American Mineralogist, Volume 58, pages 905–908, 1973

Non-Linear Variation of Cell Parameters with Composition in Alkali Feldspar Series

THOMAS A. VOGEL, ROBERT EHRLICH,

Geology Department, Michigan State University, East Lansing, Michigan 48823

WILLIAM C. LUTH

Geology Department, Stanford University, Stanford, California 94305

Abstract

For a given alkali feldspar series of constant degree of internal order (structural state) the unit cell parameters are strongly linear functions of composition. Residual variation about such regression lines exhibits a systematic non-random pattern which is similar from one structural series to another. Alkali feldspar at all structural states can be divided into two families (0.0–0.4 and 0.4–1.00 mole fraction $KAlSi_3O_8$) even for those series which do not exhibit a monoclinic-triclinic transition.

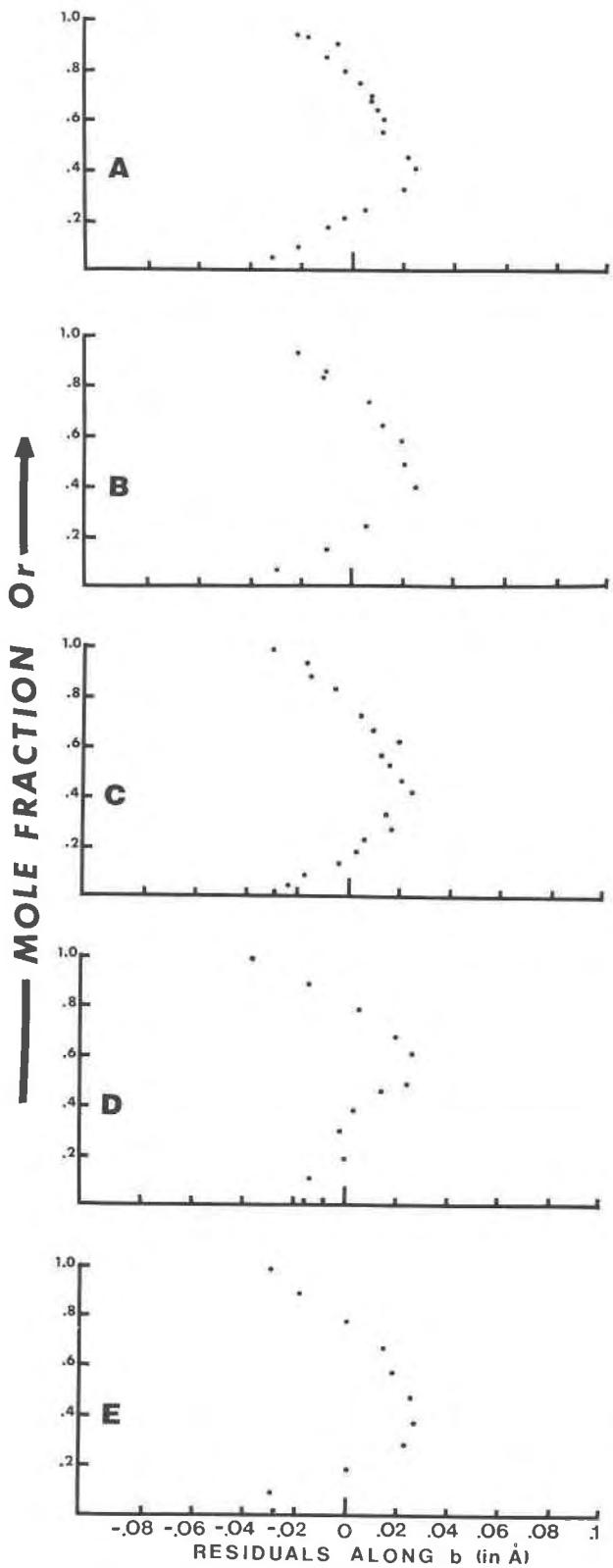
Introduction

Donnay and Donnay (1952) first studied the variation of cell dimensions with compositions for high-temperature alkali feldspars. Wright and Stewart (1968) demonstrated that the relationship between alkali feldspar compositions (mole fraction $KAlSi_3O_8$ or N_{OR}) and *b, c* cell dimensions can be expressed as a series of nearly parallel straight lines. Each line represents the response of an alkali feldspar of a constant degree of disorder to varying proportions of the two cations. These functions possess extremely high correlation coefficients (Table 1) indicating that most of the variation of the cell parameters are linearly related to composition. However, Wright and Stewart (1968) pointed out that there is a distinct change of slope at $N_{OR} = 0.4$ on a plot of any cell parameter against composition. This conclusion was based on simple inspection of the plots of cell parameters against composition of four series. In light of the availability of two additional series (Waldbaum, 1966; Luth and Querol-Suñé, 1970) and of the high correlation coefficients of all of the series, we decided to subject the data to analyses of residuals of least-squares regression lines in order to test for the presence of non-linear effects. If present, this analysis should amplify these effects and serve as an additional source of information concerning details of cell parameter response to changing composition in the alkali feldspars. If no significant residual variations are present, then the array of points about the computed regression line should be random. That is, there should be no systematic pattern of deviations from the line.

Data for five complete feldspar series were used in this analysis (Waldbaum, 1966; Orville, two series, 1967; Wright and Stewart, 1968; Luth and Querol-Suñé, 1970). The alkali-exchange method of producing various compositions was used for three series. One series of Orville (1967) and the Luth and Querol-Sune (1970) series were produced by hydrothermal crystallization from gels or glasses. These five series represent the full spectrum of structural states and compositions (Table 1).

Relations between Cell Dimension and Composition

