

## Product Information

# teXsan for Windows

## Structure Analysis Software

### 1. Introduction

**teXsan for Windows** is a complete single crystal structure analysis software package. It includes all of the tools required to reduce raw data, solve and expand the structure, perform least squares refinement, tabulate the results and present them in a variety of formats. It also contains several graphics programs and a toolkit of crystallographic utilities to facilitate structure development and analysis of the results. The suite of programs is encapsulated in a modern graphical user interface and represents the next stage in the evolution of teXsan from its original VMS roots via the more recent Motif-based UNIX version. It retains the philosophy of design and functionality of its predecessor and extends the

usefulness of the package by supporting the current generation of low-cost, high-performance personal computers.

Modern data collection techniques, e.g. CCD and IP area detectors, and automatic data collection software, have led to the development of high-throughput crystallography for small molecule analysis. The amount of data generated in an up-to-date X-ray laboratory can far exceed the capacity of a single crystallographer. While high-throughput crystallography dramatically reduces the time it takes to determine a crystal structure, it can easily saturate the computing facility of a typical laboratory. **teXsan for Windows** was developed to address the needs of these labs. It operates under Windows 95 or Windows

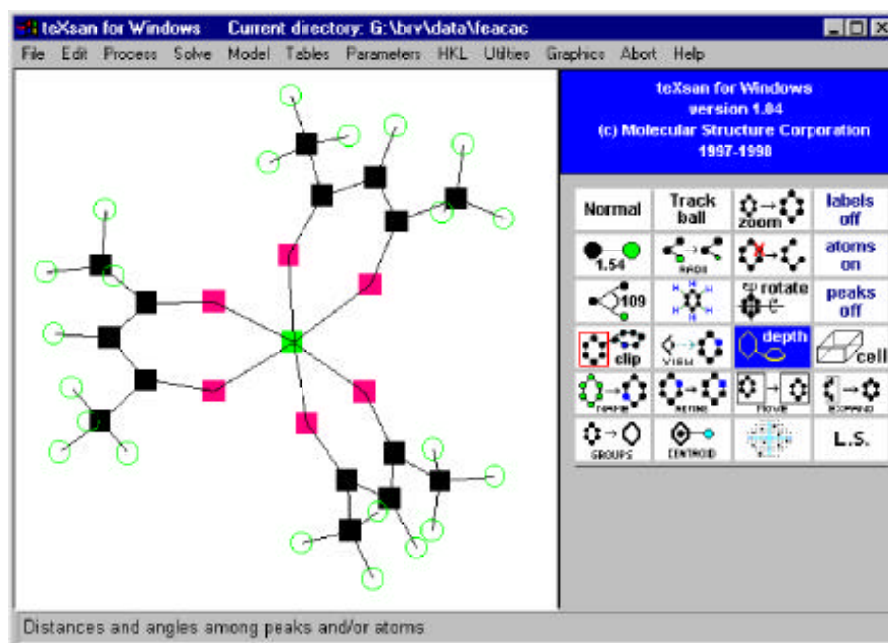


Fig. 1. The teXsan for Windows interface.

NT<sup>1</sup>, two current operating systems for personal computers. This allows a busy laboratory to operate a large number of low-priced, high-performance personal computers utilizing a true native 32-bit operating system. In addition, operating the program in the Windows environment allows the user to run teXsan concurrently with other popular programs (word processors, for instance) and can make use of the Windows clipboard for pasting text and graphical results from teXsan into documents.

Perhaps the most important characteristic of software for a crystallography laboratory running at full capacity is that it is easy to learn for the novice. Analyzing a large number of structures normally requires that students become proficient crystallographers. If the structure analysis software is hard to use, students will become frustrated, discouraged, and will make mistakes. **teXsan for Windows** has been developed with both the student and the seasoned crystallographer in mind. Menus have been designed from a usability engineering standpoint and the package is well-documented through the use of context-sensitive help, a feature which was an integral part of the design process, not an afterthought.

