ANNALES
UNIVERSITATIS MARIAE CURIE-SKŁODOWSKA
LUBLIN — POLONIA
VOL. XXIV/XXV, 25 SECTIO AA 1969/1970

Z Katedry Chemii Nieorganicznej i Analitycznej Wydziału Farmaceutycznego AM w Lublinie
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Graphical Transformation of Composition Scales in Binary and Ternary Systems

Graficzne przekształcanie skal stężeniowych w układach dwu- i trójskładnikowych

Графическое преобразование концентрационных шкал в двойных и тройных системах

In investigations on solvent composition effects in chromatography a graphical method for the transformation of composition scales has been elaborated; since most of these transformations are usually done by calculations which are sometimes tedious and time-consuming, the author is of the opinion that this method may be worth popularizing.

Solvent mixtures are usually prepared on volume basis, for practical reasons. When, however, a theoretical interpretation of the experimental data is needed, it is advisable to express the composition in terms of mole fractions which bear a straight relation to the number of molecules of the components; for this reason, mole fractions are extensively used in physical chemistry of solutions, representation of phase equilibria etc. The two scales differ markedly especially in the case when one of the components is water, a solvent of a comparatively low molar volume (18 ml/mole).

A. BINARY MIXTURES

The diagram (Fig. 1) is suitable for direct and easy determination of transformed molar composition scales for binary mixtures containing s_B = 2, 5, 10, 20, 30, 40, 50, 60, 70, 80, 85, 90, 93, 95, 97 and 99 per cent by volume of one of the components (it is assumed that no volume changes occur on mixing, which is practically true in most cases).

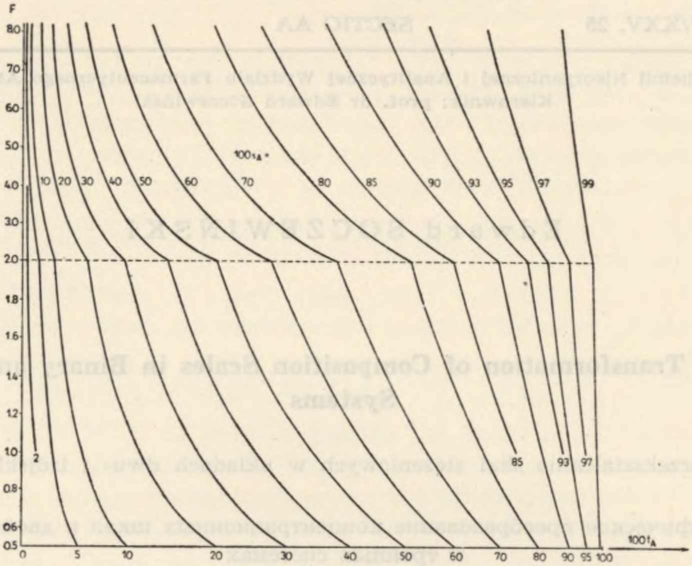

Fig. 1. Standard diagram for the transformation of composition scales

In order to find the compositions expressed in terms of mole fractions for binary mixtures of two given solvents *A*, *B*, the ratio of their molar volumes is calculated ($v^\circ_B/v^\circ_A > 1$) and the set of points on the level corresponding to this value on the ordinate is copied (Fig. 2); the new set of points on the composition axis represents the molar fractions corresponding to the sixteen volume compositions listed above and indicated on the sixteen lines in the diagram.

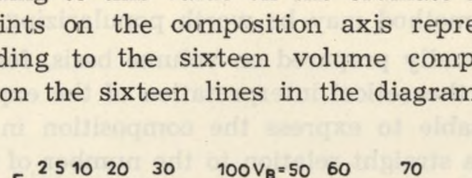

Fig. 2. An example of composition scale transformation ($v \rightarrow x$) $F = v^\circ_B/v^\circ_A = 1.33$. As a result of transformation, the composition points are shifted to the left, so that, for instance, $v_B = 50$ corresponds to $x_B = 0.43$

It is self-evident that the points are shifted in the direction of the component of lower molar volume and that the shift is more pronounced when the ratio of molar volumes (*F*) of the component solvents is greater.

