17.2-9 THE USE OF MAXIMUM ENTROPY IN THE A-PRIORI PHASING OF SMALL MOLECULES.
By G. Bricogne, LURE, Bâtiment 209D, 91405 Orsay Cedex, France and C.J. Gilmore, Department of Chemistry, University of Glasgow, Glasgow G12 8QQ, Scotland.

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:

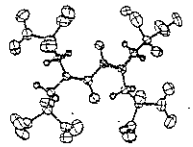
(1) It is possible to accurately extrapolate new phases via the technique.

(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 ($|E_h| < 0.5$). 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.N. Bhat, NIH, NIDDK, Bethesda, MD20892, and H.L. Ammon, Chemistry Department, U. of Maryland, College Park, MD20742, USA.

The Compound tetrakis, $C_{10}H_8N_{10}F_4O_{18}$, a high energy propellant, crystallizes in space group Pc (a=7.888A, b=6.779A, c=21.595A, β =108.21°). Cu data were collected on a Picker diffractometer (Max θ=63°). Numerous attempts to solve the structure with MULTAN, and later with MITHRIL, were unsuccessful. The structure was solved using the consistent electron density method (CEDM) (Bhat, Acta Cryst. 1984, A40. C 15; Bhat, ACA Symposium, 1985, H1. 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, ρ, was calculated. (b) Negative values of ρ were set to a constant value and the electron density values were squared. (c) From this modified ρ an unbiased map, ρ' which is analogous to an OMITMAP (Bhat & Cohen, J. Appl. Cryst. 1984, 17, 244) was calculated. Using ρ' as ρ, step (b) and (c) were repeated for several cycles. (d) A new set of phases was calculated from ρ 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 1.4A resolution and a molecular model was fit to it with the graphics program, FRODO. This model has been refined to R=0.047 for 1791 data $\geq 3\sigma$. An ORTEP diagram of the molecule is given.



17.2-11 THE SOLUTION OF CRYSTALSTRUCTURES WITH PSEUDO-SYMMETRY BY SIMPEL. By R.A.J. Driessen and H. Schenk, Lab for Crystallography, University of Amsterdam, Nieuwe 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 paritygroups. In the case of a pseudo translation these reflections are systematically weak as is reflected in the results of the normalization 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 paritygroups, type sss, and the other containing one reflection from the strong paritygroups and two from the weak ones, type sww. It was found that both types of triplets, calculated from normalized structure factors for randomly generated isotropic point atom structures with different degrees of pseudotranslational symmetry, are equally reliable as a function of their E_3-value.
For imaging the structure a vast number of phased reflections of both types is needed. Therefore the E-values are often rescaled for each paritygroup separately, in order to obtain a more equal distribution of all paritygroups at the upper part of the E- and E_3-range. Although often succesful, this procedure increases the number of type sww triplets largely, however, their reliability has dramatically decreased in comparison with triplets of the type sss at the same E_3-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 ZWO foundation.

17.2-12 THE PHASING OF SAS DATA VIA DIRECT METHODS. Suzanne Fortier and Marie E. Fraser, Dept. of Chemistry, Queen's University, Kingston, Canada, K7L 3N6.

It has been known for some thirty years that structure amplitude differences due to anomalous scattering can be used to obtain phase information. In the single-wavelength anomalous scattering (SAS) case, given the anomalous scatterer substructure and the Friedel pair amplitudes, two possible values are obtained, in general, for the individual phases. In recent years, several approaches based on the application of direct methods to SAS data have been proposed for the resolution of the two-fold ambiguity (Hauptman, H., Acta Cryst. A38, 632 (1982); Karle, J., Acta. Cryst. A41, 387 (1985); Fan Hai-Fu, Han Fu-Sun, Qian Jin-Zi, Yao Jia-Xing, Acta Cryst. A40, 489 (1984); Langs, D.A., Acta. Cryst. A42, 362 (1986); Giacovazzo, C., Acta. Cryst. A39, 585 (1983); Fortier, S., Fraser, M.E. and Moore, N.J., Acta. Cryst. A42, 149 (1986). The theoretical basis of the structure invariant probabilistic estimates is examined so as to relate parameters of the formulae to standard SAS parameters and compare the direct methods - SAS results to the results of the standard SAS method in which the phase closest to the anomalous scatterer substructure is selected.