Least-squares lines were determined for composition (N_{OR}) and the cell dimension *a, b,* and *c* for each series. In each instance, N_{OR} was considered to be the independent variable. Residuals, representing the deviation of each point from the line in the "*Y*" direction, were determined for each line. The residuals were then plotted with respect to N_{OR}. Such arrays for the *b* and *c* direction exhibit a simple and distinct pattern of deviation with respect to composition. The most strikingly non-random deviations from linearity are evident for relationships between N_{OR} and the *b* and *c* cell dimensions (Figs. 1 and



2). The patterns of such deviations are strongly monotonic above and below $N_{OR} = 0.4$. In each case the greatest positive deviation occurs in the composition range $N_{OR} = 0.4$ to 0.5, systematically decreases to zero at N_{OR} values of approximately 0.2 and 0.8, then becomes negative with the greatest negative deviations occurring at the extreme values ($N_{OR} = 0.0$ to 1.0). The pattern of deviation with respect to cell dimension a is more complex (Fig. 3) although similar and clearly non-random. A general characteristic of all such arrays is that the cell dimension increases more and more disproportionately as composition departs from the end-member values.

This regular pattern of deviations is present for all of the alkali feldspar series heretofore reported, regardless of structural state or method of synthesis. The patterns of deviations demonstrated below are so regular within and between lines that their non-random nature is clearly evident by visual inspection. These results so violate the fundamental concept of randomness (Draper and Smith, 1966) that further discussion is unnecessary.

Our results indicate that, in fact, the relationship between N_{OR} and cell dimensions is not linear. However, in light of the high linear correlation coefficients (Table 1) the non-linear component, whilst present, cannot be a strong contributor to the relationship. The important fact, then, is not that a relationship previously thought to be linear is non-linear, but that maxima and minima associated with such departures carry additional information concerning lattice parameter response to changing composition.

Whether the reversals in trend of the deviations are the result of a discontinuous function, or a manifestation of a continuous function of high order, cannot be determined from the data arrays available. Resolution of this can only come when a large number of determinations are made in close proximity to the points of reversal. At this time all that can be said is that the composition in the vicinity of $N_{OR} = 0.4$ is near the critical reversal point for the patterns of deviation of all reported alkali feldspar series.

FIG. 1. Residuals in the b direction of the linear relation between b and N_{OR} plotted against N_{OR}. A. Sanidine-high albite (Luth and Querol-Suñé, 1970); B. Orthoclase series (Wright and Stewart, 1968); C. Orville-1: Sanidine-high albite (Orville, 1967); D. Microcline-low albite (Waldbaum, 1966; Waldbaum and Robie, 1971); E. Orville-2: Microcline-low albite (Orville, 1967).