The numerical values of the new compositions can also be found

Table 1

$100.s_B$	2	5	10	20	30	40	50	60	70	80	85	90	93	95	97	99
F \ t_B	$\frac{1}{1+49F}$	$\frac{1}{1+19F}$	$\frac{1}{1+9F}$	$\frac{1}{1+4F}$	$\frac{3}{3+7F}$	$\frac{2}{2+3F}$	$\frac{1}{1+F}$	$\frac{3}{3+2F}$	$\frac{7}{7+3F}$	$\frac{4}{4+F}$	$\frac{17}{17+3F}$	$\frac{9}{9+F}$	$\frac{93}{93+7F}$	$\frac{19}{19+F}$	$\frac{97}{97+3F}$	$\frac{99}{99+F}$
1.2	1.67	4.20	8.48	17.2	26.4	35.7	45.5	55.6	66.1	76.9	82.5	88.2	91.7	94.0	96.4	98.8
1.5	1.34	3.38	6.90	14.3	22.2	30.8	40.0	50.0	60.9	72.7	79.1	85.7	89.9	92.6	95.6	98.5
1.7	1.18	3.02	6.14	12.8	20.1	28.2	37.0	46.8	57.8	70.2	77.0	84.1	88.7	91.7	95.0	98.3
2.0	1.01	2.57	5.27	11.1	17.7	25.0	33.3	42.8	53.8	66.7	73.9	81.8	86.9	90.5	94.2	98.0
2.5	0,81	2.06	4.26	9.1	14.6	21.0	28.6	37.5	48.4	61.5	69.4	78.3	84.2	88.5	92.8	97.5
3	0.68	1.72	3.58	7.7	12.5	18.2	25.0	33.3	43.7	57.2	65.4	75.0	81.6	86.3	91.5	97.1
4	0.51	1.30	2.70	5.9	9.7	14.3	20.0	27.3	36.8	50.0	58.7	69.2	76.8	82.6	89.0	96.2
5	0.41	1.04	2.18	4.8	7.9	11.8	16.7	23.1	31.8	44.4	53.1	64.3	72.7	79.2	86.7	95.2
6	0.34	0.87	1.82	4.0	6.7	10.0	14.3	20.0	28.0	40.0	48.6	60.0	68.9	76.0	84.3	94.3
7	0.29	0.75	1.56	3.4	5.8	8.7	12.5	17.6	25.0	36.4	44.7	56.2	65.5	73.1	82.2	93.4
8	0.25	0.65	1.37	3.0	5.1	7.7	11.1	15.8	22.6	33.3	41.5	53.0	62.4	70.4	80.2	92.5
9	0.23	0.58	1.22	2.7	4.5	6.9	10.0	14.3	20.6	30.8	38.6	50.0	59.6	67.8	78.2	91.7
10	0.20	0.52	1.10	2.4	4.1	6.3	9.1	13 0	18.9	28.6	36.2	47.3	57.0	65.5	76.4	90.8

by projecting the shifted points onto the abscissa axis (as in Fig. 2). For equal molar volumes of the two solvents ($F = 1$) both composition scales are identical.

If it is preferable to plot the component of lower molar volume on the right hand side (i.e., $v^\circ_B/v^\circ_A < 1$), the new diagram is simply turned upside down with respect to Fig. 1. For plotting the transformation diagram in any convenient scale, Table 1 may be used.

The diagram can also be used for other composition transformations. As a matter of fact, molar, volume and weight fractions (x, v and w, respectively), are transformed by analogous formulas of the type

$$t_B = \frac{1}{1 + \frac{S_A}{S_B} F} = \frac{1}{1 + \frac{1 - S_B}{S_B} F}$$

where s, t are two concentrations and F is a correction factor given in Table 2.

Table 2

Transfomation $s \longrightarrow t$	Factor F	Shift of points towards the component possessing
$u_B \longrightarrow x_B$	$\frac{v^o_B}{v^o_A} = \frac{M_B \cdot d_A}{M_A \cdot d_B}$	lower molar volume
$x_B \longrightarrow u_B$	$\frac{v^o_A}{v^o_B} = \frac{M_A \cdot d_B}{M_B \cdot d_A}$	higher molar volume
$w_B \longrightarrow x_B$	M_B / M_A	lower molecular weight
$x_B \longrightarrow w_B$	M_A / M_B	higher molecular weight
$w_B \longrightarrow u_B$	d_B / d_A	lower density
$u_B \longrightarrow w_B$	d_A / d_B	higher density

v — volume fractions; w — weight fractions; x — mole fractions

In all four transformations involving volume fractions it is assumed that no volume changes occurred at mixing the component solvents.

B. TERNARY MIXTURES

Transformation of composition scales in ternary (Gibbs) diagrams is a more difficult task. If series of, say, volume compositions are plotted on two sides of the triangle (e.g., *AC* and *BC*) and the points are connected with the opposite angles, then a symmetrical network of composition lines is obtained, each line corresponding to a constant proportion of two components (Fig. 3a). The size of the triangle is chosen so that its side is equal in length to the composition axis in Fig. 1.

