The present communication deals with a new algorithm which is able to estimate two-phase seminvariants in all the space groups and drastically reduces computing time.
The new procedure identifies all the one-phase structure seminvariants of first rank and calculates the three-phase structure invariants involving at least one-phase seminvariant: therefore the list of triplet invariants directly provides all the pairs ($\underline{u}_1$, $\underline{u}_2$) which are two-phase seminvariants of first rank.
The probabilistic formula used is an effective modification of older formulas. The result is that a large number of reliable two-phase seminvariants is usually available for active use with a reliability often comparable with triplet invariants estimates.

17.2-6 INVESTIGATION OF PHASE INVARIANTS FROM A POWER SERIES EXPANSION OF THE ENTROPY FUNCTIONAL. By I.R. Castleden, Department of Physics, University of Western Australia, Nedlands 6009, Australia.

The entropy functional for N atoms

$$S = - N \int_V p(x) \log\{ Vp(x)\} d^3x$$

where p(x) is single atom probability density can be expanded as a power series about a 'point' $p_0(x)$. This expansion is equivalent to a asymptotic expansion of the probability density of N independently distributed atoms. Expressed in terms of the Fourier components of p(x) and $p_0(x)$ S is represented as a sum of invariants. The ability of these invariants to predict correct phases can be tested in a similar manner to the invariants encountered in direct method calulations.
The phase indications from the invariants of a second order expansion of the entropy are tested using a routine that compares them to actual phases values. The program is similar to the XTAL program REVIEW (Hall, S.R., 1986, Tech. Rep. TR-1364.2, University of Maryland). A number of known structures are tested. For each structure a selection of expansion points $p_0(x)$ are used ranging from the uniform distribution to the true structure. For each point data such as the number of correct phase indications can be plotted. R-factors and figure-of-merits can also be calculated giving an indication of the likelihood that structure solution methods using second order entropy expansions (Wilkins, S.W. et al. 1983, *Acta Cryst.*, A39, 47-60; Bricogne, G. 1984, *Acta Cryst.*, A40, 410-445; & Navaza, J. 1985, *Acta Cryst.*, A41, 232-244) will be applicable as routine and robust procedures.

17.2-7 DIRECT METHODS SOLUTIONS FROM VERY WEAK DATA. By M.J.Begley, Department of Chemistry, University of Nottingham, Nottingham, England.

The diffraction data obtainable from very small crystals, using conventional X-ray sources, is usually very weak and limited by the sample size. If a heavy atom is present this data is sometimes sufficient to solve the structure by the Patterson method. With no heavy atom, attempts to solve the structure by direct methods using, for example, the MULTAN80 program are usually unsuccessful because of the severe limitations of the data set. It has been suggested by Sheldrick (BCA Meeting York, 1986) that at least 50% of the theoretically measurable reflections in the resolution range 1.1 to 1.2 A should be observed for the data to be of adequate quality for direct methods solution of noncentrosymmetric structures. It is the lack of sufficient intensity data in this and higher angle ranges that causes the direct methods procedure to fail. If most of the refections in this range are unobserved then the few weakly observed reflections have calculated E values that are too low to allow them to play their proper major role in the phase determination process. A method has been developed that attempts to overcome this problem. In this, E values are calculated by a conventional normalisation process for low angle reflections only. The high angle observed reflections are then inspected and estimated E values are manually added to the data set for phase determination using the MULTAN80 program. Several examples of structures (both centrosymmetric and noncentric) that have been successfully solved from very weak data, using this procedure, will be described.

17.2-8 THE USE OF E-MAGNITUDE WEIGHTING SCHEMES IN CONVERGENCE MAPPING AND TANGENT REFINEMENT IN DIRECT METHODS. By S.R. Brown and C.J. Gilmore, Department of Chemistry, University of Glasgow, Glasgow G12 8QQ, Scotland.

Traditionally, direct methods do not exploit the standard deviations of the E-magnitudes. However, it is possible to simulate the use of $\sigma(|E_h|)$ via a simple weighting scheme applied to the triplets and quartets at convergence mapping and carried through the subsequent tangent refinement procedure.

Examination of $\sigma(|E_h|)$ as a function of Bragg angle shows the expected increase at high angle, so that a suitable weighting scheme should downweight (or even remove) phase relationships involving one or more high angle E-magnitudes. A simple weighting scheme has been incorporated into the MITHRIL direct methods program:

$$\omega = 1 \text{ if } \sin^2\theta/\lambda^2 \leqslant t$$
$$\omega = f\ (\sin^2\theta/\lambda^2) \quad \sin^2\theta/\lambda^2 > t$$

where t is a selected cut-off point (usually 0.95).

Alternatively a filtering system can be used in which certain invariants are removed.

This simple method is extraordinarily successful. Over half the structures are routinely solved by this technique. A 138 atom polypeptide structure has also been solved with minimal difficulty.