

vacuum-tight cylinder inside the layer-line screens, and a bent rocksalt crystal focused the incident beam on the sample, which consisted of parallel fibers mounted in a frame. Each spot on the film therefore corresponds to the average intensity in a small volume in reciprocal space, the size of the volume element depending on the divergence of the incident beam, the height of the irradiated sample and the distance between the layer-line screens. Fig. 1 is a Weissenberg photograph for which $|\Delta r^*|$ is of the order of 0.03 \AA^{-1} . For Fortisan the diffracted intensities were recorded on normal- and inclined-beam rotation photographs. The observed intensities were normalized, and the incoherent and the structure independent scattering I_{inc} and Σf_j^2 were subtracted. Tabulated values for I_{inc} and f_j were used.

Figs. 2 and 3 show the results of these calculations for ramie, using equations (2) and (4) respectively; only the first three terms in (4) were used. The contour plots have been compared with vector maps of different models, but so far it has been impossible to make any final decision. The chain structure proposed by Meyer & Misch (1937)



Fig. 2. Ramie. Cylindrical distribution. Negative regions are shaded. (Equation (2).)

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Crystallographic data for two compounds related to deoxyribonucleic acids.* By J. S. ROLLETT, Gates and Crellin Laboratories of Chemistry, California Institute of Technology, Pasadena 4, California, U.S.A.

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Nucleotides and alkyl diesters of phosphoric acid are being investigated in these laboratories to provide data on the dimensions of groupings in the structures of nucleic acids, nucleoproteins and viruses. Preliminary investigations of two such compounds are here reported.

Deoxycytidine 5'-phosphate, $C_9H_{15}O_7N_3P$

A specimen was kindly supplied by Prof. A. R. Todd and his co-workers. Flat needle crystals were obtained by slow evaporation of aqueous solution. The symmetry is monoclinic with

$$a = 21.5, b = 11.2, c = 7.0 \text{ \AA}, \beta = 93^\circ 15'.$$

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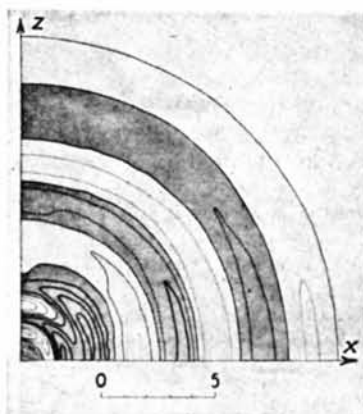


Fig. 3. Ramie. Cylindrical distribution. Negative regions are shaded. (First three terms of equation (4).)

did not fit the experimental data too well. A better agreement between model and contour plots was obtained when every other pyranose ring in the above structure was rotated, but when the twofold screw axis of the molecular chain is abandoned a large number of possibilities has to be tried. Further work on the interpretation of the distribution function is now in progress.

References

- DEAS, H. D. (1952). *Acta Cryst.* **5**, 542.
 DEBYE, P. & PIRENNE, M. H. (1938). *Ann. Phys., Lpz.* **33**, 617.
 MACGILLAVRY, C. H. & BRUINS, E. M. (1948). *Acta Cryst.* **1**, 156.
 MEYER, K. H. & MISCH, L. (1937). *Helv. chim. Acta*, **20**, 232.
 VINEYARD, G. H. (1951). *Acta Cryst.* **4**, 281.
 WRINCH, D. (1946). *Fourier Transforms and Structure Factors*. ASXRED Monograph No. 2.

Systematic absences determine the space group as $P2_1$ or $P2_1/m$, but the latter is impossible because the molecule is asymmetric.

Potassium diethyl thiono-phosphate, $(C_2H_5O)_2POSK$

A specimen was made available by Dr Francis Gunther of the Citrus Experimental Station, Riverside, California. Lath-shaped needles were obtained by evaporation of solutions in acetone at room temperature. The symmetry is monoclinic with

$$a = 21.8, b = 6.6, c = 13.4 \text{ \AA}, \beta = 90^\circ 40',$$

and the crystals are twinned on (100). Systematic absences determine the space group as $P2_1/n$.

No further work on these two compounds is contemplated.

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Re-examination of the symmetries of iron and nickel by the powder method. By F. W. VON BÄTCHELDER and R. F. RAEUCHLE, *Metallurgy Division, Naval Research Laboratory, Washington 25, D. C., U. S. A.*

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Recently, Kochanovska (1949) determined the lattice constant of iron from several reflecting planes in iron, and reported that she had found a significant difference between the measured values for the different planes above 250° C. She attributed her findings to a deviation from cubic symmetry. Because we do not believe that a deviation of the iron structure from cubic symmetry would result in the differences in lattice constant observed by her and because, in any case, the magnitude of the deviation is far larger than that expected from magnetostricture measurements, we have repeated her measurements. Similar measurements were made also on nickel, since any magnetic distortion of the lattice would, perhaps, be expected to be larger for nickel.