Another triangle of the same size is then drawn which is intended, for instance, to represent molar composition. After calculation of the molar volume ratios (v_C°/v_A° and v_C°/v_B°) the two sets of points on the sides *AC* and *BC* are transformed into the new composition scale (Fig. 3b) using the method described above. The points are now shifted

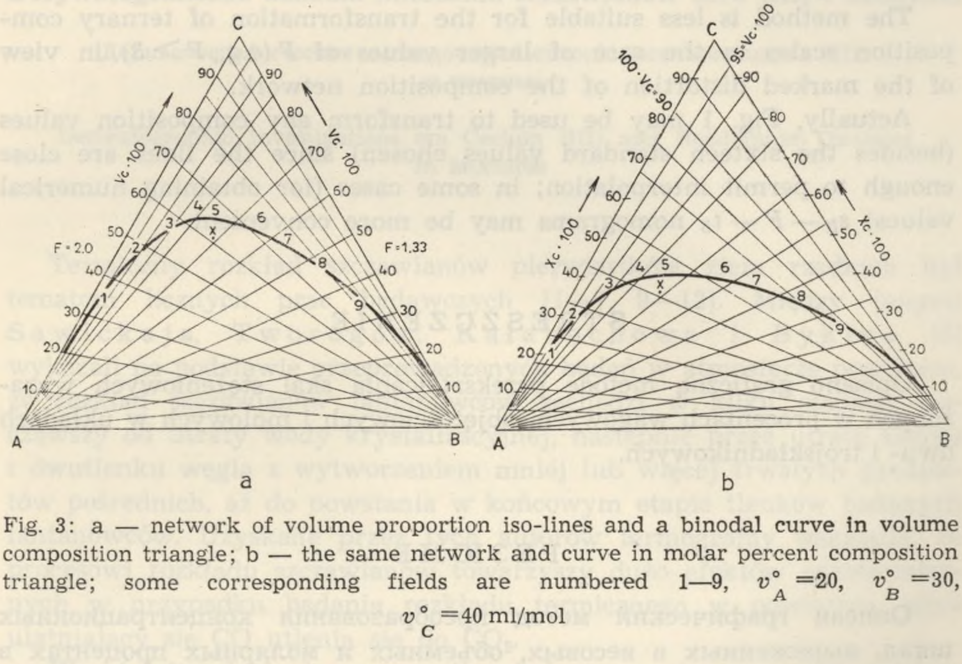

Fig. 3: a — network of volume proportion iso-lines and a binodal curve in volume composition triangle; b — the same network and curve in molar percent composition triangle; some corresponding fields are numbered 1—9, $v_A^\circ = 20$, $v_B^\circ = 30$, $v_C^\circ = 40$ ml/mol

towards the angles of components of lower molar volumes, *A* and *B*, respectively, and when the points are connected with the opposite angles of the triangle, a new, distorted network of composition lines is obtained; the new network, however, corresponds exactly to the former one since any pair of corresponding lines in the two diagrams represents composition points characterized by a constant volume (and thus also molar) proportion of two components.

If a phase diagram is drawn in Fig. 3a (volume composition scale) then the diagram can be re-drawn in Fig. 3b triangle, plotting the curve through the corresponding fields (some of the fields are numbered 1—9 in Figs. 3a, 3b) so that the diagram is obtained in the new (molar) composition scale. In analogous way, single composition points can be transformed (e.g., point X in field No 5).

It is not necessary to draw a fine network of composition lines; a compromise should be sought between the accuracy of plotting and the number of lines so as to avoid confusion. It is recommended to choose the lines so that large fields are avoided in view of lower accuracy. Some lines may be drawn a little thicker (or in colour pencil) in order to facilitate the comparison of the two networks (for instance, the lines corresponding to 20, 40, 60, and 80 v/v%).

Other transformations (e.g., $v \rightarrow w$, etc.) can be done in an analogous way, using the respective transformation factors (Table 2).

The method is less suitable for the transformation of ternary composition scales in the case of larger values of F (e.g., $F > 3$) in view of the marked distortion of the composition network.

Actually, Fig. 1 may be used to transform any composition values (besides the sixteen standard values chosen) since the lines are close enough to permit interpolation; in some cases (for obtaining numerical values) $s_B - F - t_B$ nomograms may be more convenient.

STRESZCZENIE

Opisano graficzną metodę przekształcania skal stężeniowych wyrażonych w procentach wagowych, objętościowych i molowych w układach dwu- i trójskładnikowych.

РЕЗЮМЕ

Описан графический метод преобразования концентрационных шкал, выраженных в весовых, объемных и молярных процентах в двойных и тройных системах.

Papier druk. sat. III kl. 80 g Format 70 × 100 Druku stron 6
Annales UMCS Lublin 1969 Lub. Zakł. Graf. Lublin, Unicka 4 Zam. 1662. 9.VI.70
600 + 25 egz. A-7 Manuskrypt otrzymano 9.VI.70 Data ukończenia 31.VIII.71