tributions. On the theoretical side, they concern the applicability of joint distributions, derived on the basis of restricted structural models, to the highly regular structures encountered in practice. The questions also concern whether the formulas used in practice have captured the essence of the joint distribution sufficiently well. On the practical side, there are questions concerning the accuracy and range of data, the increase of complexity, the enhanced computing requirements and the lower probabilities associated with the higher order phase invariants. We ask finally whether the strongest indications will, at least, be reliable and to what extent they can impact on a phase determination. Can they afford a facility in structure determination that is not otherwise readily accessible? Such questions have not yet been answered. There are a myriad of varieties of formulas for phase invariants and embeddings associated with the many space groups which are directly accessible and may well require prolonged investigation before evaluations and judgements of utility can be made. It is planned to describe the formulas, discuss how they are to be used, make some comparisons with the existing formulas for computing phase invariants, present some initial calculations and, perhaps, attempt to formulate some ideas concerning future developments.

17.2-02 THE USE OF QUARTETS AND QUINTETS IN RANDOM PHASING PROCEDURES. By A.A. Freer and C.J. Gilmore, Department of Chemistry, University of Glasgow, Scotland.

The use of random phasing procedures coupled with least-squares refinement has been developed (Baggio et al. Acta Cryst. (1978) A34, 883-893) into an important tool in the application of direct methods to difficult structures. As an extension of our work on utilising higher invariants in the MULTAN computer program, (Acta Cryst. (1980) A36, 470-475) we have applied negative quartets and quintets to the random phasing method in the following ways:

(a) As figures of merit to decide when to stop the least-squares (or steepest descents) refinement procedure.

(b) As figures of merit to filter out unpromising solutions so that they are not passed to the weighted tangent refinement procedure.

(c) In an active mode, whereby these invariants are themselves used in the refinement calculations.

The use of (a) and (b) can reduce the computer time needed on a typical computer run by as much as 30%. Most successful solutions show a clear minimum in these figures of merit. In this context they are more useful than the conventional reliability indices.

The use of (c) somewhat weakens (a) and (b) since the figures of merit are no longer independent of the phasing method, but the radius of convergence and the stability of refinement can sometimes be increased.

17.2-03 THE SIR PROJECT: A GENERAL PROBABILISTIC APPROACH TO THE PHASE PROBLEM. By C. Giacovazzo & G.Cascarano, Ist. Mineralogia,Università,Bari,Italy; M.C. Burla, A. Nunzi & G. Polidori, Ist. Mineralogia,Università,Perugia,Italy; B. Busetta, Lab. de Cristallographie,Université de Bordeaux,Talence,France; R. Spagna, Lab. di Strutturistica Chimica,CNR, Monterotondo Stazione (Roma), Italy; I. Vicković, University Computing Centre, Zagreb, Yugoslavia; D. Viterbo, Ist. Chimica-Fisica, Università, Torino, Italy.

In 1977 Giacovazzo (Acta Cryst. A33,933) introduced the idea of representation of a structure invariant (si) or seminvariant (ss). This idea proved to be a very general way of defining the normalized magnitudes which are most effective, in a statistical sense, in the evaluation of si or ss quantities. A very important feature of the representation method is its capability of making full use of symmetry in a general way.

The SIR (Semi Invariant Representation) project is a joint effort aiming both to the theoretical development and to the practical application of this new approach to the estimation of si's and ss's.

In its present state the SIR computer program includes the following features:

1) Evaluation of one-phase ss's and their optimization *via* special two-phase ss's.
2) Evaluation of two-phase ss's.
3) Generation of triplets and their evaluation by means of Busetta's (Acta Cryst. A32, 359, 1976) modified MDKS formula.
4) Estimation of negative quartets using the first representation (full use of symmetry) and their strenghtening by the second representation.
5) Convergence procedure using all relations and eliminating redundant information.
6) Phase extension and refinement by tangent formula.
7) Use of several figures of merit.

This is by no means the final stage of the program. The development and testing of new formulae for the estimation of other types of si's and ss's or for improving the evaluation of those already used, is in progress and will be continued in the future. We are also developing and testing new techniques for phase extension and refinement.