

02-Methods for Structure Determination and Analysis,
Computing and Graphics

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The extensive use of Fourier transform methods and the large sizes of unit cell and data sets in macromolecular crystallography make it highly desirable to use efficient methods of computation. Fast Fourier transform (FFT) methods are very useful for solution of these problems. With a few exceptions, the libraries of FFT subroutines that have been available in the past have been restricted to sample sizes (numbers of grid points per period) that were products of small, prime numbers, which results in rather large gaps between numbers that may be used for large unit cells and moderately high resolution. Efficient FFT routines for different types of numbers -- prime numbers, powers of prime numbers, or products of distinct prime numbers and their powers -- follow many different procedures, so it is not possible to write general routines that can handle all cases. Also, when many transforms are required for sample sequences all of the same size, a routine that is optimized for that particular size is desirable.

The crystallographic problem allows exploitation of certain special conditions to make computation still more efficient. Electron density is a real function, so its Fourier transform has Hermitian symmetry. Three dimensional transforms may be performed as sequences of one dimensional transforms, and the data in the intermediate steps may have a symmetric structure. For example, a 2_1 screw axis gives a data structure in which values separated by half of a lattice translation are complex conjugates, and centered lattices produce rows that are alternately symmetric and antisymmetric. Techniques for exploiting space group symmetry for space groups that have no rotation axes of order higher than two have been described by Ten Eyck (*Acta Cryst.*, 1973, A29, 183-191), but space group symmetry with three-, four- and six-fold axes may also be used to reduce the computational load.

We have developed a package of FORTRAN routines for one-dimensional FFTs for all odd number sample sizes from 11 to 99 and all even number sample sizes from 20 to 200 that have no prime factors larger than 17. The package also includes transforms from real sequences to Hermitian sequences and from Hermitian sequences to real sequences, as well as between sequences that have translational conjugate symmetry and sequences that have alternating Hermitian symmetry and Hermitian antisymmetry. These routines are utilized by transform routines for a set of space groups that contain more than 80% of reported protein crystals.

PS-02.08.09 STATISTICAL ANALYSIS AND REACTION PATHWAYS OF MOLECULES. By K.Huml*, F.Soldán and W.Hummel. Institute of Macromolecular Chemistry, Academy of Sciences of the Czech Republic, Heyrovského nám.2, 162 06 Praha 6, Czech Republic

A hypothesis concerning possible minimum energy conformations and conformational interconversions can be supported by statistical analysis of similar molecular fragments, potential energy, calculation, topology and other methods (Bürgi H.-B. and Dunitz J.D., *Acc.Chem.Res.*, 1983, 16, 153-161; Mezey P.G. *Potential Energy Hypersurfaces*, Amsterdam: Elsevier, 1987). Molecular symmetry of a fragment under study gives additional limiting conditions (Frei H., Bauder A. and Günthard H.H., *Top.Curr.Chem.*, 1979, 81, 1-97). It is believed that properly chosen model of a static and/or dynamic behaviour of the molecular fragment leads to a good mutual agreement among results reached by the methods mentioned above. Potential energy minima correspond to chemical entities which represent the most frequently occurring conformations (molecular templates). On the other hand, sporadically scattered conformations bridging stable conformations map the probable reaction pathways during the conformational interconversions.

1,2-dihydroxybenzene (catechol) and 1,2-dimethoxybenzene molecules were exploited to elucidate the procedure. Structural information was retrieved from the Cambridge Structural Database and two-dimensional potential energy maps were calculated using the molecular mechanics method.

PS-02.08.10 SHELXL-92 A NEW LEAST-SQUARES REFINEMENT PROGRAM FOR USE WITH SINGLE CRYSTAL DIFFRACTION DATA

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SHELXL-92 is a FORTRAN-77 program for the refinement of crystal structures from X-ray or neutron diffraction data, and is primarily designed for single crystal data from small structures (1-1000 unique atoms) at atomic resolution. It is intended to be easy to install and use on a wide variety of computers, and replaces the structure-refining part of SHELX-76.

SHELXL-92 is general and efficient for all space groups in all settings and there are no arbitrary limits to the size of problems which can be handled, except for the total memory available to the program. All instructions are in machine independent free format, with extensive use of default settings to minimize the amount of input required from the user. Instructions and data are taken from two standard (ASCII) text files, so that input files can easily be transferred between different computers. SHELXL-92 is a PUBLIC DOMAIN program; it is provided in source form, also as a precompiled version which has been optimized for Pc's. There are no restrictions on its use or distribution anywhere in the world for non-commercial purposes.

The program produces all the information required for efficient development of a complete structural model from a partially correct one derived using separate direct or vector methods programs such as SHELXS86. It contains many options for fully automatic handling of constraints on positional and thermal parameters and for placement of hydrogen atoms. Structural models can also be restrained to conform with chemically reasonable expectations for interatomic distances and thermal displacement parameters. These similarity restraints can be particularly useful in refinements of macromolecular structure. The atom designation rules, which accommodate standard practices, help minimize the instructions required to invoke constraints and restraints. All tables necessary for electronic mail submission to both *Acta Cryst. (C)* and the CSD are provided in CIF format and a companion program CIFTAB can produce hard copy in formats suitable for other journals.

PS-02.08.11 'CRYSTALS' in control

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