. L. Odell, *J. Chromatogr.*, 57 (1971) 1–10.
18 M. S. Vigdergauz, in H. G. Struppe (Editor), *Gas-Chromatographie 1968*, Akademie-Verlag, East-Berlin, 1968, pp. 625–642.
19 M. S. Vigdergauz and A. A. Martynov, *Chromatographia*, 4 (1971) 463–467.
20 M. B. Evans, *Chromatographia*, 11 (1978) 183–197.
21 H. Van den Dool and P. D. Kratz, *J. Chromatogr.*, 11 (1963) 463–471.
22 G. Castello and G. D'Amato, *J. Chromatogr.*, 54 (1971) 157–167.
23 G. Castello and G. D'Amato, *J. Chromatogr.*, 58 (1971) 127–135.
24 M. L. Lee, D. L. Vassilaros, C. M. White and M. Novotny, *Anal. Chem.*, 51 (1979) 768–774.