The coordination numbers of Na and K atoms in low albite and microcline as determined from a procrystal electron-density distribution

ROBERT T. DOWNS, AARON ANDALMAN,* AND MARC HUDACSKO*

Geophysical Laboratory, Carnegie Institution of Washington, 5251 Broad Branch Road NW, Washington, DC 20015, U.S.A.

ABSTRACT

Procrystal models for the electron-density distributions of low albite and microcline were constructed by placing spherically averaged Clementi-Roetti atomic wave functions at experimentally observed atomic positions. The topography of the model electron-density distribution was analyzed to locate $(3,-1)$ critical points between the Na or K positions and the positions of the surrounding framework O atoms. Because the number of $(3,-1)$ critical points associated with a given atom corresponds with its coordination number, the analysis indicated that Na is fivefold and K is sevenfold coordinated. In particular, the results indicate that the Oco atom in low albite is not coordinated with Na, whereas in microcline it is coordinated with K. This suggests that in low albite the Oco atom is underbonded and thus a possible hydrophilic site, whereas in microcline the bonding requirements of Oco are satisfied. Details of the local bonding explain the effects of pressure, H, and H_2O on ordering of Al and Si, as well as compressibility systematics.

INTRODUCTION

The feldspar minerals consist of end-member phases $NaAlSi_3O_8$ (albite), $KAlSi_3O_8$ (microcline, orthoclase, and sanidine), and $CaAl_2Si_2O_8$ (anorthite). These minerals, combined with quartz, comprise ~85% of the volume of the Earth's crust. They represent the prototype aluminosilicate framework structures for which it is well established that the Al and Si atoms are each coordinated to four O atoms and each O atom is coordinated to two of these tetrahedrally coordinated cations. Considerable work has been done to study the nature of the tetrahedral bond, especially that of the Si-O bond in the SiO_2 polymorphs (see, for instance, Gibbs et al. 1994).

The stability of these feldspar phases is constrained by pressures that exceed 4.0 GPa and temperatures >1000 °C, limiting their stability field in the Earth to no more than about 30 km depth. In all cases these feldspars undergo complex multiphase transitions to new structures where the Al is sixfold coordinated. The dynamics of these transformations are poorly understood, and currently there is much research on these changes. At surface conditions the feldspar structures react with aqueous solutions to break down into the important mineral phases that mostly constitute soils (Blum 1994). They are the primary source of the essential inorganic elements, such as Na, K, Ca, etc., that are necessary for sustaining life on our planet.

In spite of the importance of feldspars, relatively little is understood about the bonding of the alkali cations. In fact, unlike for the tetrahedral cations, not even the coordination numbers of the alkali cations have been established conclusively. This uncertainty is primarily a result of the wide range of possible bonding distances that are exhibited, and it also results because the geometries of these sites do not match those of the traditional coordination polyhedra typified by octahedra, tetrahedra, and so on (Smith and Brown 1988). The reported coordinations of Na and K in feldspars usually vary between fivefold and ninefold.

One attempt to solve this problem for low albite was undertaken by Gait et al. (1970), who assumed that it is an ionic crystal subject to Pauling's rules. Taking into account possible shielding effects, they varied the Al-Si content of each nonequivalent tetrahedral site and the coordination of Na from fourfold to 17-fold to minimize the "electrostatic charge imbalance," and they concluded that low albite should be largely ordered with 82% Al in one site and with an Na atom that is sixfold coordinated. This coordination included five O atoms that are within 2.7 Å of the Na atom plus the Oco atom, which is about 3 Å from Na. The Oco atom is also coordinated to one Si and one Al atom, so the hypothesized bond to Na was necessary for charge balance. Another O atom, Odm, is also about 3 Å from Na, but because it is coordinated to two Si atoms, it was determined not to be coordinated to Na.

