The maximum entropy formalism can be seen as a real-space equivalent of traditional (reciprocal space) direct methods (Bricogne Acta Cryst. 1984; A40, 410-445). It does, however, offer several advantages that are not available in conventional direct methods including the full use of all invariants at every point in the phasing process without their explicit generation, the natural incorporation of the standard deviations of the normalised structure factors, and the constant updating of the prior distribution of atoms that guarantees that the approximate joint distribution of structure factors remains valid even for large deviations from uniformity.

We report here, our experiences using the exponential modelling method applied to several small molecule structures in the Sheldrick difficult structures database. Our initial conclusions are as follows:

1. It is possible to accurately extrapolate new phases via the technique.
2. The method is independent of the data resolution. This is important for structures where it is impossible to obtain data sets at atomic resolution.
3. It is possible to correctly extrapolate phases for very weak reflections (|E| < 0.5). This implies that much larger structures should be accessible to the maximum entropy method than are feasible with traditional methods.

17.2.10 AB INITIO PHASE DETERMINATION USING THE CONSISTENT ELECTRON DENSITY METHOD. By T.K. Bhat, NH, NIOZ, Benthose, MD20092, and H.L. Ammon, Chemistry Department, U. of Maryland, College Park, MD20742, USA.

The compound tetrakis, C$_8$H$_8$N$_4$Mg$_2$P$_4$A$_8$, a high energy material, crystallizes in space group P (a=7.886A, c=6.779A, c=21.595A, b=10.217A). Cu data were collected on a Picker diffractometer (Max B=6.3°).

Numerous attempts to solve the structure with MARTIN, and later with MITHRIL, were unsuccessful. The structure was solved using the consistent electron density method (CEDM) (Bhat, NH, Acta. Cryst. A40, C 15; Bhat, NH, J. Appl. Cryst. 1984, H, 21). The CEDM is a Fourier method with restraints applied to the electron density distribution. It does not involve conventional direct methods. The procedure was initiated with a few, low resolution reflections assigned random phases. (a) Using these amplitudes and phases, H, an electron density map, p, was calculated. (b) Negative values of p were set to a constant value and the electron density values were corrected. (c) From this modified p an unbiased map, p' which is analogous to an OMIT map (Bhat & Cohen, J. Appl. Cryst. 1984, 17, 244) was calculated. Using p' as p, step (b) and (c) were repeated for several cycles. (d) A new set of phases was calculated from p for H and for some additional (about 15%) reflections to obtain a new set of reflections, H'. With H' as H, steps (a) through (d) were repeated. The electron density map was examined when the set H included all the reflections to about 1.4σ. A molecular model was fit to it with the graphics program, FOx. This model has been refined to R=0.047 for 1791 data > 3 σ. An ORTEP diagram of the molecule is given.

17.2.11 THE SOLUTION OF CRYSTALSTRAKTURES WITH RUDER- SYMMETRY BY INVERSE. By R.A.J. Driessen and R. Schamp, Lab for Crystallography, University of Amsterdam, Nieuw Achtergracht 166, 1018 WV Amsterdam, The Netherlands.

In general structures with pseudosymmetry are more difficult to crack by direct methods than structures without. The presence of an additional translation in the unit cell gives rise to the systematic absence of all reflections in particular paragroups. In the case of a pseudo translation these reflections are systematically weak as is reflected in the results of the normalisation procedure. The triplets for a structure with a pseudo translation (e.g. pseudo I) can be divided into two types: one containing three reflections from the strong paragroups, type A, and the other containing one reflection from the strong paragroups and two from the weak ones, type B. It was found that both types of triplets, calculated from normalised structure factors for randomly generated isotropic point atom structures with different degrees of pseudotranslational symmetry, are equally reliable as a function of their E-range.

For imaging the structure a vast number of phase reflections of both types is needed. Therefore the E-values are often recalculated for each paragroup separately, in order to obtain a more equal distribution of all paragroups at the upper part of the E- and E-range. Although often successful, this procedure increases the number of type B triplets largely, however, their reliability has dramatically decreased in comparison with triplets of the type A at the same E-value level. Instead the original E-values should be used in a modified procedure. The procedure starts with selecting equal numbers of reflections of both types, calculating all phase relationships and using this information to calculate phases of both types as reliable as possible. It includes the use of two different sets of acceptance criteria for new phases in order to achieve phase propagation for all reflections. The research has been sponsored by SON, the chemical SMS foundation.