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The unit-cell dimensions and space group of zinc diethyldithiocarbamate. By S. H. SIMONSEN and JACK WAH HO, *The University of Texas, Austin, Texas, U.S.A.*

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Transparent crystals in the form of elongated plates were prepared by recrystallization of zinc diethyldithiocarbamate (Ethasan-U, furnished by the Monsanto Chemical Company) from chloroform. The extinction direction was the direction of elongation and was designated as the *b* axis. The crystal was optically negative with a nearly uniaxial figure using sodium light; no extinction angle was apparent. The refractive indices were:

$$\alpha \text{ (almost } ||c) = 1.659 \pm 0.003; \beta \text{ (} ||b) = 1.733 \pm 0.003; \\ \gamma = 1.737 \pm 0.003.$$

Powder photographs were taken with filtered copper radiation and a single crystal was used for rotation and equi-inclination Weissenberg photographs of the levels $h0l$; $h1l$; $h2l$; and $hk0$. Laue photographs were taken with the beam parallel to the *a* and *b* axes.

The density, determined by flotation, was 1.50 g.cm.^{-3} , requiring four formula weights $\text{Zn}^{++}[\text{S}_2\text{CN}(\text{C}_2\text{H}_5)_2]_2^-$ per unit cell (4.03 calculated).

Zinc diethyldithiocarbamate is monoclinic with:

$$a = 10.02 \pm 0.02; b = 10.80 \pm 0.05; c = 16.00 \pm 0.02 \text{ \AA}; \\ \beta = 111^\circ.$$

Characteristic extinctions were noted which are those required by the space group $C_{2h}^2-P2_1/c$.

The principal lines measured on the powder photograph are listed in Table 1.

Table 1. *Principal lines of powder pattern of zinc diethyldithiocarbamate*

<i>d</i>	<i>I/I</i> ₀	<i>d</i>	<i>I/I</i> ₀
9.34	0.29	3.37	0.10
8.79	1.00	3.26	0.10
7.46	0.72	3.16	0.15
7.25	0.66	3.11	0.15
6.18	0.45	3.01	0.10
5.07	0.18	2.92	0.12
4.83	0.19	2.84	0.19
4.67	0.08	2.79	0.05
4.44	0.27	2.70	0.15
4.29	0.38	2.37	0.08
3.81	0.29	2.29	0.10
3.68	0.19	2.08	0.12
3.53	0.12		

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The double Patterson function. By DAVID SAYRE, *Johnson Foundation for Medical Physics, University of Pennsylvania, Philadelphia, Penna., U.S.A.*

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Since the paper of Patterson (1935) it has been known that the periodic function $P(\mathbf{x})$ is given by

$$P(\mathbf{x}) \equiv \int d(\mathbf{t})d(\mathbf{t}+\mathbf{x})d\mathbf{v} = V \sum_{\mathbf{N}} |F(\mathbf{N})|^2 \exp [i2\pi\mathbf{N} \cdot \mathbf{x}],$$

and that therefore this most useful function can be computed immediately from the available X-ray data. I should like to call attention to a less useful but similar function which can be calculated approximately from the data.

Let us call the function

$$DP(\mathbf{x}, \mathbf{y}) \equiv \int d(\mathbf{t})d(\mathbf{t}+\mathbf{x})d(\mathbf{t}+\mathbf{y})d\mathbf{v}$$

the *double Patterson* of the structure $d(\mathbf{x})$, a name calling attention to the fact that this function occupies a space of twice as many dimensions as $d(\mathbf{x})$ or $P(\mathbf{x})$. From the definition it is seen that a peak in DP at the point \mathbf{x}, \mathbf{y} means the existence in d of an atom which has one neighbour at a distance \mathbf{x} and another neighbour at a distance \mathbf{y} ; it does not mean merely that there are two atoms separated by \mathbf{x} and two others separated by \mathbf{y} . The function DP thus carries considerably more information about d than does P .

Now it is very easy to show that

$$DP(\mathbf{x}, \mathbf{y}) =$$

$$V^2 \sum_{\mathbf{N}} \sum_{\mathbf{M}} F(\mathbf{N})F(\mathbf{M})F(-\mathbf{N}-\mathbf{M}) \exp [i2\pi(\mathbf{N} \cdot \mathbf{x} + \mathbf{M} \cdot \mathbf{y})],$$

and that, therefore, the phases of the Fourier coefficients of DP cannot be known precisely at the start of a structure problem. But it has been shown by several authors (for instance, Karle & Hauptmann, 1950) that the phase of $F(\mathbf{N}+\mathbf{M})$ tends to be the same as that of $F(\mathbf{N})F(\mathbf{M})$, and that this tendency is stronger the larger the magnitudes of the three F 's involved. Hence the Fourier coefficients of DP , especially the large ones, tend to be real and positive, and therefore

$$DP(\mathbf{x}, \mathbf{y}) \approx V^2 \sum_{\mathbf{N}} \sum_{\mathbf{M}} |F(\mathbf{N})||F(\mathbf{M})| \\ \times |F(-\mathbf{N}-\mathbf{M})| \exp [i2\pi(\mathbf{N} \cdot \mathbf{x} + \mathbf{M} \cdot \mathbf{y})],$$

the right-hand side being obtainable immediately from the diffraction data.