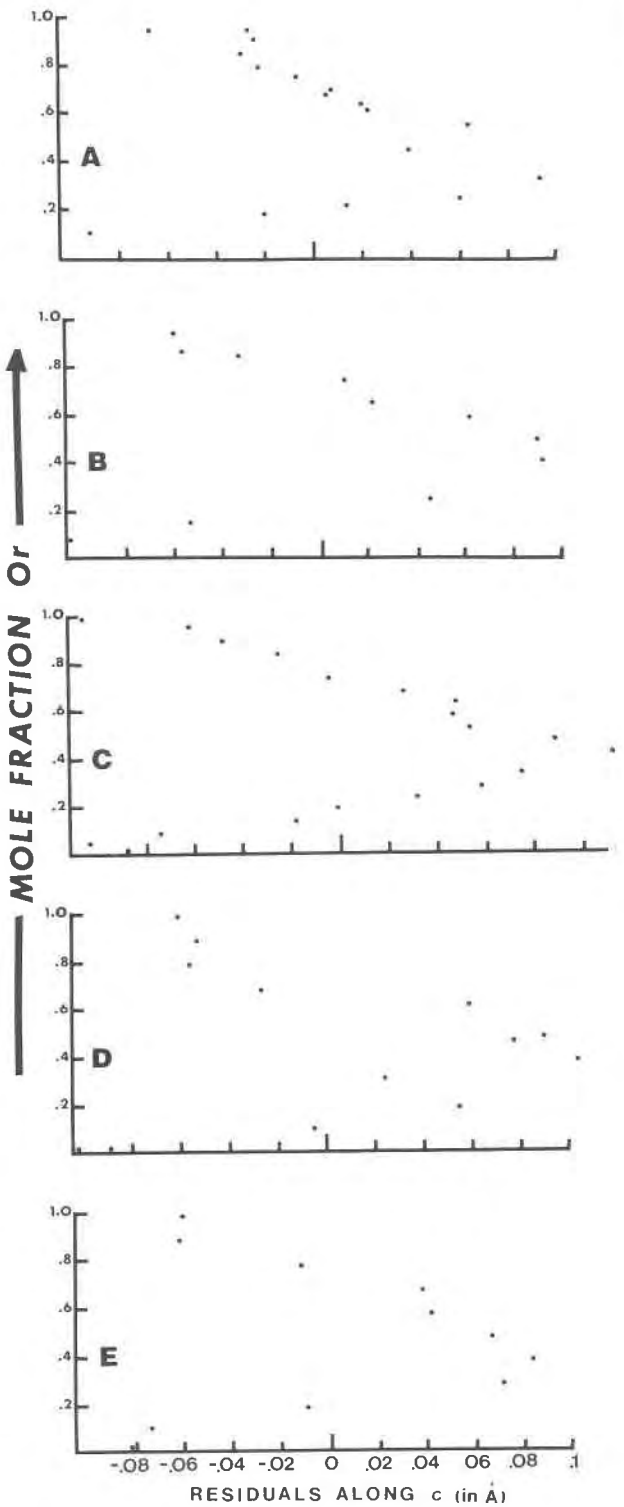


FIG. 2. Residuals in the c direction of the linear relation between c and N_{OR} plotted against N_{OR}. See Figure 1 for sources of data.

TABLE 1. Correlation Coefficients of the Five Series

	a	b	c	n
Sanidine-High Albite (Luth and Querol-Sune, 1970)				
N_{OR}	.999	.930	.931	19
a	--	.937	.937	
b	--	--	.989	
Orthoclase Series (Wright and Stewart, 1968)				
N_{OR}	.999	.920	.936	11
a	--	.924	.937	
b	--	--	.995	
Sanidine-High Albite (Series 1, Orville, 1967)				
N_{OR}	.999	.944	.948	19
a	--	.946	.947	
b	--	--	.998	
Microcline-Low Albite (Waldbaum, 1966)				
N_{OR}	.999	.968	.948	13
a	--	.975	.957	
b	--	--	.968	
Microcline-Low Albite (Series 2, Orville, 1967)				
N_{OR}	.998	.935	.961	11
a	--	.955	.976	
b	--	--	.955	

