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REPLY

Ordering in spinels—A Monte Carlo study: Reply

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We thank the authors of the comment for their interest in our work and their valuable discussion.

Andreozzi et al. (2000) first comment that their measurements were taken at room temperature after quenching. We had missed this important point and so one of the sets of experimental data (shown by empty squares) in Figure 2a of our paper (Lavrentiev et al. 2003) should be disregarded. We stress that this affects *none* of the results presented in our paper.

Their remark that "the lattice parameter of $MgAl_2O_4$ decreases when intracrystalline disorder increases" has prompted us to carry out some additional calculations. We carried out two (*NPT*) Monte Carlo simulations at 1000 K. The methodology was as described in our paper, except that the initial configurations were chosen with the degree of disorder (Q) appropriate to that at 1700 K (Q = 7/16) and at very high temperature (Q = 1/16), and cation exchanges during the course of the simulation were not permitted. Together with the result for full equilibration allowing cation exchanges (from Lavrentiev et al. 2003) these values indicate that at a given temperature the lattice parameter decreases slightly with increasing cation disorder, in agreement with Andreozzi et al. (2000) The magnitude of this decrease is an order of magnitude less than that of the positive thermal expansion.

Andreozzi et al. (2000) state that a very accurate lattice thermal expansion coefficient could be calculated from their specific thermal expansion coefficients for T and M sites. Since these were determined using as input the data of Redfern et al. (1999), there is little point in carrying out such calculations. The simulations reported in our paper refer to "equilibrated" samples and the proper comparison is directly with the in situ measurements of Redfern et al. (1999).

Finally, our comment relating to "...difficulties in preparing stochiometric samples and in the experimental determination of the order parameter" was intended as a general remark, bearing in mind the large scattering of available inversion data even for temperatures above 1000 K, as emphasized by Andreozzi et al. (2000) (e.g., p. 1170, "Inversion data with respect to temperature available in the literature for $MgAl_2O_4$ spinel are often conflicting"). Redfern et al. (1999) discuss problems of non-stoichiometry. Andreozzi et al. (2000) conclude that the same experimental technique may give embarrassingly different results and given this unsatisfactory situation it is not unreasonable to refer to a number of possible explanations. A critical survey either of experimental techniques or of the available data was far from the scope of our original article and is also true of this reply.

REFERENCES CITED

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