Recently, Downs et al. (1994) determined the crystal structure of albite as a function of pressure up to 5 GPa. They reported that pressure induces a volume decrease in low albite that topologically requires a bending of the Al-Oco-Si bridging angle. Furthermore, because the lengths of only the five shortest Na-O bonds change with increasing pressure, it was suggested that the Na atom

---

might be bonded to only these five O atoms and that, in particular, Oco was not one of them. This would leave the Oco atom bonded to only one Si and one Al atom, meaning that at higher pressures not only would the Si-Oco-Al angle be under stress, but its component Oco atom would be underbonded and, possibly, a hydrophilic site.

In this study we make use of Bader's postulate that a bond exists between a pair of atoms if and only if a certain topological feature, a $(3,-1)$ critical point, exists in the electron density between the atoms. We computed model electron-density maps for low albite and microcline and located the $(3,-1)$ critical points between the Na and the K atoms and their respective neighboring O atoms. The number of critical points can be used to determine the coordination number of an atom. Bonding features were then compared and related to crystal-chemical behavior.

BONDING CRITERIA

A bond can be considered to exist between a pair of atoms if they, in some sense, intimately share common electrons. In such a case these electrons continually pass from one atom to the other. There must then exist a saddle point in the space between the bonded atoms in which the electron density is accumulated such that a maximum exists in the plane perpendicular to the bond path and, because of the high density localized in the immediate neighborhood of the nuclei, a minimum along the bond path (Cremer 1987). This accumulation of electron density between pairs of atoms acts as an electrostatic glue that holds the nuclei together (Feynman 1939). For this reason, Bader and coworkers provided a topologically based postulate that two atoms are bonded if and only if a $(3,-1)$ critical point can be located in the electron density along the bond path between the pair of atoms. A $(3,-1)$ critical point is a point in the three-dimensional space of electron density at which the gradient is zero and the curvature is positive along the bond path but negative in the perpendicular directions. See Bader (1990) and Bader and Laidig (1990) for a review and references therein for additional details.

It follows that if we had access to a reasonable electron-density function for albite and microcline, then we could locate the $(3,-1)$ critical points around the Na and K atoms and determine to which O atoms they are coordinated. However, the electron densities of albite and microcline have not yet been determined experimentally, and, currently, it is not computationally feasible to calculate reliable maps with a first-principles calculation. Therefore, we decided to model the electron density as the superposition of spherically averaged (Gibbs et al. 1992) Roothan-Hartree-Fock wave functions (Clementi and Roetti 1974), expressed as linear combinations of Slater-type functions, centered at experimentally determined atomic positions, the so-called procrystal model (Hirshfeld and Rzotkiewicz 1974). This is the reference electron density used to model an isolated atom prior to

crystal formation, and it is equivalent to the independent atom model in electron scattering and the spherical atom approximation in X-ray crystallography (Spackman and Maslen 1986). It is the model assumed in most crystal-structure refinements.

In spite of its simplicity, the procrystal, and the related promolecule (the model as applied to molecules), electron density has proven capable of accurately modeling many bonding and electrostatic properties of crystals and molecules. Gibbs et al. (1992) and Feth et al. (1993) compared the locations of $(3,-1)$ critical points calculated from the procrystal model, constructed with spherically averaged Clementi-Roetti wave functions, with the locations observed in experimentally determined total electron-density maps for NaCl, RbCl, LiF, KCl, KBr, MgO, NiO, CuCl, CuBr, BeO, CaF_2, SiO_2 (coesite and stishovite), and $CaB_2Si_2O_8$ (danburite). For each crystal studied, the $(3,-1)$ critical points in both the observed and the theoretical maps were located at equivalent positions, within 0.03 Å of the other. Similar results were also obtained when comparing the locations of $(3,-1)$ critical points from promolecule electron densities with those from densities derived from ab initio calculations of various oxide, sulfide, nitride, fluoride, and many diatomic molecules (Spackman and Maslen 1986; Gibbs et al. 1992; Nicoll et al. 1994). Furthermore, Spackman and Maslen (1986) demonstrated that calculations using the promolecule electron density provide reasonable estimates of electrostatic energies and atomic radii and charges.

