

Product Information

TEXSAN™ STRUCTURE SOLUTION PACKAGE

The TEXSAN™ crystallographic software package contains the most comprehensive set of programs now available for use in the analysis of single crystal X-ray data. The TEXSAN™ philosophy is simple: the power of a crystallographic algorithm is directly proportional to its ease of use. The initial design goal was to develop a menu-driven user interface that would not only allow parameters to be easily modified but would lead to user through the logical flow of a crystal structure analysis. This saves the experienced crystallographer valuable research time and gives the novice a framework on which to build crystallographic skills.

Data Processing

The program PROCESS performs initial data manipulation. When coupled to a RIGAKU AFC diffractometer, this program can be automatically run at the end of data collection. PROCESS performs many calculations associated with the reflection file and can lead directly to a structure solution.

- reduction of raw intensity data
- parity class, Wilson and N(Z) analyses
- automatic space group selection
- analysis of standard reflections
- analysis of equivalent reflections
- empirical absorption correction
- automatic structure solution

Structure Solution and Expansion

The TEXSAN™ Structure Solution Library supports the most comprehensive set of programs presently available. It was developed with the philosophy that the user should be provided with as many solution tools as possible.

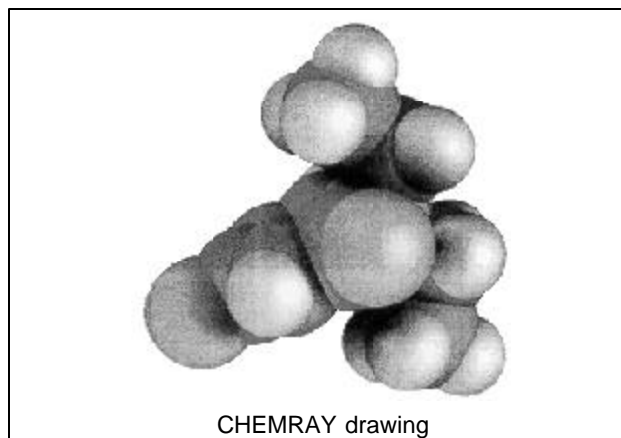
- MITHRIL—ab initio direct methods suite which includes MULTAN, YZARC, MAGEX, active use of quartets and quintets, RANTAN, etc.
- DIRDIF—difference direct methods and phase expansion; orientation/translation functions for known fragments
- PHASE—automatic Patterson deconvolution

- SIR—ab initio direct methods utilizing the semi-invariant representation theory
- SAPI—ab initio direct methods with an emphasis on pseudo-symmetry problems
- Sim—weighted and unweighted Fourier calculations
- high—level software interface with SHELXS, PATSEE, and SAYTAN (MULTAN87) packages

Structure Refinement

The standard method of refinement utilizes the technique of full matrix or block diagonal least squares. For the initial stages of refinement or for crystals that are limited in observed data, there is also the option of a Fourier refinement.

- full matrix or block diagonal matrix -accelerated full matrix refinement
- rigid body refinement utilizing a data base of stored fragments
- automatic analysis of E_{obs} versus F_{calc} during refinement
- convergence check
- matrix damping and/or individual parameter damping
- automatic Fourier calculation and distance and angle calculation following least squares



Modeling

ATOMED is a fully interactive atom-manipulation program for constructing the model that describes the crystal structure.

- graphics mode for building and viewing structures
- idealized hydrogen atom generation
- menu-driven parameter constraints
- facility for constraining atomic and group populations

Reflection Manipulation

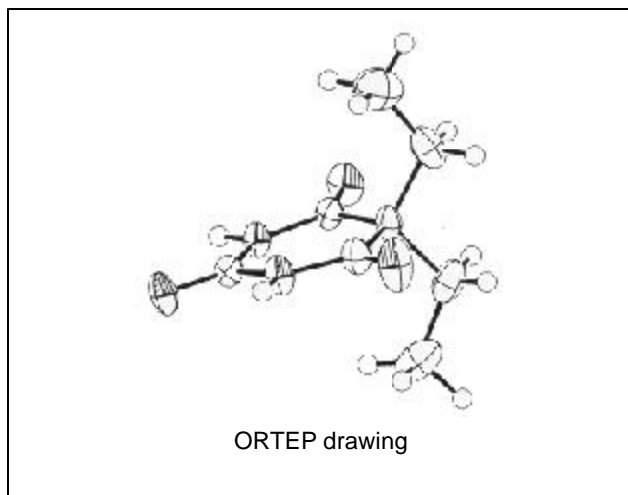
HKL is an interactive program for manipulation and modification of the reflection file. This one program contains all of the functions necessary for the user to apply corrections, remove reflections, or obtain listings.

- Ψ scan, DIFABS, numerical and analytical absorption corrections
- fifth-order polynomial decay correction
- averaging and redundant reflection flagging
- reflection removal and addition
- transformation of reflection indices, cell constants and atomic coordinates
- reflection listing and alternate file generation

Lab Management

Utilities are available to aid in the management of an X-ray laboratory.

- current status utility for monitoring projects
- data base utility for structural parameter storage



Graphics

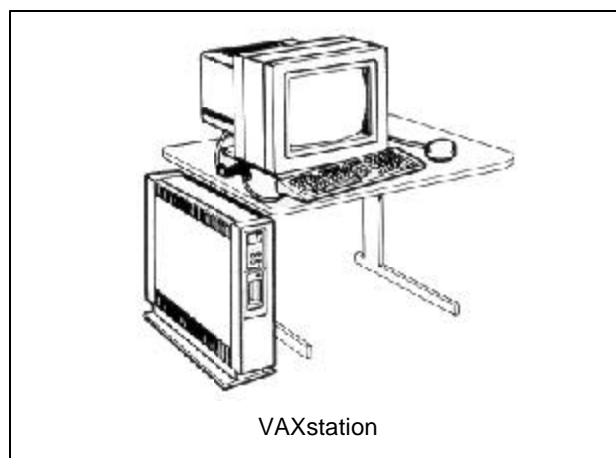
At any stage of the analysis, the user can view the structure using either a graphics terminal or a hard-copy graphics device.

- menu-driven and interactive PLUTO presentation
- menu-driven and interactive ORTEP presentation
- high-resolution CHEMRAY ray-casting presentation
- TEXSAN™ GED graphics editor for mouse manipulation of graphics images
- laser printer and workstation support of graphics

Structure Completion

When a structure has been completed, the program FINISH is used to perform all of the tasks that are normally carried out at the end of a structure analysis.

- calculation of distances, angles and planes with estimated standard deviations along with publication quality tables
- generation of tables of coordinates, thermal parameters and structure amplitudes
- report generation
- calculation of drill coordinates for model construction
- table-editing utility



Hardware Requirements

The TEXSAN™ package runs on any VAX*, MicroVAX*, or VAXstation* computer. TEXSAN™ is the only crystallographic package that utilizes the powerful VAXstation windowing and graphics facilities in a highly integrated fashion. Various other graphics devices are supported, including Tektronix terminals, Hewlett-Packard pen plotters, and DEC laser printers, as well as PostScript language laser printers.

Future Development

TEXSAN™ has been developed at MSC, the world's leading commercial single crystal X-ray laboratory. The staff of MSC is constantly expanding TEXSAN™ to incorporate the latest advances in small molecule crystallography. Currently, a macromolecular software package (BIOTEX™) is being developed which will interface to TEXSAN

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For particulars of the above, please address your inquiry to: MSC or RIGAKU CORPORATION