For non-centrosymmetric structures this approximation is rather drastic, for it gives DP a false center of symmetry. But for centrosymmetric structures it is probably fairly accurate. In the case of a model one-dimensional structure, out of the 95 non-negligible terms only 18 very small terms should have been negative.

It is not seriously proposed that this function be used in actual structure work, for the labor of calculating four- or six-dimensional functions would be too great. What is interesting is the fact that a geometrical interpretation has been found for certain analytical relations among the F 's; that is, a link has been made between the so-called 'reciprocal-space methods' and 'direct-space methods' which may be of use in further work on the phase problem.

As an example of such a use, I shall indicate how one might explain the fact, noted by Cochran (1952), that the sign relationships among the F 's appear to hold better with highly unequal atoms than with equal ones. The

height of the origin peak of DP essentially measures the preponderance of positive Fourier coefficients over negative ones. But the height of the origin peak is proportional to $\sum Z_j^2$, where Z_j is the weight of the j th atom, and this quantity is greater for a set of unequal Z 's than for a set of equal Z 's of the same total weight.

Triple and higher multiple Pattersons also exist.

References

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Book Reviews

Works intended for notice in this column should be sent direct to the Editor (P. P. Ewald, Polytechnic Institute of Brooklyn, 99 Livingston Street, Brooklyn 2, N.Y., U.S.A.). As far as practicable books will be reviewed in a country different from that of publication.

Erzmikroskopisches Praktikum. By H. SCHNEIDERHÖHN, Pp. xii+284, with 48 figs., 39 tables and 64 microphotographs on special paper. Separately added **Erzmikroskopische Bestimmungstabellen**, pp. v+24. Stuttgart: Schweizerbart'sche Verlagsbuchhandlung. 1952. Price, bound, DM. 40-60.

The descriptive part of Schneiderhöhn & Ramdohr's *Lehrbuch der Erzmikroskopie*, Volume II, appeared in 1931. Three years later this standard work was completed with Volume I, in which the theoretical and methodical problems were treated. In these volumes practically the complete knowledge of ore microscopy at that time was compiled and presented in an instructive and systematic manner. It could be expected, therefore, that this work would become a classic in the literature of this young branch of science, and that the need for it would be felt for many years. Unfortunately, this work has been out of print for some time, so it was good news when in 1950 an entirely rewritten and enlarged edition of Volume II appeared under the title *Die Erzminerale und ihre Verwachsungen* by Ramdohr. Now Schneiderhöhn presents a new edition of Volume I, likewise under a new name, though the old title would have been appropriate since it deals with the fundamental knowledge which is indispensable to a successful worker in this field.

Compared with the first edition, about 80 per cent of the book appears unaltered. This is, first of all, due to the high standard and the completeness of the original work. Secondly, the nature of this matter is such that technical improvements have been made rather than theoretical ones. Some chapters have been abridged by omitting part of the theoretical discussions. This is the case with the chapter on ore microscopes and accessory instruments (which deals only with the products of Leitz) and with that on optical investigation methods. At the same time, however, these chapters, as well as the other material, have been brought up to the level of current knowledge. This is also shown by the bibliography which comprises 262 separate articles, 83 of which have been published since 1933. The chapter on microchemical and spectro-

graphic analyses and that on the orientation of random sections are only briefly summarized in this book, which is no serious loss. However, the epoch-making work of L. von Hamos in the field of Röntgen spectrography since 1933 would have been worth mentioning.

The 39 tables in the text elucidate the subject in a graphic way. As to Table 15, which aims at giving a comparison between photocell and photometer reflectivity values, the cited literature has not been interpreted correctly. According to this table each of the listed minerals has been investigated with a photocell, whereas in the original work it has emphatically been pointed out that only some of these minerals have been studied by photocell methods. The author's conclusions are consequently erroneous.

Concerning the usefulness of micro hardness methods for reliable determinative purposes, the author concludes that a generally applicable method can be obtained only after exhaustive and critical experiments on very extensive material of undoubted nature.

Emphasis has been laid upon the importance of well-polished surfaces and this problem has therefore been treated in detail. Since the preparation of polished sections is usually left to others it is recommended that the author and the publishers agree to the separate publication of the 43 pages of this chapter (*Die Anfertigung von Erzanschliffen*).

This edition contains three new chapters (pp. 39), which, in a general way, deal with the tasks of ore microscopy, with morphological features of ore minerals, and with their intergrowths, exsolutions and textures. These subjects have been treated with much more detail in Ramdohr's work, to which the reader is referred in many cases. The author's classification of ore mineral textures, however, is new. Its viability beside the classifications of Bastin (1950) and Schwartz (1951) will have to be proved. To illustrate these chapters, 64 excellent microphotographs are added. The explanations of Figs. 52, 53, 63, 64 and 104 are given as for sitaparite; this must be bixbyite. Names like sitaparite should not be used any more in modern literature.

The determinative tables which are appended are an