Conclusion

In all alkali series from monoclinic potassic feldspar toward the sodic end members, the symmetry becomes triclinic. The transition occurs near N_{OR} of 0.4 (Wright and Stewart, 1968; Orville, 1967; Luth and Querol-Suñé, 1970), which is approximately the location of the reversals in the patterns of the residuals. However, the same reversals also occur in the same position in the more ordered alkali series, which does not contain the monoclinic—triclinic transition. The pattern of residuals of the triclinic series imitates, in all respects, the pattern of the monoclinic-triclinic series. Evidently the same structural factors which cause the symmetry change in the disordered series are also present in the ordered series. From inspection of the residuals, this structural arrangement is such that the composition $N_{OR} = 0.4$ produces the largest cell parameters (*i.e.*, a, b, and c residuals are most positive) for its composition, provided increase in cell parameters resultant from general increase in N_{OR} are accounted for. Similarly, the composition $N_{OR} = 0.0$ and 1.0 represent the smallest cell parameters, or the volumetrically most efficient structures, for their composition (*i.e.*, the residuals are most

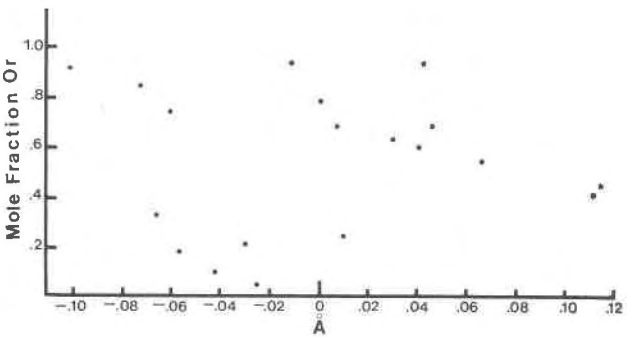


FIG. 3. Typical pattern of residuals in the a direction of the linear relation between a and N_{OR} plotted against N_{OR}. Data from Luth and Querol-Suñé, 1970.

negative at these compositions). In the more disordered feldspar series, near $N_{OR} = 0.4$, the excessively expanded cell is unstable and the monoclinic–triclinic transition occurs.

Thus, regardless of the structural state of the alkali feldspars, they consist of at least two separate and distinct families. Although the linear correlations of any alkali feldspar series is high ($r > 0.90$), these families within each series can be easily distinguished based on analyses of the residual of the regression analysis. These analyses strongly support Wright and Stewart's (1968) conclusion that the structural arrangement that leads to the monoclinic—triclinic transition in more disordered alkali feldspar series is dependent only on composition and independent of Al:Si ordering.

Acknowledgment

This work has been supported by the National Science Foundation (GA 1684).

References

DONNAY, GABRIELLE, AND J. D. H. DONNAY (1952) The symmetry change in the high-temperature alkali feldspar series. *Amer. J. Sci., Bowen Volume,* 115–132.

DRAPER, N. R., AND H. SMITH (1966) *Applied Regression Analysis.* John Wiley and Sons, New York.

LUTH, W. C., AND F. QUEROL-SUÑÉ (1970) An alkali feldspar series. *Contrib. Mineral. Petrology,* **25,** 25–40.

ORVILLE, P. M. (1967) Unit cell parameters of the microcline-low albite and the sanidine-high albite solid solution series. *Amer. Mineral.* **52,** 55–86.

WALDBAUM, D. R. (1966) *Calorimetric investigation of the alkali feldspars.* Ph.D. dissertation, Harvard University.

———, AND R. A. ROBIE (1971) Calorimetric investigation of Na-K mixing and polymorphism in the alkali feldspars. *Z. Kristallogr.* **134,** 381–420.

WRIGHT, T. L., AND D. B. STEWART (1968) X-ray and optical study of alkali feldspar: I. Determination of composition and structural state from refined unit-cell parameters and 2V. *Amer. Mineral* **53,** 38–87.

Manuscript received, December 11, 1972; accepted for publication, March 27, 1973.