Short Communications

Contributions intended for publication under this heading should be expressly so marked; they should not exceed about 1000 *words; they should be forwarded in the usual way to the appropriate Co-editor; they will be published as speedily as possible.*

Acta Cryst. (1976). A**32**, 510

The Debye–Waller factors of sodium fluoride.

By R. C. G. KILLEAN, *School of Physical Sciences, University of St. Andrews, North Haugh, St. Andrews, Scotland*

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Errors reported by Sharma [*Acta Cryst.* (1975). A**31**, 157] in a previous paper [Sharma, *Acta Cryst.* (1974), A**30**, 299–300] are noted and commented on. It is pointed out that Sharma has given insufficient detail in his paper for an independent check to be made of his new values for the Debye–Waller factors and that these values do not support his earlier discussion.

Two recent papers by Sharma (1974*a*, *b*, denoted S1 and S2 respectively) in conjunction with an erratum (Sharma, 1975) are deserving of comment. As pointed out by Post (1975), it is essential that sufficient detail on calculation techniques be given in a paper in order that a reader can assess the validity of calculated results. This is even more the case when an author has been required to publish an erratum. In this case, where the erratum changes the main numerical results of S2, it is essential that independent checks on the calculations can be made so that these results can be evaluated.

Examination of S1 and S2 shows that the two papers present identical results for the Debye–Waller factors for the sodium and fluorine ions and that they list identical structure factor tables. This in itself would not be remarkable but for Sharma's statement that while no correction for TDS was made in S1, TDS corrections were made in S2. Presumably the purpose of the erratum is to give the correct Debye–Waller factors obtained from the TDS-corrected structure-factor data, data which do not appear in either S1 or S2. Sharma concluded in S2 that his Debye–Waller factors are significantly different from those of Meisalo & Merisalo (1966) but, using the latest values in Sharma's erratum, this is no longer the case. Indeed, for the fluorine ion the hypothesis fails at even the 'possibly significant' level (Cruickshank, 1965). It must be concluded that Sharma's erratum is not just correcting typographical errors.

It would be desirable under these circumstances to make an independent check of the new calculation of the Debye–Waller factors but the data required to do this are not available. Clearly, because of the errors in S2 already admitted and the discrepancy noted above, the results reported by Sharma should be analysed with caution.

In conclusion, it is perhaps curious that no reference in S2 is made to S1 with which, ignoring the TDS issue, it is in substance identical.

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Acta Cryst. (1976). A**32**, 510

Reply to Killean's comment *The Debye–Waller factors of sodium fluoride.*

By V. C. SHARMA, *Department of Physics, University of Benin, Benin City, Nigeria*

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Comments made by Killean [*Acta Cryst.* (1976). A**32**, 510] on papers by Sharma [*Acta Cryst.* (1974), A**30**, 299–300; *Acta Cryst.* (1975), A**31**, 157] are discussed.

Killean's (1976) comments on papers by Sharma (1974*a*, *b*, 1975, hereafter referred to as S1, S2 and S3 respectively) are discussed.

1. Killean (1976) points out that sufficient details on the calculation techniques were not given. A closer study of S2 should reveal that reasonable details along with the necessary references were given in that paper. The TDS corrections were made by the usual analytical method developed by Cooper & Rouse (1968) which requires no such *geometrical* parameters as understood by Killean (1975). Furthermore, he has no evidence to suggest that TDS corrections in sodium fluoride using the analytical method will differ significantly from the ones using the numerical method of Cooper & Rouse (1968). In fact, this point is irrelevant, as