We measured the Mo $K\alpha_1$ spectral line by TCD in the position (1,1,1) and (1,1,3) and by DCS in position (1,1). The DCS width is larger than the widths taken with TCD. This is in agreement with smaller widths of the smearing functions shown in Table 1.

Table 1 *Widths* (w_R) *of the smearing functions*

Experimental arrangement with germanium crystals cut parallel to the (111) planes; Mo $K\alpha_1$ radiation.

Position	w_R
(1, −1)	0·17 mÅ
(1,1,1)	0·15
(1,1,3)	0·05

Conclusions

The paper of Das Gupta & Welch seemed to support their statement that the fundamental widths of the X-ray emission lines taken with DCS are in error. In view of our own analysis and experiments this statement is not convincing.

Note:– The role of the vertical divergence, the use of x_3 instead of the (unsuitable) position of the maximum B, and perhaps other questions should be treated in detail, but were omitted here because of their complexity.

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Role of the dispersion correction in analysis of X-ray diffraction data.

By M. LINKOAHO, *Laboratory of Physics,* *Helsinki University of Technology, Otaniemi, Finland,* and M. MERISALO, *Department of Physics, University of Helsinki Helsinki 17, Finland*

The role of the dispersion correction in the analysis of X-ray diffraction data of lithium fluoride has been considered by applying the recent theoretical and experimental values of the dispersion corrections.

In applying modern methods in the analysis of X-ray diffraction data the dispersion corrections are introduced as parameters. Their contributions are commonly taken into account by assuming the theoretical values. Of these, the most often used and probably the most reliable are those of Cromer (1965) and Cromer & Liberman (1968). Recently, Bonse & Hellkötter (1969) have determined the real part of the dispersion corrections from measurements of the refractive index for Cu $K\alpha$ radiation. Their result for fluorine in lithium fluoride, $\Delta f' = 0\cdot18 \pm 0\cdot02$, is in indisputable disagreement with the theoretical value $\Delta f' = 0\cdot081$ (Cromer & Liberman, 1968).† In this note we consider the effects of this difference on conclusions arrived at in the analysis of the recent X-ray diffraction study for lithium fluoride (Merisalo & Inkinen, 1966).

First, the Debye–Waller coefficients B [in exp $\{-B(\sin\theta/\lambda)^2\}$] have been determined by employing the difference Fourier method (see *e.g.* Kurki–Suonio & Fontell, 1964; Järvinen & Inkinen, 1967). The resulting values are listed in Table 1 along with the values calculated by Merisalo (1968) from the eigenfrequency– eigenvector data reported by Karo & Hardy (1963). It is obvious from Table 1 that the adoption of the experimentally determined result for the dispersion correction of fluorine gives particularly close agreement of the experimental and theoretical B and B_+/B_- values. Further, the experimental Debye–Waller coefficients and their ratio are found to be strongly dependent on the values of the dispersion correction applied. Thus any comparison between a theoretical vibration model and experimental results is of little value unless the dispersion corrections are known reliable enough. It should be realized that the ratio of the Debye–Waller coefficients is probably the best test of the various theoretical vibration models (Karo & Hardy, 1969).

Table 1. *The experimental and theoretical Debye–Waller coefficients of lithium fluoride at* 300 °K *in* (Å)² *for the cation* (B_+) *and anion* (B_-) *together with their ratio* (B_+/B_-)

	C & L	B & H	K & H
B_+	1·04	1·02	1·01
B_-	0·67	0·82	0·83
B_+/B_-	1·55	1·24	1·22

L: with the dispersion corrections calculated by Cromer & Liberman (1968).

H: with the dispersion corrections measured by Bonse & Hellkötter (1969).

H: calculated from the normal mode data of Karo & Hardy (1963).