Lattice constants were determined at room temperature, using Jette & Foote's (1935) modification of Cohen's method. The {310}, {211}, and {220} reflections of iron were obtained on the same film by interchanging X-ray

tubes with different target materials during exposure. The {420}, {331}, {222} and {400} planes of nickel were similarly recorded together. No systematic dependence of the lattice constant on h , k and l could be observed other than the $\varphi \sin 2\varphi$ dependence which is interpretable in terms of geometric and adsorption errors. The final lattice parameters adjusted to 25° C. are:

$$\text{Iron: } a_0 = 2.8665 \pm 0.0001 \text{ \AA.}^*$$

$$\text{Nickel: } a_0 = 3.5238 \pm 0.0003 \text{ \AA.}^*$$

Measurements of lattice constants at higher temperatures were made from films exposed in a flat-plate back-reflection camera with a 0.01" pinhole, which was positioned to place the required diffraction ring on the focusing circle. Lattice constants for the above mentioned planes were obtained in the temperature range 24–362° C. for iron and 24–455° C. for nickel. The high-temperature lattice constants were standardized by recording a room-temperature diagram on a sector of each film. The results so obtained agree well with the mean linear expansion coefficients reported by Austin & Pierce (1934) for iron and by Jordan & Swanger (1930) for nickel. A curve showing our data together with those of Austin & Pierce for iron is given in Fig. 1. The deviation of individual points from either of the curves lies well within our experimental error ($\pm 0.0005 \text{ \AA.}$). We conclude that there is no significant difference among the lattice constants of iron calculated for the various planes at any temperature. Thus our results do not support Kochanovska's conclusion that deviation from cubic symmetry develops in iron as the temperature is raised or that the deviation can be observed by X-ray techniques.

Similar results have been obtained for nickel.

References

- AUSTIN, J. B. & PIERCE, R. H. H. JR. (1934). *Trans. Amer. Soc. Metals*, **22**, 447.
 JETTE, E. R. & FOOTE, F. (1935). *J. Chem. Phys.* **3**, 605.
 JORDAN, L. & SWANGER, W. H. (1930). *Bur. Stand. J. Res., Wash.* **5**, 1291.
 KOCHANOVSKA, A. (1949). *Physica*, **15**, 191.

* All units are Angström units. The wavelength values used were:

	$K\alpha_1$	$K\alpha_2$
Cr	2.28962 Å	2.29352 Å
Fe	1.93597	1.93991
Co	1.78890	1.79279
Ni	1.65783	1.66168
Cu	1.54050	—

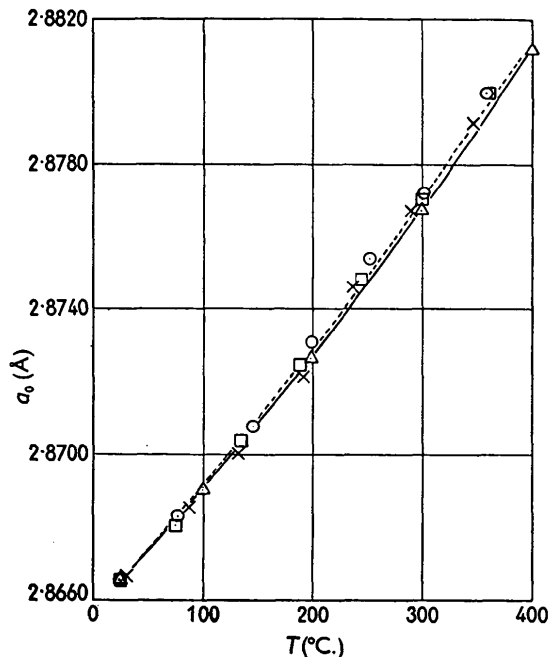


Fig. 1. Plot of lattice constant as a function of temperature for iron. Circles: 310 plane; Co radiation. Squares: 211 plane; Cr radiation. Crosses: 220 plane; Fe radiation. Triangles and full line: Austin & Pierce's (1934) data. Broken line: adjusted experimental data.

Notes and News

Announcements and other items of crystallographic interest will be published under this heading at the discretion of the Editorial Board. Copy should be sent direct to the British Co-editor (R. C. Evans, *Crystallographic Laboratory, Cavendish Laboratory, Cambridge, England*).

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