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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  $1.50 \text{ g.cm.}^{-3}$ , 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> <sub>0</sub>	<i>d</i>	<i>I/I</i> <sub>0</sub>
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.