SYNOPSES

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Calculation of *T*-site occupancies in alkali feldspar from refined lattice constants

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TETRAHEDRAL site occupancies in alkali feldspar from refined lattice constants can be measured assuming $t_1O+t_1m+t_2O+t_2m = t_1O+t_1m+2t_2 = 1$ and using the indicators of structural state $\Delta(bc) = t_1O+t_1m$ (or $\Delta(b^*c^*)$ in all circumstances in which it is more convenient than $\Delta(bc)$) and $\Delta(\alpha^*\gamma^*) = t_1O-t_1m$, as widely discussed in Smith's (1974) and Ribbe's (1975) works on the basis of the most recent structural investigations.

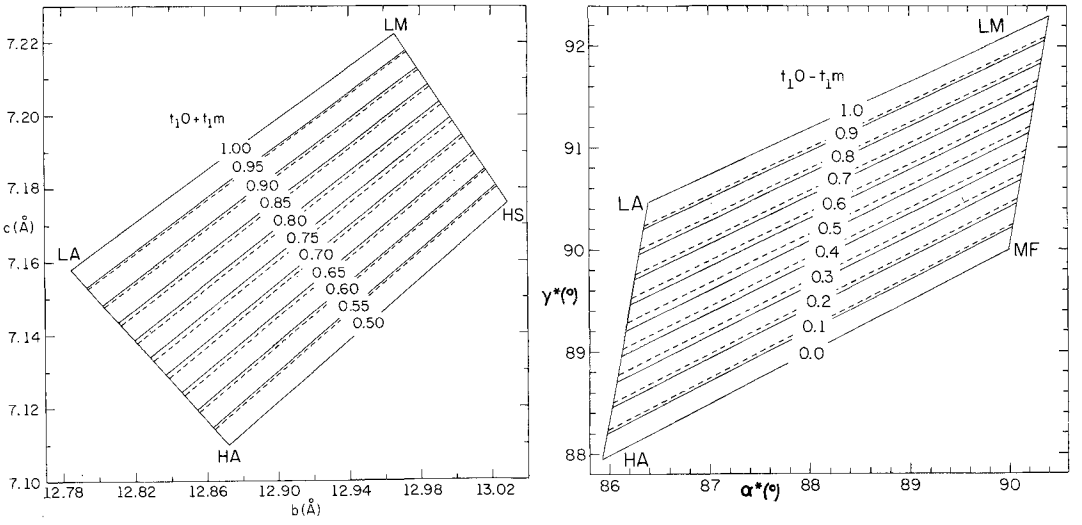
The relevant equations proposed by Luth (1974) for calculating all these indicators from refined lattice constants b and c (or b^* and c^*), α^* and γ^*, respectively, have been considered since they appeared approximate when first examined. As Luth (1974) has not explained how he obtained these formulae for the unit-cell dimensions of the alkali feldspar end-members quoted in his paper and in Ribbe's (1975) work, a procedure that enables them to be derived has been reconstructed in the present paper.

This procedure was then applied to obtain Luth's equations for alkali feldspar reference end-members proposed by Smith (1974). Figs. 1 and 2 show the opposite behaviour for the equations of the iso-$\Delta(bc)$ and iso-$\Delta(\alpha^*\gamma^*)$ straight lines, which furnish true values only at each extreme of the indicators considered.

As values of these indicators are commonly rounded off in the literature until they contain three or four decimal places, it also seems worthwhile pointing out that the inaccuracies introduced by using Luth's equations can be several tens of times higher than the approximations with which the results are usually written.

As an alternative, a new method of calculation is proposed that represents a rigorous treatment. It is based on the solution of the equation of the iso-Δ straight line, i.e. according to the cases iso-$\Delta(bc)$ (or iso-$\Delta(b^*c^*)$) and iso-$\Delta(\alpha^*\gamma^*)$ straight lines, on which the representative point of a given alkali feldspar lies in the irregular quadrilateral of the reference end-members plotted on the bc (or b^*c^*) and $\alpha^*\gamma^*$ diagrams, respectively. Expressed as a function of the unknown indicator Δ, of the extreme values which Δ can assume ($0 \leqslant \Delta(bc) \leqslant 0{\cdot}5$ and $0 \leqslant \Delta(\alpha^*\gamma^*) \leqslant 1$), and of the quadrilateral vertex coordinates, the equation of this iso-Δ straight line written out explicitly with respect to Δ assumes a quadratic form. Therefore, in practice there are two real and unequal solutions, one of which is included in the extreme ranges of Δ and of course is the solution to accept.

This method can also be applied for calculating Smith's (1974) indicator $Or(b^*c^*)$, which is involved in cell dimensions of perthites and anomalous specimens. This indicator is derived from refined lattice constants b^* and c^*, and in this case, too, the procedure proposed leads to a quadratic equation, which in practice gives two real and unequal solutions, one of which falls in



FIGS. 1 and 2: FIG. 1 (*left*). Plot of *bc* of alkali feldspar using the end-member co-ordinates for high-sanidine (HS), low-microcline (LM), low-albite (LA), and high-albite (HA) as given by Smith (1974). The quadrilateral, contoured for t_1O+t_1m, shows the differences between the straight lines representing $\Delta(bc)$ values calculable with the proposed method (solid lines) and those obtainable from the equation of Luth (1974) (dashed lines). FIG. 2 (*right*). Plot of $\alpha^*\gamma^*$ of alkali feldspar using the reference points for monoclinic feldspars (MF), low-microcline (LM), low-albite (LA), and high-albite (HA) as given by Smith (1974). The quadrilateral, contoured for t_1O-t_1m, shows the differences between the straight lines of $\Delta(\alpha^*\gamma^*)$ values calculable with the proposed method (solid lines) and those obtainable from the equation of Luth (1974) (dashed lines).

the interval between the extreme values of $Or(b^*c^*)$ ($0 \leqslant Or(b^*c^*) \leqslant 1$), and of course is the solution to accept.

The calculation procedure for estimating the error terms in $\Delta(bc)$ (or $\Delta(b^*c^*)$), $\Delta(\alpha^*\gamma^*)$, and $Or(b^*c^*)$ is also given in an attached Appendix. The expressions that permit these error terms to be calculated are derived by the Law of Propagation of Errors, using variances and also covariances, since covariances are usually available on the output of the most up-to-date lattice constant refinement programs.

The formulae devised in the present investigation for calculating both structural indicators $\Delta(bc)$, $\Delta(b^*c^*)$, $\Delta(\alpha^*\gamma^*)$, and Smith's (1974) indicator $Or(b^*c^*)$ entail tedious computations. As these quantities are being increasingly used in common mineralogical and petrological practice, a computer program available in Fortran IV has also been prepared, which allows these indicators and their respective variances to be calculated.

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The full text in the 'miniprint' section of this volume, pp. M14–16.

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