The results show that:

(i) \( P_{13} \) formula gives a more reliable estimate for both positive and negative quartets, although an underestimation still exists.

(ii) There is a considerable increase in the availability of quartets \( (P_{13} P_{13}) \) having a high associated probability. This increase is most dramatic in the range \( 1.0 > p^* > 0.89 \).

(iii) There is also a pronounced increase in the availability of negative quartets.

(iv) In cases of limited data, the multiplicity of third neighbourhoods can generate strong indications in situations where \( P_7 \) alone is of limited use.

(v) Multiplicity of individual estimates also enhances the phase estimation procedure.

Practical experience indicates that as few as 50 negative quartets with good estimated probabilities is enough to solve difficult structures.

17.10 PHASE RELATIONSHIPS FOR SUPERSTRUCTURES

By V. Gramlich, Institute for Crystallography and Petrography ETH, CH-8092 Zurich, Switzerland.

Statistical relationships between phases of structure factors are usually derived for structures with rationally independent atom coordinates. Prominent deviations of the mean squared normalized structure factors from unity for certain index parity classes (in general a 'strong' subset of 'main' reflections and 'weak' cosets) are a characteristic feature of systematic rational dependence.

A formula for phase determination has been derived in which the different mean coset intensities are explicitly taken into account:

\[
P\{\varphi(h_n)\} = \frac{1}{(2\pi i)} \exp(\frac{\varphi(h_n) - \beta}{N})
\]

with

\[
\varphi(h_n) = -\sum_{n=0}^{\infty} \frac{n!}{n!} \exp\left\{i\left[\frac{\pi}{2} \cos(n(h_n) + \varphi(h_n) - \beta)\right]\right\}
\]

and

\[
K(h_n h') = \frac{2\pi}{\sqrt{N}} \sum_{m=0}^{N-1} B_n B_{-n} E(h_n) E(h') E(h_n - h')
\]

\( P(\varphi(h_n)) \) is the von Mises distribution of the phase of the structure factor \( E(h_n) \)

\( n \) is an appropriate numbering of the cosets (or possibly parity classes), \( n = 0, 1, \ldots, p-1 \)

17.11 ON THE ESTIMATION OF SEMINVARIANTS

BY THE AID OF HARKER RELATIONS.

By H. Burzlaff, Institut für Angewandte Physik, Lehrstuhl für Kristallographie, Loewensteinstr. 22, Universität Erlangen-Nürnberg, FRG.

As the direct inspection of seminvariant phases leads to a remarkable increase of computation time if higher symmetry is present and "upper representations" are included another approach is proposed:

(i) A Patterson function is computed on the base of \( E^2 \) values

(ii) Space-group symmetry is applied to construct a "Harker" space.

(iii) The Fourier transform of the Harker space gives information on the phases of seminvariant reflexions.

The procedure is tested on the base of some difficult structures, the result will be reported.