However, consider the case in which no bond should reasonably exist, such as that of two atoms with a large separation. If one places a pair of spherically averaged atomic wave functions at these positions, then a $(3,-1)$ critical point in the model electron density still mathematically exists between the pair. Thus, it appears that the number of $(3,-1)$ critical points calculated from the procrystal density is capable of providing an upper bound on the coordination number of a given atom.

METHOD

The positions of the atoms used in our calculations were obtained from published reports of the structure refinements of experimentally determined X-ray diffraction data for low albite (Downs et al. 1994) and maximum microcline (Blasi et al. 1987). Bond-length systematics and rigid-body analysis of the displacement parameters (Armbruster et al. 1990; Downs et al. 1990) indicate that these particular feldspar structures represent phases with completely or almost completely ordered Al-Si distributions. The procrystal electron density was computed as the superposition of spherically averaged Roothan-Hartree-Fock wave functions (Clementi and Roetti 1974), as outlined by Gibbs et al. (1992).

The location of a $(3,-1)$ critical point associated with a pair of atoms was found by first locating the point of minimum electron density along the interatomic vector. Next, the maximum was located in the orthogonal plane.

TABLE 1. Electron-density parameters at (3,−1) critical points associated with M-O bonds for low albite (M = Na) and microcline (M = K)

Bonded atom	R(M-O) (Å)	ρ (e/Å³)	∇² (e/Å⁵)	Eigenvalues (e/Å⁵)	(e/Å⁵)	(e/Å⁵)
Albite						
Oa1	2.665	0.0714	1.0652	1.318	−0.168	−0.084
Oa1	2.538	0.0886	1.5738	2.021	−0.256	−0.192
Oa2	2.368	0.1154	2.5365	3.402	−0.451	−0.414
Obo	2.459	0.0984	1.9383	2.546	−0.333	−0.274
Odo	2.438	0.1016	2.0548	2.717	−0.356	−0.307
Microcline						
Oa1	2.876	0.0839	1.2743	1.661	−0.220	−0.167
Oa1	2.882	0.0834	1.2592	1.635	−0.216	−0.161
Oa2	2.751	0.1034	1.7245	2.304	−0.318	−0.261
Obo	2.960	0.0707	1.0318	1.323	−0.173	−0.118
Oco	2.911	0.0763	1.1548	1.465	−0.199	−0.112
Odo	2.899	0.0766	1.1770	1.537	−0.204	−0.156
Odm	2.987	0.0660	0.9617	1.208	−0.158	−0.088

Note: The parameters are R(M-O), the bond length; ρ, the electron density; ∇², the Laplacian; and the three eigenvalues.

A minimum was then located along the line parallel to the interatomic vector and passing through the maximum in the plane. These steps were repeated in an iterative fashion until the maximum in the plane and the minimum along the line converged to a value less than a tolerance of 10^{-7} bohr. Electron densities were computed at 27 points along the edges, corners, and faces of a cube (10^{-18} bohr³) centered at the convergent point, r_c, and were fitted to the expression

$$\rho(r) = \rho_0 + (\nabla\rho)^t(r - r_c) + \tfrac{1}{2}(r - r_c)^t \mathbf{H}(r - r_c)$$

where $\nabla\rho$ is the gradient vector, $\mathbf{H}$ is the Hessian matrix of second derivatives, and the superscript t indicates a transposed vector. The magnitude of the gradient and the eigenvalues of the Hessian matrix were then calculated. If the gradient was zero and two of the eigenvalues were negative and one was positive, then we located a $(3,-1)$ critical point. If, during the search, we wandered outside the sphere centered at the midpoint of the interatomic vector and with a diameter equal to the interatomic separation, then the search was halted and it was assumed that no $(3,-1)$ critical point associated with the pair of atoms exists.

