The p_z orbitals for the lead atoms and one of the e_1 orbitals of the cyclopentadienyl ring (with the right symmetry) are arranged in such a way as to give a conjugated system. A monomeric molecule participates in the π system with four electrons.

This configuration justifies a planar structure for the polymeric chain.

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Intensity corrections for the Guinier camera. By W. H. SAS and P. M. DE WOLFF, *Laboratorium voor Technische Natuurkunde der Technische Hogeschool, Lorentzweg* 1, *Delft, The Netherlands*

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Intensity corrections for the Guinier camera

The integrated intensities as measured on a photometer record of powder diffraction lines on a Guinier film can be written as follows:

$$I = kpTF^2 \mathrm{LP}ABSG;\ L = 1/\sin^2\theta\cos\theta \qquad (1)$$

where k, p, T, F, L and P are scale-, multiplicity-, temperature-, structure-, Lorentz- and polarization factor respectively. We shall show that the combined effect of the remaining factors A, B, S, G can be approximated by a linear function of cos $(2\theta-\psi)$, ψ being the angle between specimen normal and crystal-reflected primary beam; and we present nomograms from which the normalized slope of this function can be found for $\psi = 30°$.

The factor A accounts for absorption in the specimen (thickness d, linear absorption coefficient μ):

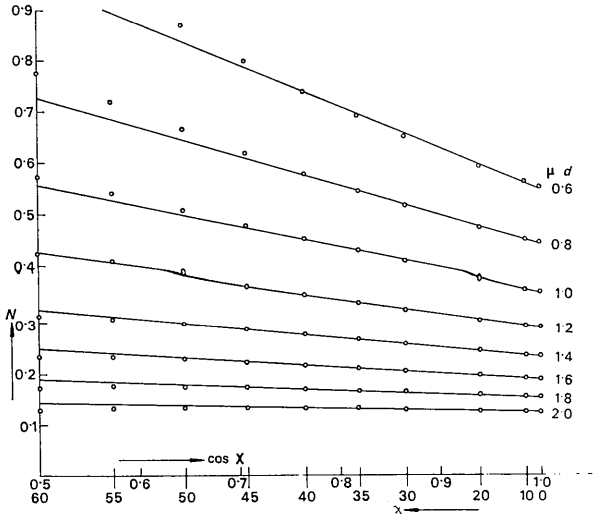

Fig. 1. The combined correction factor $N = ABSG$ (circles) as a function of cos χ for $\psi = 30°$, $\mu_1 d_1 = \mu_2 d_2 = 0{\cdot}35$, $\mu_p d_p = 0{\cdot}1$ and 8 values of μd. The linear least-squares approximation is shown by the straight lines.

$$A = \frac{1}{\mu d}\frac{\cos\psi \,.\, \cos\chi}{\cos\psi - \cos\chi}\left[\exp\{-(\mu d/\cos\psi)\} - \exp\{-(\mu d/\cos\chi)\}\right] \qquad (2)$$

where $\chi = |2\theta - \psi|$.

The factor B accounts for absorption in a layer which is often present in front of the film, *e.g.* wrapping paper or filter (thickness d_p, linear absorption coefficient μ_p).

$$B = \exp\{-(\mu_p d_p/\cos\chi)\}\,. \qquad (3)$$

S is the oblique incidence factor for integrated intensities:

$$S = \frac{[1-\exp\{-(\mu_1 d_1/\cos\chi)\}]}{[1-\exp\{-\mu_1 d_1\}]} \times \frac{[1+\exp\{-(\mu_1 d_1+\mu_2 d_2)/\cos\chi\}]}{[1+\exp\{-(\mu_1 d_1+\mu_2 d_2)\}]} \qquad (4)$$

where d_1 and d_2 are the thicknesses of one layer of emulsion and of the base, respectively and μ_1, μ_2 are the corresponding linear absorption coefficients (*International Tables for X-ray Crystallography*, 1962). G is a geometric factor:

$$G = 1/\cos\chi \qquad (5)$$

(*International Tables*, 1962), arising from the fact that the θ-dependent factor in (1) is valid for a constant specimen–film distance, whereas in the Guinier camera that distance varies as cos χ. Since a photometer measures the energy over a constant height of the diffraction line, the corresponding fraction of the total energy in the Debye–Scherrer cone contains the extra factor $1/\cos\chi$.*

If we define $N = ABSG$, then N is a function of cos χ, with parameters ψ, μd, $\mu_1 d_1$, $\mu_2 d_2$, $\mu_p d_p$, because A, B, S, G are all functions of cos χ. For $\mu_1 d_1 = \mu_2 d_2$ as well as for $\mu_2 d_2 = 0$ and a great number of different combinations of

* Hellner (1954) gave an entirely different expression for the geometric factor, which has been cited and tabulated by Sagel (1958). Professor Hellner (private communication) now states that his formula resulted from an erroneous derivation and kindly pointed out to us that the correct expression was given first by Hägg & Regnström (1944).

