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A program for plotting Fourier maps. By K. ANZENHOFER, *Abteilung für Röntgenstrukturforschung am Max-Planck-Institut für Eiweiss- und Lederforschung, München, Germany*

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There is no analytic expression for contour lines, where

$$\varrho(\mathbf{r}) = \sum_{\mathbf{h}} F_{\mathbf{h}} \exp(-2\pi i(\mathbf{h}\mathbf{r}))$$

is a constant ϱ_c . To get automatically plotted Fourier maps, one must try to obtain the correct curves ϱ_c from the commonly used lattice representation of three-dimensional Fourier syntheses by interpolative methods. We have therefore developed a program for the IBM 7090 computer, which performs this task and prepares a plot tape for a peripheral device, *viz.* a magnetic tape graph plotter.

In part 1 of the program the points of a certain density ϱ_c are determined for each column and row of the density lattice by linear interpolation. Out of these points the next part collects points P_n for a curve, part 3 transforms the found sequence of points P_n by plotter subroutines into the right input mode for the plotting device. Parts

2 and 3 of the program are repeated as frequently as there are points P_n not yet connected by curves. The fundamental idea of part 2, which is the most important part, will be explained in detail in Fig. 1.

Beginning with an arbitrary point P_0 , the next point P_1 must lie on the rectangle drawn in full lines (Fig. 1(a)). For every further point P_n there are still more restrictions on its position (Fig. 1(b)), because the sense of the curve to be determined is fixed by vector $\mathbf{P}_{n-2}\mathbf{P}_{n-1}$. Consequently, we have to examine only small pieces of three columns and rows altogether as to where the next point of the curve may be situated. These pieces are marked in Fig. 1(b) by full lines, too. Only in the case of lattice points there are more possibilities for the continuation of a curve. The program must be able to distinguish between closed curves, curves from edge to edge, and isolated points (only lattice points can be isolated). We should here emphasize that all the restric-

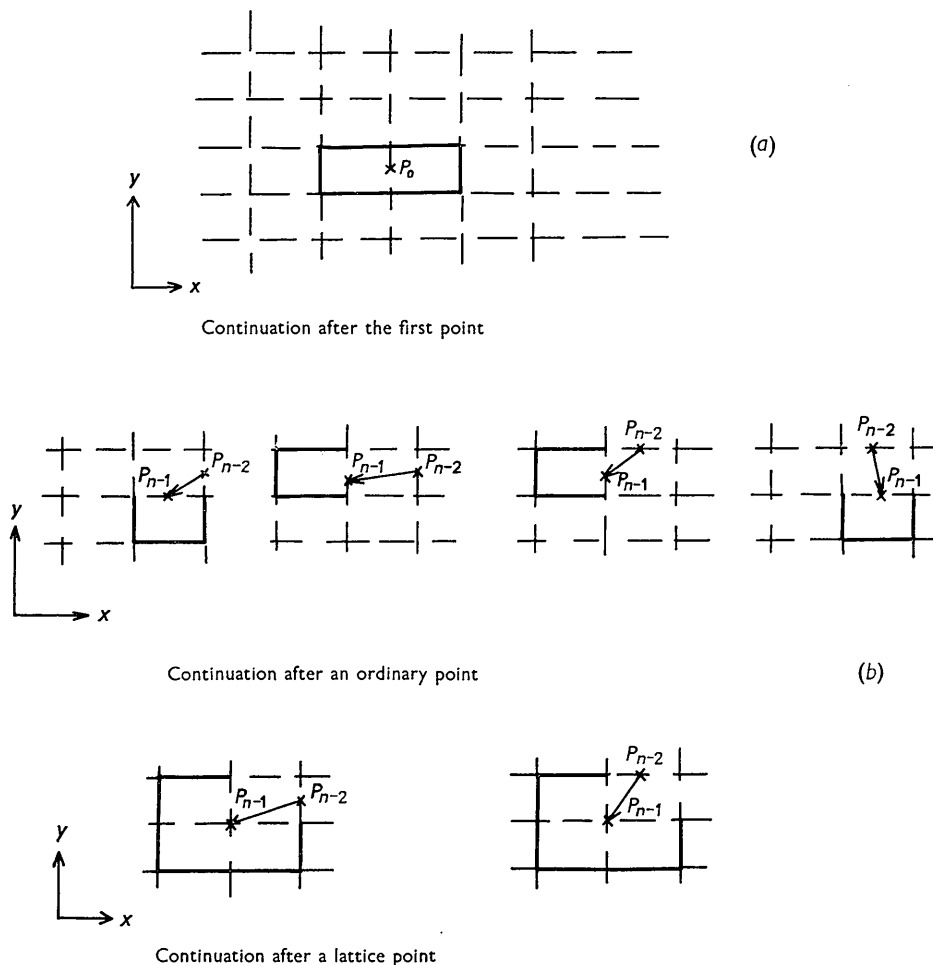


Fig. 1. Fundamental aspects for part 2 of plot.



Fig. 2. Patterson function of a test structure.

tions shown in Fig. 1(b) may only be made on account of the use of linear interpolation in the determination of the points g_c .

We give, as an example, the sharpened Patterson

function of a test structure (c projection; $a=8$, $b=6$ Å; 4 C atoms, 1 Cl atom; space group $Pna2_1$) (Fig. 2). The calculation took 1.5 min for a lattice of 31×31 points and 33 different levels.

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X-ray evidence for CrBO_3 , VBO_3 and TiBO_3 with calcite structure. By H. SCHMID, *Battelle Memorial Institute, International Division, Geneva, Switzerland*

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In the course of preparations of boracites by gas phase transport reactions in sealed quartz tubes (Schmid, 1964) we also obtained several known and some new transition metal borates *via* the gas phase.

Here we want to report on a new chromium, vanadium, and titanium borate. The experimental conditions indicated in the following are not optimal for borate formation since they were chosen with a view to obtaining boracites. Nonetheless they may serve as a guide:

The chromium borate was obtained as follows: in a sealed quartz tube (volume 0.08 l) three quartz crucibles containing 0.76 g B_2O_3 , 0.3 g ($\text{Cr}_2\text{O}_3 + \text{Cr}$) and 0.67 g CrCl_2 respectively, were arranged, one above the other, and 175 mg H_2O in the form of H_3BO_3 was placed in

the crucible containing $\text{Cr}_2\text{O}_3 + \text{Cr}$. The sealed tube was heated in a vertical tubular furnace for four days in a small temperature gradient ($T_1 \sim 990^\circ\text{C}$, $T_2 \sim 1000^\circ\text{C}$) in such a way that the colder end of the tube was on top. The cooling to room temperature took 3 hours. In the crucible, containing B_2O_3 , Cr-Cl-boracite had formed, and on the walls of the tube (coldest zone), hexagonal, grass-green platelets (about 0.05 mm thick and 0.5 mm in diameter) were detected. The crystals could easily be detached by dissolving the B_2O_3 film on the tube wall in boiling water.

The vanadium borate was formed as follows: three quartz crucibles containing 2.8 g B_2O_3 , 1.34 g ($\text{V}_2\text{O}_5 + 3\text{V}$) and 2.54 g VCl_2 respectively, were placed in a quartz