RESULTS

Low albite

Five $(3,-1)$ critical points were located in the electron-density distribution around the Na atom in low albite. A summary of the associated parameters is presented in Table 1. These points are associated with the five closest O atoms, with $R(\text{Na-O})$ ranging from 2.37 to 2.66 Å. Three of these O atoms, Oa1, Obo, and Odo, are also bonded with Al and Si atoms, with two Oa1 atoms coordinated with Na. The other remaining bonded O atom, Oa2, is also coordinated with two Si atoms. The Si-O bond lengths to Oa2 are the longest in the structure, 0.03 Å longer than the average of the others. This is probably a
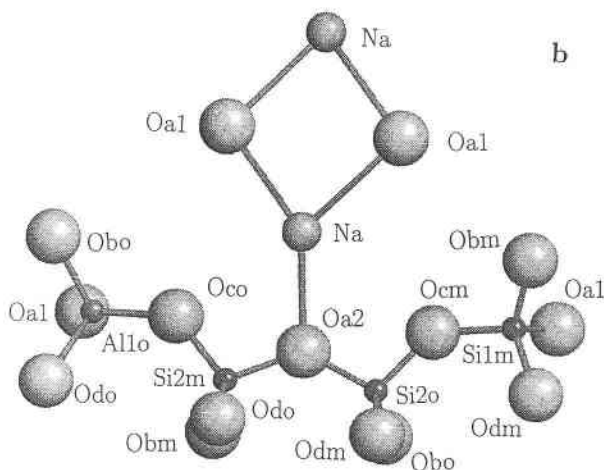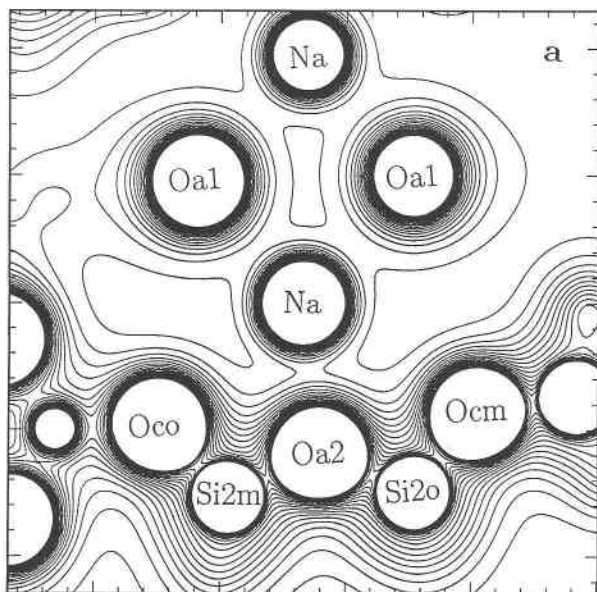
FIGURE 1. (a) Electron-density contour plot of low albite through the plane Oco-Na-Oa1. The view is approximately parallel with the [001] direction, and the pseudomirror plane (010) is vertical through Na-Oa2. Contour intervals are 0.0075 e/Å³, ranging from 0 to 0.15 e/Å³. The external scale is in steps of 0.2 Å. A (3,−1) critical point can be observed, for instance, between Na and Oa1 but not between Na and Oco. (b) Ball-and-stick representation of the portion of the albite structure relevant to **a**.

