COMMUNICATION

Coordinates for Ternary Systems

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SCHOTT has proposed a coordinate transformation for applying the method of wet residues algebraically in ternary systems (2). Advantages of an algebraic approach to the wet residue principle have been described by Hill and Ricci (1). In principle the transformation effects a superposition of rectangular upon triangular coordinates in the ternary diagram. As the manipulation of ternary systems frequently involves extensive mathematical detail, some comment upon several aspects of the coordinate transformation appears to be advisable.

The proposed transformation has been described previously by Smith (3) in connection with liquid-liquid systems. Smith obtained, in terms of Schott's variables,

$$x = \frac{p_A + 2p_C}{3^{1/2}} \quad (1)$$

which is somewhat simpler in form than Schott's equivalent Equation 6. The transformation into x, y coordinates neither simplifies calculations nor improves their precision beyond that already obtainable. This may be domonstrated by briefly considering two loci of points of particular significance in ternary systems, described in their form in a triangular diagram: (1) a line passing (ordinarily, only by extension) through any two of the sides of the triangle, (2) a line passing through one of the apexes. The former may correspond either to a tie line or the locus of resultants of the mixing of varying amounts of a given pair of mixtures lying on the line. The latter may correspond to the locus of points resulting from the addition (or removal) of one of the three components—e.g., a cloud point titration in a liquid-liquid system or a crystallization path in a liquid-solid system.

LINE THROUGH TWO SIDES

The straight line passing through the pair of points (x_i, y_i) and (x_j, y_j) considered in Schott's Equation 7 may also be expressed directly in terms of weight per cent. The straight line may be defined by any one of the determinants

$$\begin{vmatrix} p_A & p_B & 1 \\ p_{Ai} & p_{Bi} & 1 \\ p_{Aj} & p_{Bj} & 1 \end{vmatrix} = \begin{vmatrix} p_A & p_C & 1 \\ p_{Ai} & p_{Ci} & 1 \\ p_{Aj} & p_{Cj} & 1 \end{vmatrix} = \begin{vmatrix} p_B & p_C & 1 \\ p_{Bi} & p_{Ci} & 1 \\ p_{Bj} & p_{Cj} & 1 \end{vmatrix} = 0 \quad (2)$$

Therefore the tie lines given by Schott in Equations 8 and 9 may also be expressed directly as

$$-p_B - 11.000p_A + 535.30 = 0 \quad (3)$$

$$p_B + 4.185p_A - 213.44 = 0 \quad (4)$$

These lead to the identical p_A and p_B obtained by Schott, but without the complication of converting into and then back out of the x, y coordinates.

The use of weight per cent directly is even more advantageous when the intersections of the line with the two sides (obtainable by extrapolation) are known. If these be the $AC(i)$ and $BC(j)$ axes, for example, then from Equation 2

$$p_{Bj}p_A + p_{Ai}p_B - p_{Ai}p_{Bj} = 0 \quad (5)$$

defines the line. This simplification is not possible with the x, y coordinates.

LINE THROUGH APEX

Two aspects are commonly concerned with the relationship, and in the present system, using the C apex as example, they may be stated as: (1) for such a line, what is the p_A/p_B ratio along that line; (2) for a desired p_A/p_B ratio what is the required line? Assume a point x, y. From Schott's Equation 1 and 6

$$\frac{p_A}{p_B} = \frac{2y}{200 - y - 3^{1/2}x} \quad (6)$$

Thus for the various points along this line, while p_A/p_B is constant, there is not a correspondingly constant x/y ratio. The constancy of p_A/p_B along such a line is especially desirable when trial-and-error procedures are necessary. A similar conclusion holds for the ratio p_B/p_C when the apex is A. If the apex is B, although x/y is now a constant, it is unequal to the ratio p_A/p_C. Like objections to the variable transformation arise when, say, a desired ratio $p_A/p_B = r$ has been selected for a certain value for p_A.

In summary it appears that the x, y coordinate system would introduce a significant increase of labor into various calculations, of which there are often many in an exhaustive study of a ternary system. The coordinate transformation might be justified if results were more precise than those obtainable directly by weight per cent variables, but this is not so. In fact, the weight per cent variables are inherently more precise than the x, y variables, because, as Equation 1 shows, the uncertainty of x combines those of two of the weight per cent variables.

LITERATURE CITED

(1) Hill, A.E., Ricci, J.E., *J. Am. Chem. Soc.* **53**, 4305 (1931).
(2) Schott, H., J. CHEM. ENG. DATA **6**, 324 (1961).
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RECEIVED for review April 19, 1962. Accepted June 13, 1962.