

contemporaneous or later deformation had occurred in the vicinity of the postulated bends. Such deformation might possibly fit into the late Caledonian movements. This problem would be more acute for significant Tertiary (or even post-Devonian) crustal shortening or extension affecting north Britain. The known Tertiary movement is predominantly relatively minor regional extension involved in dyke injection, basin formation and normal faulting.

Collette^{9,10} has presented further evidence to suggest that the line of the Great Glen fault lies east of the Shetland Isles. It is clear that all hypotheses give rise to problems and this should encourage us to look for further evidence particularly in the vicinity of the postulated bends. Perhaps the simplest is the hypothesis advanced by Pitcher¹¹ that the Walls Boundary fault is a splay of the main fault. The main fault would then pass east of the Shetlands.

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Structure Determination by the Combination of Anomalous Scattering and Direct Methods

PHASE determination by direct methods is more difficult for non-centrosymmetric than for centrosymmetric crystals. The phase, $\alpha(h,k,l)$, can take any value for the former crystal between 0 and 2π while the choice for the latter crystal is limited to two values, 0 or π . If the structure is non-centrosymmetric and contains a small number of atoms which scatter anomalously, then $\alpha(h,k,l)$ can be determined from the Bijvoet difference, for example, $\Delta I = |F(h,k,l)|^2 - |F(\bar{h},\bar{k},\bar{l})|^2$, and the known phase α_p of the anomalous scatterers^{1,2}. From

$$\alpha'_N = \alpha_p + \pi/2 \pm \theta \quad (1)$$

and

$$\cos \theta = \frac{\Delta I}{4 |F'_N| |F_p|} \quad (2)$$

where α'_N is $\alpha(h,k,l)$, the phase of the reflexion, F'_N , if there were no anomalous scattering. F_p is the contribution from the absorption term Δf_p . The indeterminacy in equation (1) arises because the cosine is an even function. In practice, the ambiguity has been resolved by choosing α'_N to be the phase closest to α_p (ref. 3) or by calculating a double phased synthesis². An alternative, indeed the original method, is to calculate the Patterson sine function⁴.

A different approach⁵ is to recognize that the incorporation of anomalous scattering data reduces the problem to the comparative simplicity of the centrosymmetric case, or to a choice between two phases, and then to use direct methods to select the observed phase closest to the

correct value. An important difference is that the two possible phases α_1 and α_2 need no longer be π apart.

When $|\cos \theta|_{\text{obs}} \geq 1$ then $\alpha_1 = \alpha_2$ and the phase is known unambiguously. Such reflexions form a basic set from which the phase determination may proceed. For L(+)-lysine hydrochloride dihydrate, using Raman's³ data, fifty-two out of 128 phases can be determined unambiguously in this way. Similarly, from the neutron diffraction data for cadmium nitrate tetradeuterate⁶, thirty-two out of 161 phases can be determined.

From the basic set, there are two possible ways of proceeding. Phases for the remaining reflexions can be calculated and the observed phase closest to the calculated phase can be chosen or, alternatively, phases can be determined and refined without paying further attention to the observed phases. A reasonable approach would be to carry out sufficient cycles of the first alternative to determine as many phases as required, and then to refine them by the second method, because the observed phases will be liable to error. A preliminary cycle in which the basic set alone is refined should be performed because α_1 for the set may have only a small number of discrete values depending on the space group and the number of anomalous scatterers in the asymmetric unit. For example, for lysine hydrochloride, the phases of the basic set were 90° or 270° . It should be noted that no arbitrary origin-defining phases can be used because the origin is already determined when placing the anomalous scatterers.

The method described here could be useful for determining the structures of large molecules of biological interest which are often solved by combining multiple isomorphous replacement with anomalous scattering data. An obvious advantage would be in the reduction of the number of data to be collected.

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Supralinearity of Thermoluminescent Phosphor Lithium Fluoride

THE non-linear response to dose reported for many thermoluminescent phosphors^{1,2} has caused serious concern both for dosimetry and for dating techniques.

We have investigated square samples of TLD-100 phosphor 3 mm across and 1 mm thick. The thermoluminescence output induced by a ⁹⁰Sr source was measured conventionally with a photomultiplier tube in oxygen-free nitrogen and a heating rate of 20° C/s. A dose of a few kilorads was given to the phosphor and the TL output was measured. In addition to the peaks reported by Zimmerman *et al.*³, a tail was observed at the higher temperature region. A detailed study on this tail showed that there are at least two peaks in its fine structure. These two peaks were found to increase with dose to saturation at near 3 megarads. The peak positions are at 370° C and 430° C respectively. The structure of this tail and its dependence on dose can be seen from Figs. 1 and 2.

A thermal annealing experiment was performed in order to study the characteristics of these peaks. Both peaks were found to tail off exponentially at constant