consequence of the bonding of Oa2 to Na, which leaves fewer electrons available for the Si-O bonds, making them weaker and therefore longer. The Oco atom, also coordinated with Al, is indicated not to be bonded with Na. This suggests that Oco is underbonded, which is probably the reason that it is involved in the shortest Al-O bond length, 0.01 Å shorter than the average of the others. A plot of the electron density in the plane Oa1-Na-Oco, approximately looking down [001], is given in Figure 1a. Other atoms appear in this figure; they are close
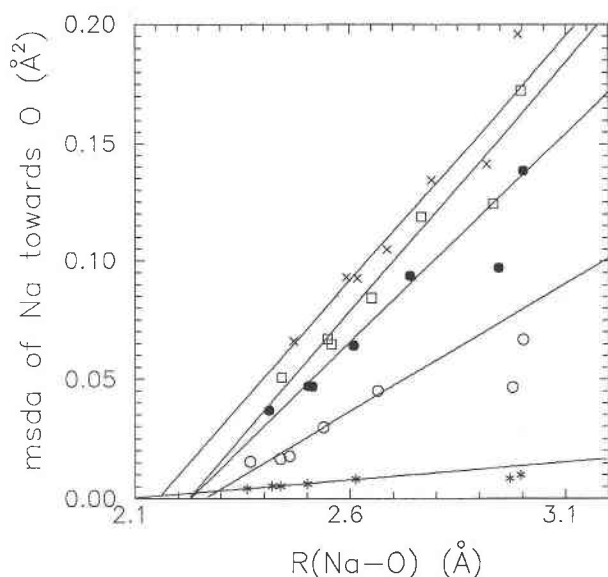
FIGURE 2. Plot of the mean-square displacement amplitudes of Na toward O vs. the corresponding Na-O bond length for the seven O atoms that are closest to Na at temperatures of 13 (asterisks), 295 (open circles), 770 (solid circles), 1020 (open squares), and 1240 K (Xs). The best-fit lines from the five nearest O atoms are superimposed to indicate the trends. The linear relations demonstrate that the five bonded O atoms lie on an ellipsoidal surface that is parallel to the vibrational ellipsoids of Na. The different slopes are a consequence of the differences in the sizes of the vibrational ellipsoids at different temperatures.
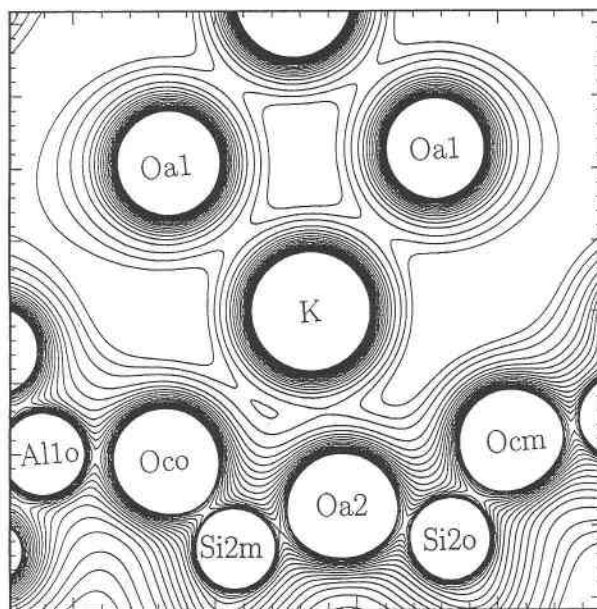

FIGURE 3. Electron-density contour plot of microcline through the plane Oco-K-Oa1, viewed with an orientation similar to that in Figure 1. Contour intervals are 0.0075 e/Å³, ranging from 0 to 0.15 e/Å³. The external scale is in steps of 0.2 Å. In contrast to low albite, $(3,-1)$ critical points can be observed not only between K and Oa1 but also between K and Oco.

to the plane, but they do not necessarily lie in it. The $(3,-1)$ critical points can be observed between the Na atom and Oa1 and Oa2, but not between Na and Oco. Figure 1b is a ball-and-stick representation of the atoms in the near neighborhood of the plane represented in Figure 1a. It is provided as an aid in the interpretation of the electron-density maps.

