6,000 photographs were taken, yielding about 60,000 tracks. From these, Professor McCusker claimed that five tracks were found which showed an ionization of about a half (unity being that from a proton). Because ionization varies as the square of the charge, this points to the existence of particles of charge $2/3$. The exact figure for the ionization of these tracks was quoted as 0.48 ± 0.05 .

The interpretation of the ionization tracks, however, is far from simple, as Professor McCusker seems readily to have admitted. There are several possible processes that can produce tracks similar to those from lightly ionizing particles, and it was inevitable that Professor McCusker's experiment would be judged on the strength of his evidence to dispose of freak events. As well as "background" due to ionization loss from relativistic particles, possible variations in the density of gas within the chamber and tracks caused by pre-expansion events are all factors which may affect the situation. Professor McCusker said he has assumed that the distribution of ionizations in the tracks was Poissonian, but there was general concern at the conference at the lack of a histogram displaying the distribution of particles with ionization. If the tracks are to be considered significant in the sense indicated by McCusker, then some direct evidence is needed to show that they are not part of some overall background distribution. Although the Sydney group is evidently aware of these problems, and McCusker seems to have answered the points on the uniformity of gas in the chamber quite deftly, the presentation of a histogram of track widths would have added much backing to the case.

This sort of experiment, of course, provides ample scope for sceptics to indulge in ritual slaughter. The absence of incontrovertible evidence is an easy excuse for unfettered criticism, and it is encouraging to note that a further experiment is being planned by McCusker's group to find the other types of quark with a charge of $1/3$. By using a high pressure chamber he expects to be able to track particles with an ionization down to below $1/10$, which would then include the quarks of smaller charge. Should tracks be found which correspond to both types of quarks and which cannot be explained as part of a simple statistical distribution, the evidence for the existence of quarks will indeed be very strong. As it is, opinion seems to be divided chiefly between cautious optimism and cautious pessimism as to how McCusker's results should be interpreted. It may be that a more detailed analysis of the existing results will be enough to sway the balance.

CRYSTALLOGRAPHY

New Structures by Computer

from a Correspondent

It frequently happens in the crystal structure analysis of organic compounds that one wishes to determine the chemical structure or molecular conformation of a compound about which accurate knowledge of a part of the molecule is already available. A computerized Patterson search method which uses such information is described in a recent paper by P. B. Braun, J. Hornstra and J. I. Leenhouts (*Philips Research Reports*, **24**, 85; 1969). Other workers, for instance C. E. Nordman and K. Nakatsu (*J. Amer. Chem. Soc.*,

85, 353; 1963) and W. Hoppe and E. F. Paulus (*Acta Cryst.*, **23**, 339; 1967), have described methods to determine the atomic coordinates for the known part of a molecule, but the computer programs of Braun *et al.* determine the atomic parameters for the unknown part of the structure as well as the known part.

The Patterson map, which may be computed very easily from the X-ray diffraction data, is essentially a vector map of the crystal structure, the peaks in a Patterson synthesis representing the interactions between atoms. Thus if there are n atoms in the unit cell there will be $n(n-1)$ peaks in the Patterson map plus an n -fold peak at the origin which represents the interaction of each atom with itself. The size of a vector peak is proportional to the product of the atomic numbers of the interacting atoms, so if there are no heavy atoms in a large molecule there will be an impossibly large number of similar peaks in the Patterson function. With these new programs for disentangling the vector map, the computer first stores a numerical copy of the Patterson function and is then given the coordinates of the known part of the molecule referred to an arbitrary set of axes. The program next calculates the coordinates of all the vectors between the atoms of this model structure, compares the calculated vectors with those which occur in the Patterson synthesis, and calculates a measure of fit. The model is then systematically rotated in steps about the axes and the process repeated. The position of the centroid of the model is found by systematic trials, and the measures of fit are short listed and refined by making small adjustments. The few models with such optimized best fits now contain the true solution. In practice it is usually, but not always, the first in the list.

The parameters of the unknown part of the molecule are then calculated by a second program. Possible positions for atoms attached to the best model are first calculated from simple chemical and geometrical considerations. Because there are usually several alternative possibilities for the bonds from each model atom, the vectors between the known atoms and each of the possible new atoms are calculated and compared with the true vector map as before. The one with the best fit is selected and this atom is added to the molecule. The process is repeated with the now enlarged model until the molecule is complete. Standard crystallographic least squares refinement methods are then used to complete the determination.

The methods described were successfully applied to the structure determination of seven retro-steroids. The initial well known chemical group consisted of nine atoms in most cases—the C and D rings. In all cases a complete list of the coordinates of up to twenty-six non-hydrogen atoms was produced by a CD3600 computer within 45 minutes, a time which a crystallographer would consider extremely reasonable for such difficult structural analyses.

Theoretical calculations in the paper show that the minimum size of model required to solve a structure with n atoms in the unit cell was approximately equal to the square root of n . It was also shown practically as well as theoretically that a structure could be solved even if some atoms in the model were completely misplaced, provided that at least the minimum number were correctly placed.