computation, it is convenient to introduce the wavelength by the use of modified coefficients, α_k', where $\alpha_k' = \alpha_k/\lambda^k$ so that the independent variable becomes sin θ.

Our tables also include f_0 values corrected for dispersion with the data of Dauben & Templeton (1955).

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References

BERGHUIS, J., HAANAPPEL, IJ. M., POTTERS, M., LOOPSTRA, B. O., MACGILLAVRY, C. H. & VEENENDAAL, A. L. (1955). *Acta Cryst.* **8**, 478.

CROUT, P. D. (1941). *Trans. Amer. Inst. Electr. Engrs.* **60**, 1235.

DAUBEN, C. H. & TEMPLETON, D. H. (1955). *Acta Cryst.* **8**, 841.

FORSYTH, J. B. & WELLS, M. (1959). *Acta Cryst.* **12**, 412.

FREEMAN, H. C. & SMITH, J. E. W. L. (1958). *Acta Cryst.* **11**, 819.

MILNE, W. E. (1949). *Numerical Calculus.* Princeton: University Press.

PATTERSON, A. L. (1935). *Z. Kristallogr.* **90**, 517.

STEINFINK, H. (1957). Private communication.

THOMAS, L. H. & UMEDA, K. (1957). *J. Chem. Phys.* **26**, 293.

VAND, V., EILAND, P. F. & PEPINSKY, R. (1957). *Acta Cryst.* **10**, 303.

VIERVOLL, H. & ØGRIM, O. (1949). *Acta Cryst.* **2**, 277.

WILSON, A. J. C. (1942). *Nature, Lond.* **150**, 152.

Acta Cryst. (1960). **13**, 54

On the structure of evaporated carbon films.

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During an investigation by the present author on multiple scattering effects in electron diffraction, several diffractograms were taken of evaporated carbon films in the thickness range 100–600 Å. It is the purpose of this note to discuss the radial distribution curves which were obtained from these diffractograms after performing correction for multiple scattering as described in a recent paper (Gjønnes, 1959). The diffractograms consisted of a series of diffuse halos with no signs of the graphite crystallites occasionally observed by Cosslett & Cosslett (1959) from similar specimens. Apart from multiple scattering effects no variations with film thickness were observed in the diffractograms. The $s(4\pi \sin \theta/\lambda)$ values for the halos were found to correspond closely to those reported by Kakinoki *et al.* (1957).

The atomic radial distribution curve shown in Fig. 1 was calculated from intensity data in the region $s = 1$–20 Å^{-1}. Normalization and subtraction of back-ground was carried out according to the procedure extensively used by Almenningen *et al.* (1955) in gas investigations.

Table 1. *Observed and calculated interatomic distances*

Observed		Graphite layer		Three-dimensional network		
r (Å)	No. of atoms	r (Å)	No. of atoms	r (Å)	Average	No. of atoms
1·45	2·9	(1·45)	3	1·40 1·52	1·44	2 1
2·49	7	2·51	6	2·42 2·53	2·49	2 4
3·1	7	2·90	3	2·80 2·92 3·24	3·09	1 2 4
3·74	12–14	3·84	6	3·58 3·82	3·77	2 8
4·52		4·35	6		4·32 4·55 4·75	10 6 7
4·95		5·02 5·22	6 6		5·00 5·17	5 14

As the intensity at small angles was neglected, the calculated radial distribution corresponds to the deviations from the even distribution (see e.g. Klug & Alexander, 1954). To obtain the total atomic distribution function one must therefore read the ordinate above the straight line in Fig. 1 corresponding to *minus* the normalized even distribution. The r-values of the peaks in the σ/r-curve are tabulated in the first column of Table 1 together with the peak areas found by decomposition and integration of $\sigma(r)$. The values in the next two columns are calculated for a single graphite layer with bond length equal to the observed nearest neighbor distance, *viz.* 1·45 Å. By comparison it is at once seen that the observed interatomic distances do not fit well with a planar hexagonal layer, and it is further noticed that the observed nearest neighbor distance is appreciably greater than that found in graphite (1·42 Å).

Attempts to account for those discrepancies by introducing variations in bond angle and deviations from planarity indicate the latter to be considerable. It thus seems reasonable to seek an interpretation of the experimental radial distribution by a three-dimensional network like those previously suggested by Gilson *et al.* (1946) or Kakinoki *et al.* (1957). The distances and weights tabulated in the last two columns of Table 1 correspond to the model proposed by Gilson *et al.* (1946). This structure consists essentially of a mixture of 6-rings and staggered 8-rings, the atomic arrangement around each 8-ring being similar to that found for tetraphenylene by Karle & Brockway (1944). The C–C bonds within and between the 6-rings were taken to be 1·40 and 1·52 Å respectively and all C–C–C angles were set equal to 120°, in close agreement with the reported values for tetraphenylene.