Secondly, the electron distributions of the atoms in lithium fluoride were studied in terms of cubic harmonics, (Kurki-Suonio & Meisalo, 1967; Kurki-Suonio, 1967, 1968). Again, the analysis was carried out by applying both the theoretical and experimental values for the dispersion correction of fluorine. As an example, the differences between experimental and theoretical radial scattering amplitudes of fluorine, Δf_0 (the spherical component) and Δf_4 (the first non-spherical component), are illustrated in Fig. 1. It is found that the Δf_0 component is sensitive to the choice of the dispersion correction while the non-spherical component Δf_4 is, to first order, independent of the

† *Note added in proof:* Creagh & Hart (1970) give an experimental value $\Delta f' = 0\cdot099 \pm 0\cdot009$

dispersion correction applied. This is to be expected as the dispersion corrections have spherically symmetric contributions in the analysis. However, significant deviations from spherical symmetry in the electron distribution of the fluorine ion may introduce some directional dependence of the dispersion correction. Hence, on the basis of the above analysis it remains uncertain to what extent the observed asphericity originates in the asphericity of the dispersion correction.

Disregarding any possible asphericity, a few additional remarks on the theoretical dispersion corrections should be made. The theoretical calculations require knowledge of the oscillator strengths and the manner in which the photoelectric absorption coefficient varies with the wavelength. The main limitation of the accuracy of these calculations is the uncertainty in the wavelength dependence of the absorption coefficients. Further, the values of Cromer (1965) and Cromer & Liberman (1968) are based on the oscillator strengths calculated from free atom wave functions. However, changes induced in the free atom wave functions when the atom is placed in a solid may manifest themselves in significant changes in the oscillator densities and thus in the dispersion corrections. In particular, this is the case for fluorine where the L-electrons are valence electrons and the probability of multiple excitations produced by X-rays is large (Åberg, Graeffe, Utriainen & Linkoaho, 1970).

On the basis of the above considerations further direct measurements of the dispersion corrections and calculations based on the solid state wave-functions are readily suggested.

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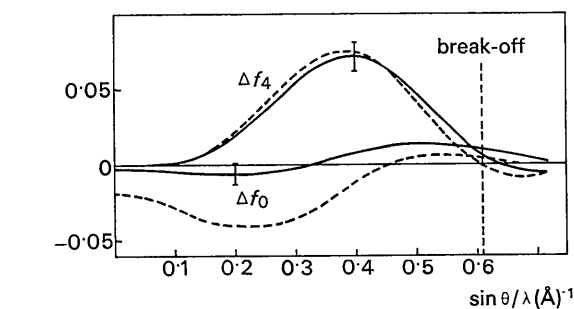CROMER, D. T. & LIBERMAN, D. (1968). Private communication.

Fig. 1. The radial scattering amplitudes Δf_0 and Δf_4 for fluorine in lithium fluoride obtained by the application of the theoretical (solid curves) and experimental (broken curves) values of the dispersion correction. The remarkable Δf_4 component indicates electron transfer from the [111] to the [100] direction. The number of electrons necessary to produce this deformation has been calculated to be 0·08 (Kurki-Suonio, 1970).

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Setting a rhombohedral crystal to its trigonal axis. By R.J.DAVIS and P.G.EMBREY, *Mineralogy Department, British Museum (Natural History), Cromwell Road, London, S.W.7, England.*

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Double oscillations at 120° intervals are used to set a rhombohedral crystal to its trigonal axis, using the separation of non-equatorial pairs of equivalent spots at $\theta = 45°$. The two exposures are made each at 30° to the directions usually used for double oscillation photographs at 180° intervals; arc corrections are derived in the usual way but are here increased by the factor sec $30° = 1·155$.

We have found by experience that when an oscillation photograph shows equatorial symmetry, non-equatorial pairs of equivalent spots can be used for setting the crystal to its axis by double oscillation photographs, provided that the spots are on a reasonably linear part of the ζ-scale, say $\zeta < 0·5$. Oscillation photographs of rhombohedral crystals taken around their trigonal axes show row-lines in which only every third layer-line is occupied by a spot. The majority of row-lines are asymmetrical about the equator and only about one-third of them show equatorial symmetry and an equatorial spot; the latter are difficult to recognize

and are usually too few to be useful for crystal setting. The spots are however repeated at 120° intervals, and double oscillation photographs at 120° intervals show all spots as equivalent pairs from which convenient pairs can be selected for use, whether or not they lie on the equator.

Crystallographers vary as to whether they prefer to take 180° double oscillation photographs with the mean beam directions parallel to, or at 45° to an arc. In either case, if the directions usually chosen are at 0 and 180° of azimuth, for 120° double oscillation photographs the exposures are made with the mean beam directions at 30 and 150°. Arc