The positions of the five bonded O atoms appear to determine the shape and orientation of the thermal vibration ellipsoid of the Na atom. The five bonded O atoms are arranged around the Na atom on an ellipsoidal surface that is parallel to the surface of the anisotropic vibrational ellipsoid of Na at all the temperatures for which the structure has been determined (13–1240 K). This is demonstrated in Figure 2, where the mean-square displacement amplitudes of the Na atom calculated in the Na-O directions are plotted against the corresponding Na-O bond lengths at temperatures of 13, 295, 770, 1020, and 1240 K (Smith et al. 1986; Downs et al. 1994; Winter et al. 1977). The displacement amplitudes follow linear trends with R(Na-O) for the five closest atoms, but the trends do not hold for the O atoms that are further away.

Microcline

A total of seven $(3,-1)$ critical points were located in the electron density around the K atom in microcline (Table 1). These points are associated with the seven closest

O atoms with R(K-O) ranging from 2.75 to 2.99 Å. The next-nearest O atom is 3.13 Å away from the K atom. All the O atoms that are bonded to an Al and an Si atom are also coordinated with K, along with two other atoms, Oa2 and Odm, that are also bonded to two Si atoms. Only the two O atoms Obm and Ocm are not indicated to be coordinated with the K atom. They display the shortest average Si-O bond lengths. A plot of the electron density in the Oa1-K-Oco plane is provided in Figure 3.

As demonstrated for low albite, the vibrational ellipsoid of K is also related to the K-O bond lengths. However, the anisotropy is much less pronounced than for Na, with the ratio of the shortest axial length over the longest, λ_s/λ_l, of 0.75 for K in comparison with 0.44 for Na. The anisotropy follows the distribution of bond lengths.

DISCUSSION

Effects of pressure on Al-Si ordering

In the first attempts to synthesize low albite hydrothermally from a glass, Tuttle and Bowen (1950) failed and instead synthesized high albite. This is the albite phase with a completely random distribution of Al and Si at the tetrahedral sites. All other attempts to synthesize low albite also failed, until Martin (1969) succeeded in experiments completed at 1.0 GPa and 350 °C. On the basis of the results of his experiments he concluded that synthesis requires a high-pressure environment with temperatures in the range of 300–400 °C. Lower temperatures did not provide sufficient energy to allow the atoms to

move, whereas higher temperatures, especially above 600 °C, provided so much energy that disordered states always resulted.

Microcline, on the other hand, has never been hydrothermally synthesized (Goldsmith 1986). All the attempts have resulted in disordered phases, except when authigenic conditions were simulated in sediments at very low temperatures by means of slow precipitation from hydroxide gels (Flehmig 1977). Because the aluminosilicate frameworks of both albite and microcline are essentially identical, the Al-Si ordering differences may be ascribed to the bonding characteristics of the alkali sites.

In their study of the response of the low albite structure to the effects of pressure, Downs et al. (1994) observed that the major compression mechanism was the bending of the Al-Oco-Si angle. The microcline structure has not yet been determined as a function of pressure, but similar topologies and strain ellipsoids (Hackwell 1995) strongly suggest that the compression mechanism should also be similar.

The bending-force constant of Al-O-Si angles is one-half that of Si-O-Si angles (Nicholas et al. 1992). Therefore, with the application of pressure, an Al-O-Si angle should bend more easily than an Si-O-Si angle. It follows that an alkali feldspar crystal with an Al-Oco-Si angle would show greater compression than one with an Si-Oco-Si angle, and, with sufficient energy to allow cation diffusion, Al-Si ordering would be induced, satisfying the $P\Delta V$ energy requirements. If, however, in an Al-O-Si linkage the bridging O atom is also coordinated to a third cation, then the angle is constrained and the bending-force constant is significantly increased (Geisinger et al. 1985).

Consequently, if Oco is coordinated with Al and Si but not with Na, then the bending-force constant of the Al-Oco-Si angle in low albite should be small. It follows, then, that a larger pressure-induced volume change is obtained through Al-Si ordering than would be obtained if the albite structure were disordered. Although most naturally occurring albite is found in a largely ordered state, it appears that the disordered high albite, common in rhyolitic rocks and as phenocrysts in extrusive rocks but not found in plutonic rocks (Tuttle and Bowen 1950), results not only because of fast cooling or annealing rates but because of the lack of significant pressure.