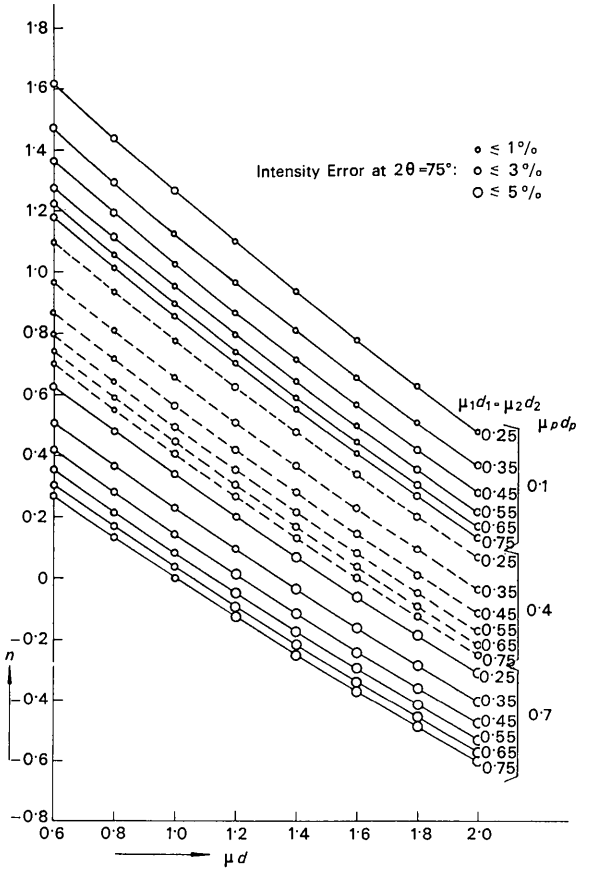

Fig. 2. Slope n of the linear approximation (normalized so as to yield $N=1$ for $\chi=0°$) for $\psi=30°$, six values of $\mu_1 d_1$ and three of $\mu_p d_p$, as a function of μd, with the condition $\mu_2 d_2 = \mu_1 d_1$. The size of the circles corresponds to the error of the linear approximation at $\chi=45°$, as shown.

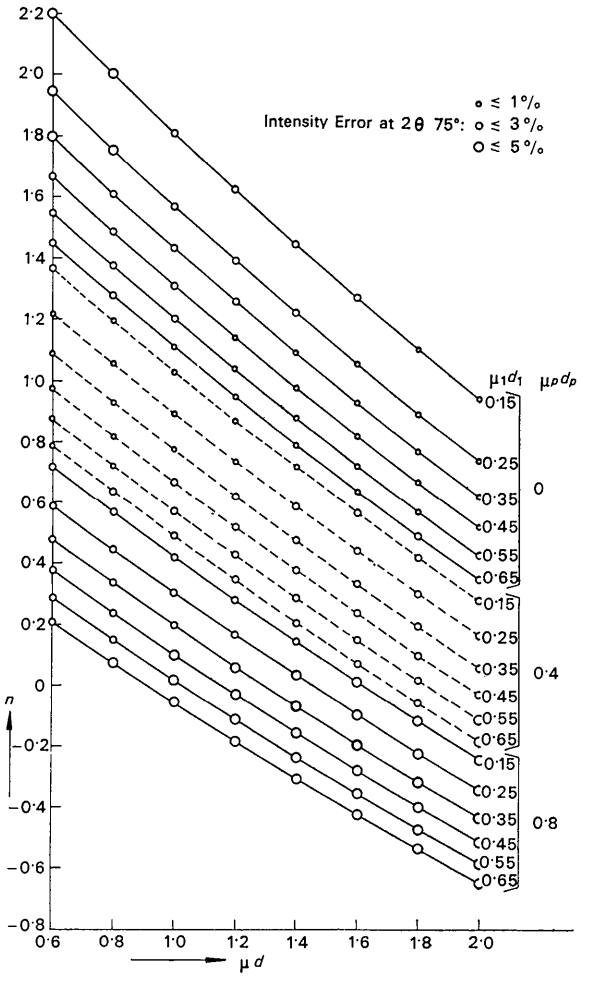

Fig. 3. As Fig. 2, the condition now being $\mu_2 d_2 = 0$.

$\mu_1 d_1$, $\mu_p d_p$ and μd, N was calculated by a computer for 10 values of χ between 0 and 60°. The value of $\psi=30°$ throughout.

Some of the results are shown in Fig. 1. The computed curves $N=N(\cos\chi)$ are seen to be almost linear in the range $\chi=0-40°$, which corresponds to the range $2\theta=$ 0–70°, covering the greater part – if not all – of useful reflexions. Therefore we approximate them by linear functions

$$N=N_0[1+n(1-\cos\chi)]\,, \qquad (6)$$

formulated so as to yield $N=N_0$ for $2\theta=\psi$, whereas N_0 can be regarded as part of a new scale factor and may be put equal to unity. The quantities N_0 and n have been calculated in each case by the method of least squares. We used a weighting factor, which was unity for $\chi=0°$, 30°, 40°, 2 for $\chi=10°$, 20° (because each of these points corresponds to two values of 2θ), and zero for all other points. The differences between the exact values of N and the function (6) turned out to be less than 1 % between $\chi=0°$ and 30° (2θ between 0° and 60°). At $\chi=45°$ ($2\theta=75°$) they rise only rarely up to 5 %, while between $\chi=45°$ and $\chi=50°$ they increase by a factor of about 2. We have plotted n as a function of μd in Fig. 2 for $\mu_1 d_1=\mu_2 d_2$ and in Fig. 3 for $\mu_2 d_2=0$, where we have indicated the error of the linear approximation at $\chi=45°$. For values of $\mu_p d_p$ between those chosen for these figures, the value of n can be found by linear interpolation. In intermediate cases ($\mu_2 d_2$ between 0 and $\mu_1 d_1$) we could again interpolate linearly between the values for n obtained from Figs. 2 and 3. Though linear interpolation both with respect to $\mu_p d_p$ and to $\mu_2 d_2$ is not exactly justified, it has been verified that the accuracy obtained is quite sufficient, the maximum ensuing error in N being less 1 %. For single-coated films with absorption coefficient μ and thickness d of the emulsion the curve $\mu_1 d_1 = \frac{1}{2}\mu d$ in Fig. 3 should be used, as is easily seen from expression (4).

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