My Part in X-ray Statistics

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It is difficult to set down memories of how an idea was born. After twenty years they become befogged and coloured by the knowledge of later events, and the strict discipline of scientific writing is hard to shake off. Nevertheless, on the occasion of the commemoration of the discovery of X-ray diffraction and at the request of the President of the International Union of Crystallography, the attempt must be made.

In 1942 Yü submitted to *Nature* a paper on the determination of absolute from relative X-ray intensities, and the Editors of *Nature* sent the paper to the Cavendish Laboratory for an opinion on its merit. The method proposed was complex and depended on the use of a set of tables not then available in Britain, but Lipson and I did recommend publication (Yü, 1942). The proposal set us arguing over a practicable method of achieving the same purpose, and a hazy idea emerged that the general level of the intensities of the various reflections from a crystal must depend on the content of the unit cell and not on the details of the atomic arrangement. Lipson (unpublished, so far as I know) suggested calculating the F's for an arbitrary arrangement of the atoms in the unit cell and comparing $\Sigma|F_{calc}|$ with $\Sigma|F_{obs}|$ for suitable groups of reflections, but I wanted a tidier approach. Statistical calculations were in my mind in connection with diffraction by disordered structures like Co and $AuCu_3$ (Wilson 1942a, 1943), and it was soon evident that the appropriate statistical variables to use were the X-ray intensities, not the structure amplitudes. A very short calculation (Wilson 1942b) showed that the mean value of the intensity expressed in units of (electrons)^2 is equal to the sum of the squares of the scattering factors of all the atoms in the unit cell. Once obtained, this relation is practically obvious from conservation of energy, and is the first example of the blindness to the implications of what I knew, that has mingled a good deal of self-dissatisfaction with my pleasure in developing statistical methods.

Knowing the mean value of the intensities immediately suggests the problem of determining the probability distribution of the intensities about the mean. I derived what I thought was the general formula for this by an application of the method of induction, and found that it gave approximate agreement for copper sulphate (Beevers and Lipson, 1934). I drafted a paper on the subject, which I remember discussing with Ewald as we travelled to London together for some function or other. When revising the draft, however, I noticed that my argument made an implicit assumption of non-centrosymmetry in the atomic arrangement, and that a centrosymmetric arrangement would give a different result. This was an important finding, but I did not see its importance. Instead I put the whole matter on one side for four or five years, feeling that distribution functions that depended on symmetry were too complicated to bother with. I ought, of course, to have looked at the matter the other way, and have seen that the distribution function provided a valuable way of detecting those symmetry elements that do not cause systematic absences.

Enlightenment came some years later, when I was in Cardiff and responsible for a research student who found difficulty in distinguishing between a centrosymmetric and a non-centrosymmetric space group having the same systematic absences. There could have been many ways out of his difficulty, but while discussing the problem with Rogers I saw my work on distribution functions from the obverse, and fruitful, point of view (Wilson, 1949). X-ray determination of the absence of a centre of symmetry was received with a little scepticism at first—did not all the textbooks say that it was impossible?—and I well remember carrying a couple of slides in my pocket to a conference of the Institute of Physics, without being able to obtain an opportunity of projecting them. The friends to whom I showed them during the intervals hid their disbelief with varying degrees of success.

Statistical methods of determining the absence of mirror planes and rotation axes provide a third instance of blindness to the obvious. In my letter in *Nature* (1942b) I wrote:

'If two atoms are close together in the projection, they ought to be counted as a single atom with atomic factor equal to the sum of their respective atomic factors. · · · certain coincidences can be predicted from the space group only, and allowed for.'

I was then considering the matter in the direction: space group known; can one avoid statistical complications? It was not until many years later, in conversation with Rogers about ridges of high density in Patterson projections, that the reverse question occurred to me:

statistical anomalies detectable; what is the space group? Once the question had been posed it was easy enough for me to write down the factor multiplying the average intensity for the groups of reflections affected by various symmetry elements (Wilson, 1950), and with rather more labour Rogers (1950) was able to prepare the statistical equivalent of vol. I of the *International Tables*.

If there is any moral it is this: systematic work will usually discover the answer to a properly posed question, but discovery of the right questions to ask is a pretty erratic random variable.

References

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