In contrast to albite, Oco is bonded to K in microcline. If, as Geisinger et al. (1985) suggested, a third cation is coordinated with the bridging O atom, then the Al-Oco-Si angle is stiffer and there is no mechanism for pressure-induced ordering. Most naturally formed potassium feldspar is found as disordered or partially disordered sanidine or orthoclase.

Effects of H and H₂O on Al-Si ordering

In low albite, if the Oco atom is not coordinated with Na, then it must be underbonded and therefore, potentially, a hydrophilic site. If any H is in the low-albite structure, it would probably be concentrated around the

Oco site. Goldsmith (1986) demonstrated that, in contrast to the pressure-induced ordering behavior of pure dry albite, Al-Si interdiffusion at pressures between 0.5 and 2.4 GPa is enhanced dramatically if H or H_2O is present. Again, a small amount of heat is necessary to drive the kinetics. The Al-Si disordering in the presence of H can be understood in terms of an underbonded Oco atom. With H attracted to the Oco atom, and with the Oco angle strained at high pressures, the Al-Oco bond is weakened, the Si-O-Al linkage can be easily broken, and diffusion can then proceed.

Compressibility systematics

The molar volume of microcline (109 cm³/mol) is larger than the molar volume of low albite (100 cm³/mol). The K-O bonds are longer [$\langle R(K\text{-}O)\rangle$ = 2.90 Å] than the Na-O bonds [$\langle R(Na\text{-}O)\rangle$ = 2.49 Å] and consequently weaker (Hill et al. 1994). Therefore, it is surprising that the bulk modulus of microcline [63(2) GPa; Hackwell 1995] is larger than that of low albite [54(1) GPa; Downs et al. 1994]. This systematic also may be ascribed to the differences in the bonding of the alkali cations to Oco. The Al-Oco-Si angle in microcline, which must narrow topologically to allow volume decrease, is constrained by the K-O bond and is thus stiffer than the same angle in low albite, which is not constrained. It follows that the microcline structure is less compressible than the low-albite structure.

REFERENCES CITED

Armbruster, T., Bürgi, H.B., Kunz, M., Gnos, E., Brönnimann, S., and Lienert, C. (1990) Variation of displacement parameters in structure refinements of low albite. American Mineralogist, 75, 135–140.

Bader, R.F.W. (1990) Atoms in molecules: A quantum theory, 400 p. Oxford University Press, U.K.

Bader, R.F.W., and Laidig, K.E. (1990) Analysis and classification of the charge distribution using quantum mechanics. Transactions of the American Crystallographic Association, 26, 1–21.

Blasi, A., De Pol Blasi, C., and Zanazzi, P.F. (1987) A re-examination of the Pellotsalo microcline: Mineralogical implications and genetic considerations. Canadian Mineralogist, 25, 527–537.

Blum, A.E. (1994) Feldspars in weathering. In I. Parsons, Ed., Feldspars and their reactions, p. 595–630. Nato ASI Series C, Mathematical and Physical Sciences, Kluwer Academic, Dordrecht, the Netherlands.

Clementi, E., and Roetti, C. (1974) Roothan-Hartree-Fock atomic wavefunctions. Atomic Data and Nuclear Data Tables, 14, 177–478.

Cremer, D. (1987) New ways of analyzing chemical bonding. In Z.B. Marsić, Ed., Modelling of structure and properties of molecules, p. 128–144. Halstead, New York.

Downs, R.T., Gibbs, G.V., and Boisen, M.B., Jr. (1990) A study of the mean-square displacement amplitudes of Si, Al, and O atoms in frame-

work structures: Evidence for rigid bonds, order, twinning, and stacking faults. American Mineralogist, 75, 1253–1267.

