

Ordering behavior in albite using the modified sequential construction method: Reply

GHOLAMABBAS RAJABALI

Department of Chemistry, Isfahan University of Technology, Isfahan, Iran

The preceding discussion by C. R. Ross (1989) of my paper on a model for ordering behavior in albite (Rajabali, 1988) raises two main points. First, Ross has suggested that values obtained for the thermodynamic functions are incorrect in the case of the three-unit-cell model, and, second, he has questioned the claimed accuracy of the Monte Carlo calculations. The first point is accepted; there are some errors in my numerical calculations for the three-squares unit. I have some comments concerning the second point, however.

In the Monte Carlo approach, the number of sites must, of course, be large, and to achieve this, one may calculate a thermodynamic parameter for different lattice sizes and then extrapolate to $1/N = 0$, where N is the number of sites in the model. Alternatively, one may choose a model that is sufficiently large that the thermodynamic property does not change on further enlargement. The number of iterations must also be large enough for the parameter to become stable, i.e., a reasonable amount of computing time is necessary. In the case of Anderson and Mazo's (1979) model, one may conclude that the Monte Carlo

(MC) approach works well because, on the one hand, better agreement is observed between the modified sequential construction method (MSCM) and the MC results than between the sequential construction method (SCM) and the MC results. On the other hand, it is expected that the MSCM approach will give better results than the SCM approach because of the reduced dependence on the way in which atoms are distributed among equivalent sites (as discussed at greater length in Rajabali, 1988).

REFERENCES CITED

- Anderson, G.R., and Mazo, R.M. (1979) Electroneutrality effects on aluminium order in sodium feldspar: A two-dimensional model. *Journal of Chemical Physics*, 71, 1062-1065.
- Rajabali, G. (1988) Ordering behavior in albite using the modified sequential construction method. *American Mineralogist* 73, 91-96.
- Ross, C.R., II. (1989) Ordering behavior in albite using the modified sequential construction method: Discussion. *American Mineralogist*, 74, 482-483.

MANUSCRIPT RECEIVED JULY 29, 1988

MANUSCRIPT ACCEPTED OCTOBER 31, 1988