17.X-7 DIRECT METHODS OUTSIDE TRADITIONAL FIELD
By Fan Hai-Fu, Institute of Physics, Academia Sinica, Beijing, China.

After 40 years of development, direct methods are now firmly established. New procedures are under examination in the Institute of Physics in Beijing.

1. In protein crystallography, the combination of direct methods with isomorphous replacement or anomalous scattering data may play an important role in the near future. The method proposed in our group (Fan (1965) Acta Phys. Sin., 21, 1114; Fan, Han, Qian & Yao (1984) Acta Crystal., A 40, 409; Fan & Gu (1985) Acta Crystal., A 41, 280) has been tested with experimental protein data in the one-wavelength anomalous scattering case yielding a thousand of initial phases with average error of about 40 degrees.

2. In high resolution electron microscopy, direct methods may become a powerful tool of image processing. It has been proved by simulation that direct methods are useful in image deconvolution and resolution enhancement (Fan, Zhong, Chen & Li (1985) Acta Crystal. A41, 163; Han, Fan & Li (1986) Acta Crystal. A42, 353; Liu, Fan & Zheng (1986) IUCR CSM Meeting, Beijing, China.

3. Modulated structures are important in both solid state physics and structural chemistry. However, there was no straightforward way to solve their structure. Recently a direct method has been proposed and used successfully to solve the phase problem of an incommensurate structure. This implies that direct methods will no longer be limited in solving 3-dimensional periodic structures. Hopefully, the method can be extended to solve the phase problem in the determination of quasicrystal structures.

17.X-8 FUTURE METHODOLOGY. SOME PROBABILISTIC AND SOME POSSIBLES. By Jerome Karle, Laboratory for the Structure of Matter, Naval Research Laboratory, Washington, D. C. 20375, U. S. A.

In the area of macromolecular structure determination, there are several developments which indicate the potential for enhanced analytical capability. In addition to the development of tunable, high-intensity sources (synchrotron radiation) and the continuing improvement of computing facilities, the results of theoretical studies of the potential of modern algebraic analysis techniques in recent years imply the potential for enhanced speed and facility in performing structure determinations. An algebraic analysis of multiple-wavelength anomalous dispersion, for example, has resulted in a set of simultaneous equations that are both exact and linear (J. Karle, Int. J. Quantum Chem. Symp., 1980, I, 257-367). Such exact algebraic analysis is valid for any number of anomalous scatterers and any variety of types of anomalous scatterer. The unknown quantities, which do not vary with wavelength, are composed of intensities, phase differences, or a combination of the two. The part that varies with wavelength occurs only as coefficients of the unknowns. The unknown phases and intensities are those that would be obtained from individual types of atoms as if each type were present in isolation from the rest. Knowledge of the intensities for the structure forced by a particular type of atom can facilitate the determination of the structure forced by this particular type of atom. Once the structure is known for any of the types of atom present, the entire structure can be readily determined. The determination of the structure of anomalous scatterers may not always be successful. In those cases, the structures of nonanomally scattering atoms may, perhaps be obtainable from known values for triplet phase invariants of the type \( h_{1}h_{2}h_{3}-k_{1}k_{2}k_{3} \). Values for triplet phase invariants may be obtained from recent algebraic analysis (J. Karle, Acta Crystal., 1984, A40, 526-531). Evaluations of triplet phase invariants have also been made from use of probability theory (H. Hauptman, Acta Crystal., 1985, A41, 288-294; V. Glocovass, Acta Crystal., 1983, A39, 583-592; S. Fortler, N. J. Moore and N. E. Fraser, Acta Crystal., 1985, A41, 571-577) and alternative algebraic analysis that make use of special mathematical and physical properties of the isomorphous replacement and the anomalous dispersion phenomena (J. Karle, Acta Crystal., 1983, A39, 802-805; J. Karle, Acta Crystal., 1984, A40, 431-437, 445-451; J. Karle, Acta Crystal., 1985, A41, 102-106). It has been further shown that by use of algebraic analysis essentially unique values can be obtained with one-wavelength anomalous dispersion data for the 2-phase invariant (J. Karle, Acta Crystal., 1985, A41, 397-398). This analysis was limited to the case of one predominant type of anomalous scatterer in a one-wavelength experiment. Another investigation has shown that with use of values obtained for 2-phase invariants in one-wavelength anomalous dispersion experiments and single isomorphous replacement experiments, knowledge of the structures of the anomalous scattering atoms or heavy atoms could afford a large number of phase conditions, and thereby enhance the determination of a native or nonanomally scattering structure (J. Karle, Acta Crystal., 1986, A42, 246-253). This could also provide a possible strategy for use of triplet phase invariants.