Downs, R.T., Hazen, R.M., and Finger, L.W. (1994) The high-pressure crystal chemistry of low albite and the origin of the pressure dependency of Al-Si ordering. American Mineralogist, 79, 1042–1052.

Feth, S., Gibbs, G.V., Boisen, M.B., Jr., and Meyers, R.H. (1993) Promolecule radii for nitrides, oxides and sulfides: A comparison with effective ionic and crystal radii. Journal of Physical Chemistry, 97, 11445–11450.

Feynman, R.P. (1939) Forces in molecules. Physical Review, 56, 340–343.

Flehmig, W. (1977) The synthesis of feldspars at temperatures between 0°–80°C, their ordering behaviour and twinning. Contributions to Mineralogy and Petrology, 65, 1–9.

Gait, R.I., Ferguson, R.B., and Coish, H.R. (1970) Electrostatic charge distributions in the structure of low albite, $NaAlSi_3O_8$. Acta Crystallographica, B26, 68–77.

Geisinger, K.L., Gibbs, G.V., and Navrotsky, A. (1985) A molecular orbital study of bond length and angle variations in framework structures. Physics and Chemistry of Minerals, 11, 266–283.

Gibbs, G.V., Spackman, M.A., and Boisen, M.B., Jr. (1992) Bonded and promolecule radii for molecules and crystals. American Mineralogist, 77, 741–750.

Gibbs, G.V., Downs, J.W., and Boisen, M.B., Jr. (1994) The elusive SiO bond. In Mineralogical Society of America Reviews in Mineralogy, 29, 606 p.

Goldsmith, J.R. (1986) The role of hydrogen in promoting Al-Si interdiffusion in albite ($NaAlSi_3O_8$) at high pressures. Earth and Planetary Science Letters, 80, 135–138.

Hackwell, T.P. (1995) Feldspars at high pressures and temperatures. Ph.D. dissertation, University College London, U.K.

Hill, F.C., Gibbs, G.V., and Boisen, M.B., Jr. (1994) Bond stretching force constants and compressibilities of nitride, oxide, and sulfide coordination polyhedra in molecules and crystals. Structural Chemistry, 6, 349–355.

Hirshfeld, F.L., and Rzotkiewicz, S. (1974) Electrostatic binding in the first-row AH and A_2 diatomic molecules. Molecular Physics, 27, 1319–1343.

Martin, R.F. (1969) The hydrothermal synthesis of low albite. Contributions to Mineralogy and Petrology, 23, 323–339.

Nicholas, J.B., Winans, R.E., Harrison, R.J., Iton, L.E., Curtiss, L.A., and Hopfinger, A.J. (1992) Ab initio molecular orbital study of the effects of basis set size on the calculated structure and acidity of hydroxyl groups in framework molecular sieves. Journal of Physical Chemistry, 96, 10247–10257.

Nicoll, J.S., Gibbs, G.V., Boisen, M.B., Jr., Downs, R.T., and Bartelmehs, K.L. (1994) Bond length and radii variations in fluoride and oxide molecules and crystals. Physics and Chemistry of Minerals, 20, 617–624.

Smith, J.V., Artioli, G., and Kvick, Å. (1986) Low albite, $NaAlSi_3O_8$: Neutron diffraction study of crystal structure at 13 K. American Mineralogist, 71, 727–733.

Smith, J.V., and Brown, W.L. (1988) Feldspar minerals: I. Crystal structures, physical, chemical and microtextural properties, 828 p. Springer-Verlag, New York.

Spackman, M.A., and Maslen, E.N. (1986) Chemical properties from the promolecule. Journal of Physical Chemistry, 90, 2020–2027.

Tuttle, O.F., and Bowen, N.L. (1950) High-temperature albite and contiguous feldspars. Journal of Geology, 58, 572–583.

Winter, J.K., Ghose, S., and Okamura, F.P. (1977) A high-temperature study of the thermal expansion and the anisotropy of the sodium atom in low albite. American Mineralogist, 62, 921–931.