The agreement between the latter model and the observed radial distribution may be judged from Table 1. As a further illustration we have calculated σ/r-curves for this model and a turbostratic packing (see Biscoe & Warren (1942) or Franklin (1951)) of graphite layers, with $r = 1·45$ Å and an interlayer distance of 3·40 Å.

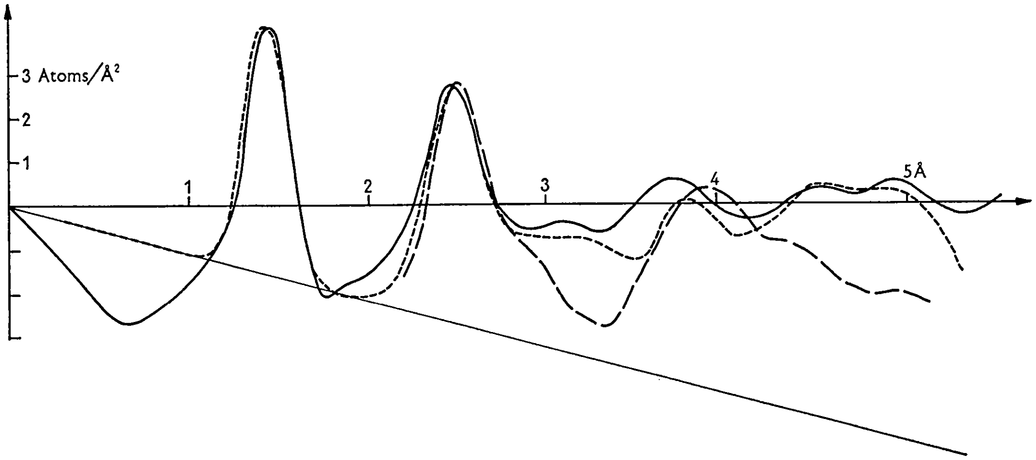

Fig. 1. Experimental and calculated σ/r-curves. Full line: Experimental curve. Dotted: Calculated for three-dimensional network. Broken: Calculated for turbostratic packing of graphite layers. Straight line: *minus* the even distribution $4\pi\varrho_{\text{atomic}}/r$.

The peaks were approximated by Gaussian curves, and the half widths were taken as a descending function of r.

It has to be mentioned that good agreement with the experimental radial distribution appears to be achievable also for the other three-dimensional networks containing 7-rings or other types of 8-rings. It does not seem justified from the present data, however, to make any discrimination between these models and the one considered here. In any case, the structure is very likely to contain a great number of irregularities and very little long-range order as also suggested by Blue & Danielson (1957) from measurements of electrical properties. It should perhaps be noted that films produced during one of the evaporation experiments rendered diffractograms displaying more pronounced halos than usual. A radial distribution curve calculated from these diffractograms indicated a faint split of the nearest-neighbor peak whereas the remaining features did not differ appreciably from the other curves.

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References

Almenningen, A. & Bastiansen, O. (1955). *Acta Chem. Scand.* **9**, 815.

Biscoe, J. & Warren, B. E. (1942). *J. Appl. Phys.* **13**, 364.

Blue, M. D. & Danielson, G. C. (1957). *J. Appl. Phys.* **28**, 583.

Cosslett, A. & Cosslett, V. E. (1959). IV International Conference on Electron-microscopy. (In the press.)

Franklin, R. E. (1951). *Acta Cryst.* **4**, 253.

Gilson, J., Holohan, M. & Riley, H. L. (1946). *J. Chem. Soc. Lond.* p. 456.

Gjønnes, J. (1959). *Acta Cryst.* **12**, 976.

Karle, I. L. & Brockway, L. O. (1944). *J. Amer. Chem. Soc.* **66**, 1974.

Kakinoki, J., Ino, T., Katada, K. & Hanawa, T. (1957). *Acta Cryst.* **10**, 829.

Klug, H. P. & Alexander, L. E. (1954). *X-ray Diffraction Procedures*, p. 590. New York: Wiley.

Acta Cryst. (1960). **13**, 55

Crystallographic data for 5-oxiphenazine.

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5-oxiphenazine is a yellow substance, which melts at 226·5 °C. and is obtainable as single crystals from ethylmethylketone. The crystals used in this study were obtained from a sample prepared by Mr S. Locchi, using the method of Wohl & Aue (1901). These were small needles elongated along b, bounded on the sides by prominent $\{100\}$ and $\{102\}$, and small $\{001\}$ faces, and on the ends by $\{011\}$ and $\{111\}$ faces. Although most of the crystals were poorly formed, and some faces occurred as curved surfaces, a few suitable for goniometric measurements for single-crystal X-ray photographs were found.

By goniometric measurements the following constants were determined: crystal system: monoclinic; axial angle: $\beta = 108° 52'$; axial ratios: $a:b:c = 1{\cdot}632:1:3{\cdot}115$. Rotation, equi-inclination Weissenberg and precession photographs were taken, using Cu $K\alpha$ radiation. The cell dimensions were determined from the rotation and zero-level Weissenberg photographs, the camera radius of