17.5–7 A 'BEST TEST' TO DISTINGUISH BETWEEN THE CENTRIC AND ACENTRIC WILSON DISTRIBUTIONS. By S.Parthasarathy and N.Elango, Department of Crystallography and Biophysics, University of Madras, Guindy Campus, Madras-600 025, India.

It is known that X-ray intensities from a crystal containing similar atoms follow either the centric or the acentric Wilson distribution depending on whether the crystal is centrosymmetric or not. Crystallographers exploit this property to resolve space group ambiguities of a crystal from a statistical study of the observed intensities. A number of statistical parameters of the two Wilson distributions (e.g. Wilson's ratio, variance, higher moments of intensities) as well as other quantitative statistical criteria for goodness of fit (e.g. chi-square test, Kolmogorov test, Neyman-Barton smooth test etc.) have been suggested in the literature for this purpose. From the point of view of the Theory of Statistics none of these can be classified as a 'best test'. A 'best test' (also called the most powerful test) is the one for which the critical region is such that the type II error is minimized. Such a test can be constructed using Neyman-Pearson Lemma. In this paper a best test to distinguish between the two Wilson distributions is discussed. The effect of data truncation due to unobserved reflections is also taken into account in the theoretical treatment.

17.5–8 INFORMATION AND CRYSTAL STRUCTURE ESTIMATION

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One of the most fundamental concepts in science is the concept of information. The proof by Shannon (*The Mathematical Theory of Communication*, 1948, Bell Syst. Tech. J. 27, 379-423; 623-656) that there exists a unique and consistent measure of the information content in a probability distribution, followed by the development by Jaynes (see *Collected Works: Papers on Probability, Statistics, and Statistical Physics*, 1982, Dordrecht-Holland: Reidel) of a general information-theoretic approach to problems of statistical inference, provides a very powerful framework for treating such problems of which statistical mechanics, image processing, and crystallographic inversion (i.e. structure estimation) may be regarded as particular examples.

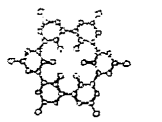
We shall describe some of the fundamental concepts involved in information-theoretic based approaches to the crystallographic inversion problem and show how practical methods of structure refinement may be developed which are aimed at macromolecular structure determination (Wilkins, Varghese and Lehmann, Acta Cryst. 1983, A39, 47). Particular attention will be given to the roles of prior information, event-space and choice of constraint functions (Steenstrup and Wilkins, 1984, Acta Cryst. A40) with a view to relating recent articles on the inversion problem (e.g. Britten and Collins, Acta Cryst., 1982, A38, 129, and Piro, Acta Cryst., 1983, A39, 61).

17.6–1 CHARACTERISATION OF ROTATIONAL DISORDER IN MOLECULAR CRYSTALS. By J.C.A. Boeyens and D.C. Levendis, Department of Chemistry, University of the Witwatersrand, Johannesburg, South Africa.

Rotational disorder occurs in many crystals containing planar aromatic molecules. Evidence of disorder often shows up as large anisotropic thermal parameters or unusual bond lengths and angles. Detection of steric rotational disorder may be difficult by crystallographic means, and refinement converges to the average of the superimposed disorder arrangements. However, by calculation of the appropriate maps of the potential energy environment as a function of concerted ring rotation the forms contributing to the disorder can be identified (as in the room-temperature ferrocene crystal). Subsequent rigid-body crystallographic refinement converges to models that fit the observed electron density as well as the average structure. This has been demonstrated for the charge-transfer complex, anthracene:tetracyanobenzene. Further work shows that the presence of rotational (static) disorder can be established by energy-map calculations and rigid-body refinement in several classes of molecular crystal, including organometallic sandwich complexes, charge-transfer complexes and hydrocarbons such as perylene and biphenyl.

17.6–2 MOLECULAR VOLUMES AND 'HOLE' SIZES IN HOSTS AND HOST-GUEST COMPLEXES*. By E.Maverick, K.Mirsky and K.N.Trueblood, Department of Chemistry and Biochemistry, University of California, Los Angeles, CA 90024, USA.

The method of calculation of molecular packing energies and molecular volumes (A. Gavezzotti, J. Am. Chem. Soc. (1983) 105, 5220) has been applied to several spherands, hemispherands and other chemically- and structurally-related compounds and their complexes (for examples, see D.J.Cram and K.N.Trueblood, Topics in Current Chem. (1981) 98, 43). Such calculations have been helpful in two respects. First, they provide a convenient way to describe 'pre-organization' of the host, by characterizing the 'hole' size with and without a guest; and second, they help in some cases to resolve difficulties in describing solvent or counter-ion species when they are disordered in the crystal structure.
An example of the second type of calculation follows. We found that the macrocycle below crystallizes in the space group Pa3, although the included solvent (CH_2Cl_2) must be disordered, since it is near the 3-fold axis. Relative energies calculated for several solvent positions helped us to choose the best model.



$C_{42}H_{30}F_6$

Fluorine atoms projecting inward, methyl groups outward

Other structures we have studied in this manner include analogous spherands with methoxy groups projecting inward, with and without Li+ and Na+ guest ions; hemispherands (part spherand, part cyclic ether); augmented spherands with guest Li+ ions; spherands and hemispherands containing urea moieties; and 'bowls.'

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