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Concluding Remarks

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In reviewing the papers and discussions of the last few days, I am struck by the fact that the title of the conference was wider than what has in fact taken place. We have only considered accurate intensity measurements on, and structure factors of, well-ordered three-dimensional crystals. Disordered crystals have not been considered at all: here, of course, the problems are quite different because what you measure depends very much on the limits of integration in reciprocal space.

It is clear that our ability to make observed and calculated structure factors agree is much better than our ability to get an accurate measure of either. This fact has shaken our confidence in ourselves and in what we measure, especially in view of the outcome of the three projects about which we have heard. We needed a reduction in our over-confidence.

There has not been enough comment on the shakiness of our knowledge of F_{calc}, especially of the thermal position, even though Dawson has drawn our attention to some of the problems involved. Our normal procedure is to replace $f(\hat{s})$ by $f(s)$, but we do not even know enough about the latter. More notice must be taken of the imaginary part of the atomic scattering factor; the real part is merely a part of the form factor curve where the inaccuracy is very large in any case, but the imaginary part is very important. Dispersion effects, especially in weak reflexions are very important and in these days of automatic diffractometers there is no excuse for confining one's measurements to one octant.

There are many experimental errors for which we do not correct adequately, such as thermal diffuse scattering with which we cannot deal easily because it peaks under the Bragg peaks.

We have forgotten that the attainment of accurate structure factors has no value in itself – other than the pleasure which one gets from well-made measurements. The only thing of value is the information extracted, and the required accuracy depends on the ultimate aim.

The normal procedure among crystallographers is to believe implicitly in the sets of F_{obs} and of F_{calc} and to regard only the scale factor as having to be determined. You run these sets through your calculations, and very often you obtain negative temperature factors. Usually you then throw out the strong reflexions and get reasonable values of B, but then you know nothing about the accuracy of your results.

Looking at the many structures which have been published in *Acta Cryst.* during the last few years, it is evident that the positional parameters are reasonably good – even though the actual errors are probably about five times greater than the estimated ones. However, the thermal parameters are all nonsense and must all be done again in a sensible way.

Post referred to the importance of simultaneous reflexions which I pointed out some years ago. More work is obviously needed on how to deal with this problem.

I have the distinct impression that many people believe that my extinction formulae are completely adequate except for very severe extinction. I must warn them that these formulae only work as far as they go: they are very crude, especially when the absorption is high. I was happy to hear from Professor Kato that he intends to have the perfect extinction formula within a year. I am sure he will get there and it will be very useful.

The most important thing to learn from this meeting is to distrust everything in the literature and not to take oneself or one's work too seriously.