

Comparison of the compositions of crystalline aluminosilicate rocks and their minerals in a planar triangular projection

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Abstract

The problem of comparison of the composition of crystalline rocks with the composition of the constituent minerals of these rocks is considered. It is proposed to present the composition of rocks and the compositions of the constituent minerals in the form of a triangle on the plane. The experience of presentation of compositions in phase diagrams was taken as a basis for the construction. Analysis of the crystallochemical characteristics of clinopyroxenes and garnets has shown that three parameters are enough for depicting the compositions of these and other minerals. For this purpose, similar composition components of rocks and their minerals are summarized in molecular proportions and are plotted on the triangle $DO-1/2(R_2O_3)-XO_2$, where $DO = (MgO + CaO + FeO + MnO + NiO + \dots) + 1/4(Na_2O + Al_2O_3) + 1/4(K_2O + Al_2O_3)$, $1/2(R_2O_3) = 1/2(Al_2O_3 + Fe_2O_3 + Cr_2O_3 + \dots) - (1/4(Na_2O + Al_2O_3) + 1/4(K_2O + Al_2O_3))$, and $XO_2 = SiO_2 + TiO_2$. The compositions of minerals are expressed as the sums of their components: $Ol = Fo + Fa + Lar + Neph + \dots$, $Px = Di + En + Wol + Ged + Gip + Jd + Eg + \dots$, $Ga = Pyr + Gross + Alm + Spe + Ski + Knr + Mj + \dots$, etc. A step-by-step calculation algorithm is proposed, which permits evaluation of the contents of bi- and trivalent iron during probe microanalyses of garnets and pyroxenes. Comparison of the compositions of deep-seated rocks and their minerals shows their good consistency. The proposed schematic projection permits a visual comparison of the compositions of rocks with low contents of carbonates and water, from ultrabasic (e.g., dunites) to acid (e.g., granites) ones.

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Introduction

Results of rock and mineral analyses are usually presented as weight contents of their components. At the same time, the compositions of rocks and minerals can be compared only as molecular proportions of the contents of these components. Zavaritskii (1944) elaborated algorithms for recalculation of these parameters, and Bulakh (1967) calculated formula factors, based on mineral compositions. At present, this problem is paid no attention, because the above two publications are considered to be highly informative.

Nevertheless, the problem of comparison of mineral compositions, rock compositions, and, particularly, compositions of rocks and their minerals is still urgent. This is due to the desire to create a universal system. The number of significant parameters in such a system cannot be presented graphically

in 3D space, which deprives these systems of visualization and does not permit one to analyze the results correctly.

Moreover, the development of methods for analysis of rocks and minerals led to mass replacement of chemical analyses by indirect analytical methods, such as X-ray fluorescence analysis (XRF) and electron probe microanalysis (EPMA) of minerals. These are partial analyses with regard to their techniques. The main problem of these techniques is that there is no analysis of the contents of elements in accordance with their valence state. Therefore, the rock compositions determined by XRF cannot be processed and compared with each other by classical correct methods, and the results of EPMA of most minerals cannot be recalculated to formula factors. These analytical data cannot be used in physicochemical modeling and mineral geothermobarometry. This restriction is totally ignored in most publications dealt with the above problems.

In most analyses of rocks and aluminosilicate minerals, this problem might be solved by determining the proportion of bi-

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and trivalent iron, but such techniques are not applied today, although they are theoretically realizable.

Some researchers propose estimation of the content of trivalent iron cation from the ideal mineral formula (Brandelik, 2009; Droop, 1987; Finger, 1972; Lindsley, 1983; Nenova, 1997; Papike et al., 1974). These techniques differ in the order of calculation operations, but the calculation is made by the same algorithm: First, the number of cations is determined and the sum of their valences is calculated; then, the amount of tri- and bivalent iron is calculated from the difference between the sum of the cation valences and the ideal formula (the sum of oxygen valences). With this algorithm, the total error in the determination of all cations is obviously involved in the parameters used for the calculation of the amounts of bivalent and trivalent iron.

Thus, calculation of the contents of bi- and trivalent iron in mineral, based on its ideal formula and EPMA data, is a disputable technique. Although when other techniques are inapplicable, the above one can be used, with publication of the original analytical data and their recalculation algorithm.

The experience of works with synthetic substances prepared from reagents of special-purity grade showed that electron probe microanalysis (EPMA) never yields the total content of their components equal to 100%. For two-thirds of the examined points, the total content is 97–98%. Researchers usually reject such analytical data, explaining them by the complex structure of the sample, thin intergrowths of phases, small grain size, etc. In principle, this is reasonable. However, such data show that the actual accuracy of a particular analysis is much lower than the instrumental accuracy and that an EPMA yielding the total content of components close to 100% is not always the most accurate. This factor is not well realized by researchers, as evidenced from some EPMA results (Brandelik, 2009; Droop, 1987) of natural clinopyroxene yielding the total content of components greater than 100% (the initial content is 100.02%, and the recalculated content is 100.36%). It is obvious that not all elements of a natural mineral can be analyzed. This means that the total content of components in the reference sample must always be less than 100%.

