Acta Cryst. (1969). B25, 403

A method for stereo plotting of three-dimensional electron density*.

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(*Received* 16 *September* 1968)

A method is described for generating random points in space, the number of points per unit volume being proportional to the value of the electron density. Stereo plotting of these points provides a useful three-dimensional representation of the electron density.

Three-dimensional Fourier syntheses are usually plotted as contours in a series of parallel sections. When looking for a particular grouping of atoms in such maps it is often difficult to see at a glance whether such a grouping is present. In particular, if one were studying a series of E maps having several different phase assignments, it would be desirable to have the Fourier output plotted in such a way that one could quickly select the one most likely to be correct.

In order to represent the electron density, ϱ, random dots are plotted in such a way that the number of dots per unit volume is proportional to ϱ. Three random numbers between 0 and 1 are generated and scaled to represent a point xyz within the boundaries of the Fourier synthesis. The electron density at the grid point nearest to xyz is designated as q. A fourth random number, p, is generated and scaled to be within the range 0 and ϱ_{max}. If $p \leqq q$ a dot is plotted at the point xyz. The process is repeated until the desired number of points has been plotted.

Application of the symbolic addition procedure in the structure determination of hydrazinium fluoroborate (Roof & Conant, 1969) yielded 48 signs, including three unknown signs a, b and c, out of some 600 reflections. Eight E maps were computed. Fig. 1 shows the correct sign choice; a tetrahedral BF_4 group and an N–N group are clearly visible. It was found desirable, in this example, to omit any points at which $\varrho < 0{\cdot}2\,\varrho_{max}$. With so few terms in the summation there were many small spurious peaks and hence some undesirable background. This three-dimensional solution differs from the earlier two-dimensional results of Conant, Corrigan & Sparks (1964) by a shift of origin of $\frac{1}{4}$ in z.

It does not seem worthwhile to give any programming details here because so much of the strategy depends on the Fourier program one uses, the local plotting subroutines and plotting facilities, and the particular computer. The principle, however, is simple and should be easily applicable in individual cases.

The method used here is very similar to that used in a Monte-Carlo integration. Also, this method is generally applicable in plotting a function of three variables; it has been used to plot hydrogen-like electron densities for orbitals $l = 0$ to 5 and for all appropriate values of $|m|$ (Cromer, 1968).

* Work performed under the auspices of the U.S. Atomic Energy Commission.

References

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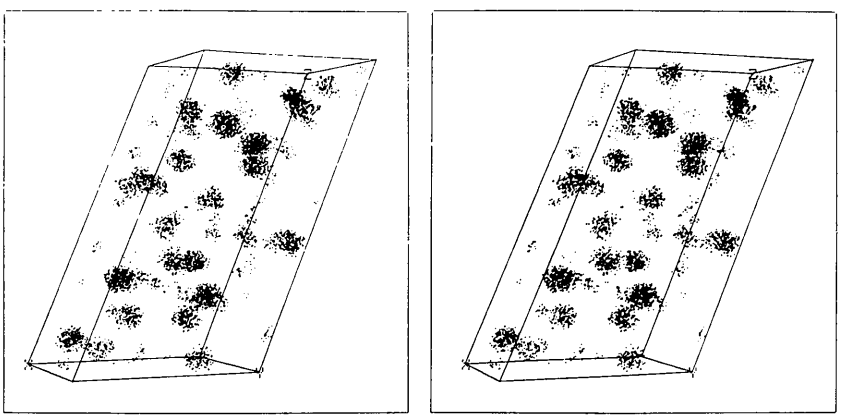

Fig. 1. A 48-term E map for hydrazinium fluoroborate, space group $C2/c$, plotted in the range $x = 0$ to $\frac{1}{2}$, y and $z = 0$ to 1. In this example, approximately 300000 random points were generated and about 5000 points have been plotted.