will enable the extension in the Ethiopian Rift to be determined.

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The Great Glen Fault in the Shetland Area

The Bouger anomaly map of the continental shelf to the west of Orkney and Shetland recently published by Bott and Watts[1] provides gratifying confirmation of the geology of this area which I proposed earlier[2]. My predictions were based on an interpretation of the aeromagnetic map of the area and include not only most of the deep sedimentary basins proposed by Bott and Watts but also the great NW–SE trending strip of Lewisian rocks labelled *A* by Bott and Watts.

The chief difference between the gravity map[1] and my interpretation map based on the aeromagnetic map of the area concerns this anomaly *A*. On the gravity map anomaly *A* continues across the north of Shetland to about 0° 40′ W. The equivalent feature on the aeromagnetic map ends to the east of 1° 00′ W.

After consideration of both the geological evidence and of the aeromagnetic map I correlated the Great Glen fault with a very powerful fault of transcurrent type exposed in Shetland and called the Walls Boundary fault. In conformity with the pattern of the aeromagnetic map I extended the Walls Boundary fault north of Shetland along a line striking only slightly east of north. This extrapolation takes it through part of Bott and Watt's anomaly *A*. Because their anomaly is not displaced along this line they suggest that the Great Glen fault must pass to the east of Shetland and not through it.

This suggestion completely ignores the known geology of the area; it fails to take the Walls Boundary fault into account. This fault has all the hall-marks of a great transcurrent fault. It must continue to the south and north of Shetland for considerable distances. There is nothing on the aeromagnetic and gravity maps to set a limit to the extension of the Walls Boundary fault to the south. On both maps the line of best fit for it is a smooth curve from Shetland to Inverness passing close to the west of Fair Isle.

The extrapolation of the Walls Boundary fault to the north of Shetland can be made with less certainty. The line which best fits both the gravity and the aeromagnetic maps lies to the east of my original line[2]. It passes through 1° 00′ W and 61° 00′ N and skirts the eastern end of gravity anomaly *A*.

With this projected line for the fault the nearly N–S strike of the fault in Shetland becomes a local deflexion of strike from the general NNE strike to the north and south of Shetland. The change from concave west to concave east can be seen in Shetland, where the fault is intermittently exposed over 59 km. For 31 km after it enters Shetland from the south the fault has a strike of 004°. For 28 km before it leaves Shetland to the north the strike is 011°. The maximum strike necessary to carry it past anomaly *A* is 020°.

This configuration for the fault in the Shetland area has the advantage that the Nesting fault (a 16 km displacement transcurrent fault (2)) and other major parallel faults in Shetland become the *en echelon* branches which would be expected if such a deflexion of strike took place.

I maintain that Bott and Watts's gravity map not only confirms the presence of the deep sedimentary basins and crystalline gneiss ridges on the shelf to the west of Shetland which I predicted[2] but also provides additional evidence of the connexion between the Walls Boundary fault and the Great Glen faults and shows that to the north of Shetland the fault resumes the strike it had to the south of Shetland.

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We apologize to Dr Flinn for any disquiet we may have caused by omitting to refer to his recent paper[1]. We agree with him that the aeromagnetic map[2] distinguishes regions of shallow and deep magnetic basement by the smoothness of the contours. We disagree, however, with his use of the general anomaly level as an indication of sediment thickness, which is the distinction between his pattern *A* anomalies which "probably overlie deep sedimentary basins" and pattern *B* which "covers sedimentary basins less deep than those of pattern *A*". The usual geophysical approach is to estimate the depth to the basement using well established quantitative techniques[3]. One of the main points of our report[4] was to present evidence for three deep Mesozoic basins marked *C*, *D* and *E* on our map. These basins are not delineated in Flinn's interpretation, although they do occur within wider tracts which he interprets as sediment covered.

Flinn has suggested a new line for the Great Glen fault which does not cross gravity "high" *A* north of the Shetlands. This raises a problem which needs to be recognized.

To quote Allen[5], "probably the most impressive feature of thoroughgoing transcurrent faults is their extreme linearity over literally hundreds of kilometres". Large transcurrent faults should now be interpreted as transform faults which play an essential part in the scheme of global tectonics as boundaries between plates of lithosphere moving laterally relative to each other[6]. If there is no significant internal deformation within the plates, the fault plane must lie on a small circle with reference to the pole of rotation about which the relative motion can be described. The trace of the fault plane can only deviate from a small circle if either one or both of the plates suffer internal deformation during the movement, or if the fault plane has been horizontally displaced at a later stage. Thus Benioff[7] interpreted the bend in the San Andreas fault in terms of sinistral movement on the Garlock fault which started to develop later than the San Andreas, accompanied by severe distortion where they intersect. The bends of the Alpine fault of New Zealand[8] can be interpreted in terms of splaying of the fault and deformation currently occurring near the bends.

The new line of Flinn involves changes in direction of the fault south and north of the Shetlands. The bend to the north is particularly sharp. Flinn's line would be acceptable if it could be demonstrated that the required 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 Pitcher[11] 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, α(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 α(h,k,l) can be determined from the Bijvoet difference, for example, $\Delta I = |F(\text{h,k,l})|^2 - |F(\bar{\text{h}},\bar{\text{k}},\bar{\text{l}})|^2$, and the known phase α'_P of the anomalous scatterers[1,2]. From

$$\alpha'_N = \alpha'_P + \pi/2 \pm \theta \tag{1}$$

and

$$\cos\theta = \frac{\Delta I}{4\,|F'_N|\,|F''_P|} \tag{2}$$

where α'_N is α(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 $\Delta f''_P$. 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 synthesis[2]. An alternative, indeed the original method, is to calculate the Patterson sine function[4].

A different approach[5] 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's[3] data, fifty-two out of 128 phases can be determined unambiguously in this way. Similarly, from the neutron diffraction data for cadmium nitrate tetradeuterate[6], 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 ^{90}Sr 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