Of special interest are the analytical potentialities of energy-dispersive electron probe microanalysis (ED-EPMA). The measurement accuracy of electron probe is much worse than that of crystalline detectors, but the progress in the design of these detectors makes it possible to reach a satisfactory quality of analysis. The advantage of ED-EPMA is that the determined atomic (molecular) proportions of element contents show a minor dependence on the quality of the surface of the sample being analyzed. Therefore, for geothermobarometric measurements, thermodynamic calculations, and crystallochemical studies requiring the accurate determination of the molecular proportions of component contents, ED-EPMA of minerals is preferable to EPMA.

In addition to calculation of the content of trivalent iron from the ideal mineral formula, there are other methods for estimating the content of trivalent iron in minerals such as clinopyroxenes and garnets which do not depend strongly on the ideal formula of minerals. These methods can be developed

if one takes into account the clinopyroxene and garnet structures (Bragg and Claringbull, 1965) and depicts the phase compositions as phase diagrams.

In a simplified representation, the pyroxene structure contains paired chains of silicon–oxygen tetrahedra, with six- and eight-coordinated positions in between, usually occupied by bivalent cations. Trivalent cations (aluminum) enter both the four-coordinated positions (at the place of silicon cations) and the six-coordinated position. Monovalent cations (sodium) occupy the eight-coordinated positions.

Pyroxenes have a compositional formula $M_1M_2TTO_6$, where the position M_1 is a more or less regular octahedron with coordination number 6, which is occupied by bivalent and trivalent cations Mg^{2+} , Al^{3+} , Fe^{2+} , Fe^{3+} , Mn^{2+} , Cr^{3+} , etc., the position M_2 with coordination number 8 is occupied by larger cations Ca^{2+} , Na^{1+} , Mg^{2+} , Fe^{2+} , Mn^{2+} , etc., and the position T is chains of tetrahedra with coordination number 4, which are occupied by cations Si^{4+} and Al^{3+} . Substitution of cations in all structural positions is intricate, and the pyroxene structure is complicated by the distortion of the silicon–oxygen chain orientation and by coordination ordering.

Garnet structure consists of a framework formed by silicon–oxygen tetrahedra binding the octahedral positions occupied by trivalent cations (mainly Al^{3+} , Cr^{3+} , and Fe^{3+}), with eight-coordinated positions in between, which are occupied by bivalent cations.

Thus, both clinopyroxene and garnet structures have three structural positions occupied by corresponding cations. This makes it possible to describe the compositions of these minerals via three independent parameters and present their projections as a planar triangle.

First, let us consider a composition triangle for the system $MgO-Al_2O_3-SiO_2$ system (Fig. 1). Phase relations in this system at the atmospheric pressure and other pressures of up to 40 kbar are described by Doroshev and Malinovskii (1974).

The phase compositions expressed in mol.% of components MgO , $1/2(Al_2O_3)$, and SiO_2 have integer ratios of these components and correspond to points with the following compositions: enstatite— $2(MgO) + 2(SiO_2)$, forsterite— $2(MgO) + 1(SiO_2)$, pyrope— $3(MgO) + 2(1/2(Al_2O_3)) + 3(SiO_2)$, spinel— $1(MgO) + 2(1/2(Al_2O_3))$, etc.

Enstatite and pyrope lie on the composition triangle diagonal connecting the vertex $1/2(Al_2O_3)$ with the enstatite end-member $1/2(Mg_2Si_2O_6)$. Solid solutions of aluminous orthopyroxenes, localized in the $Mg_2Si_2O_6$ (enstatite)– $MgAl_2SiO_6$ (Mg-tschermakite) join, fall on the same diagonal. No deviation of their compositions from this line is observed. Protoenstatites show a minor deviation toward high SiO_2 contents at the atmospheric pressure (Biggar, 1985). This deviation is close to the accuracy of composition determination.

Solid solutions of the majorite ($Mg_3MgSi_3O_{12}$) component in pyrope are solutions of the enstatite end-member $1/2(Mg_2Si_2O_6)$ in pyrope garnet ($Mg_3Al_2Si_3O_{12}$). When Si^{4+} enters the six-coordinated structural position instead of Al^{3+} , the excess positive charge must be compensated by the synchronous substitution of Al^{3+} by Mg^{2+} . Magnesium cation

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