CHEMISTRY

F. M. PERELMAN

1960

SovietRxiv

Fig. 1. Optimal model for representing simple five-component systems (of type 5 || 1)

Figure 1: Fig. 1. Optimal model for representing simple five-component systems (of type 5 || 1)

Abstract

Full Text

CHEMISTRY

F. M. PERELMAN

REPRESENTATION OF MULTICOMPONENT SYSTEMS BY MEANS OF MODELS

(Presented by Academician N. V. Tananaev, 25 XI 1959)

In the investigation of systems formed by three or four components, models are often used which make it possible to represent the dependence between composition and properties more vividly than can be done on a graph. As the number of components (and other equilibrium factors) increases, models may prove still more useful, since in this case multidimensional spatial figures serve to represent composition. Thus, five-component systems of various types are represented mainly by means of three different four-dimensional figures (^1): 1) a pentatope—for simple systems, i.e., those formed by five metals, or oxides, or salts with one common ion; 2) a tetradic hexahedroid—for reciprocal systems of four cations and two anions (or of four anions and two cations), i.e., of eight simple salts; 3) a prismatic hexahedroid—for reciprocal systems of three cations and three anions, i.e., of nine simple salts. Let us denote the different types of five-component systems, respectively, as: 5 || 1; 4 || 2; 3 || 3.

Fig. 1. Optimal model for representing simple five-component systems (of type 5 || 1)

These four-dimensional figures can be projected onto six coordinate planes. Analysis shows, however, that the projections obtained are not equivalent in their visual clarity and practical suitability. In each case only one of the plane projections, which I have called optimal (^2), makes it possible to depict all components on the same scale, gives a clear representation of the limits of distribution of individual phases of the systems, and permits quantitative calculations.

Depending on the nature of the system and the properties of the four-dimensional figure, construction of the complete state diagram is carried out by means of several projections of the optimal type: for systems 5 || 1—three, 4 || 2

Fig. 2

Figure 2: Fig. 2

Fig. 3

Figure 3: Fig. 3

–four, 3 || 3–nine. It is possible, however, to project the figures listed above not onto a plane, but into three-dimensional space. Referring them to a Cartesian coordinate system with axes x, y, z, T, one can obtain projections of the model onto four coordinate spaces: xyz, xyT, xzT, yzT. Like the projections of the same figures onto a plane, these spatial projections also differ from one another in their degree of visual clarity.

It has been found that for the pentatope only the projection onto the coordinate space xzT is optimal (see Fig. 1). It is a tet-

polyhedron, three vertices of which correspond respectively to three components of the system (E, D, and C), while the fourth vertex represents the remaining two components (A and B) in aggregate. Thus, in order to represent the state diagram of system 5 ‖ 1 as a whole, it is necessary to construct two models of the type shown in Fig. 1.

The tetrahedral hexahedron also has only one projection–onto the coordinate space xzT–that permits quantitative calculations (see Fig. 2). This is a triangular prism; four of its vertices, D, C, D_1, C_1 (two in the upper and two in the lower base), correspond to four simple salts of the system; the remaining two vertices represent two salts each in aggregate (AB and A_1B_1).

Fig. 2. Optimal model for representing reciprocal systems of five components forming eight simple salts (of type 4 ‖ 2)

Fig. 3. Optimal model for representing reciprocal systems of five components forming nine simple salts (of type 3 ‖ 3)

(AB and A_1B_1). Thus, in order to represent system 4 ‖ 2 as a whole, it is necessary to construct two models of the type shown in Fig. 2, since the initial system is formed by eight simple salts. Finally, the prismatic hexahedron can be projected clearly onto two coordinate spaces: xyT and xzT. In both cases similar models are obtained. One of them is shown in Fig. 3.

On the triangular prism the original nine simple salts are arranged as follows: three salts (A_2, B_2, C_2) at the vertices of the upper base, and the remaining six pairwise at the three vertices of the lower base (AA_1, BB_1, and CC_1). Therefore, to represent the complete state diagram of system 3 ‖ 3, it is necessary to have three models of the type shown in Fig. 3. The models indicated in Figs. 1, 2, and 3 can be constructed on the basis of data on the constituent ternary systems represented on the faces of the tetrahedron or of both prisms. Thus preliminary state diagrams of the corresponding five-component systems will be obtained, giving a general orientation picture of the five-component system as a whole.

Such models are very useful for predicting compositions with desired properties and for indicating the most promising directions for the investigation of multicomponent systems.

Institute of General and Inorganic Chemistry
named after N. S. Kurnakov
Academy of Sciences of the USSR

Received
20 XI 1959

CITED LITERATURE

1. V. P. Radishchev, *Izv. sektora fiz.-khim. analiza*, **22**, 33 (1953).

2. F. M. Perelman, *Methods for Representing Multicomponent Systems. Five-Component Systems*, Publishing House of the Academy of Sciences of the USSR, 1959.

Note: Figure translations are in progress. See original paper for figures.