## 2. Features

The main interface of **teXsan for Windows** contains a graphics window for viewing models and electron density maps, a set of tools for model building and manipulation, as well as a menu bar with pull-down menus organized in the sequence in which a typical structure analysis is performed. A toolbar for easy access to frequently used procedures is also provided.

From data processing to structure solution, modeling, refinement, and finally to tabulation and reporting of results, **teXsan for Windows** is organized to lead the user step-by-step through the structure analysis procedure. Programs and utilities have been provided with a logical set of default parameters so that, in many cases, no action is required by the user beyond selecting the process to run.

In addition to the Windows standard menus (File, Edit, Help), the following options are available:

### (1) Process

**teXsan for Windows** accepts data from numerous sources, including diffractometers, CCD and imaging plate area detectors. Program dimensions have been increased from earlier versions to allow for large area detector data sets. The PROCESS module reduces raw intensities or converts data processed by other software into standard internal format. This program also analyzes the intensities for decay, calculates psi-scan transmission factors, automatically selects a space group and tabulates agreement of

<sup>1</sup> Windows is a trademark of Microsoft Corporation.

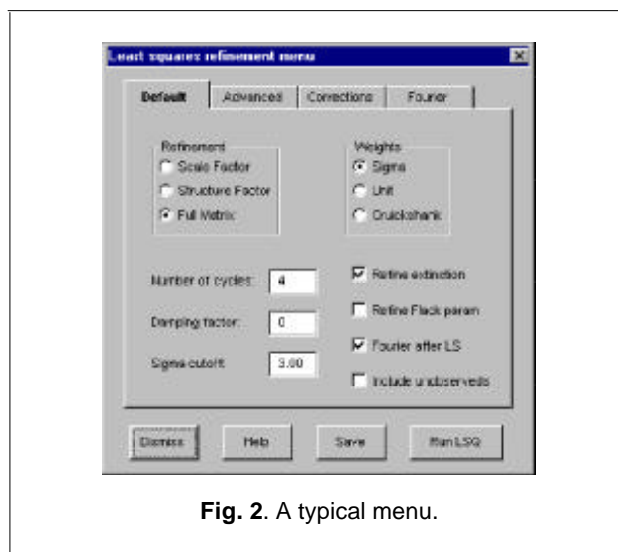


Fig. 2. A typical menu.

any equivalent data. Statistical information about intensity distributions is provided so that alternate space group choices may be explored.

### (2) Solve

**teXsan for Windows** supports a number of ab initio direct methods programs, including SIR, SAPI, SAYTAN<sup>2</sup> and SHELXS<sup>3</sup>, thus giving the user a large set of tools with which to tackle tough structures. Each package can be run in default mode, where the minimal required instruction set is created by the interface, in hard mode, where a more sophisticated input file is created automatically, tailored to the particular multisolution program, or individual parameters can be modified using the interface menus. Other supported structure solution methods include molecular replacement (orientation and translation functions), automated Patterson deconvolution (both using the DIRDIF package) and automated or manual partial structure expansion, using DIRDIF and SIR algorithms.

### (3) Model

The crystal model is developed using a sophisticated interactive graphical tool chest, where peaks are interpreted and assigned, geometry information is displayed, refinement characteristics are modified and the structure is manipulated in real time. The refinement utilities of **teXsan for Windows** have been expanded to include all of the important functions necessary for problem structures in addition to well-behaved structures. These options include: weighted geometry restraints, rigid body constraints, riding hydrogen atoms, TLS analysis, a Flack parameter, and normal matrix analysis to identify nearly singular matrices. Refinement may be performed

<sup>2</sup> SAYTAN (MULTAN88) is an optional direct methods program requiring an additional license fee.

<sup>3</sup> SHELXS and SHELXL must be obtained directly from their author, Prof. George Sheldrick.

against  $F$  or  $F^2$ . Alternately, the popular SHELXL<sup>2</sup> refinement package (1993 or 1997 versions) can be interfaced to **teXsan for Windows**.

## (4) Tables

A structure report, complete with experimental details and tabulated results, can be easily generated in a number of different formats, including Rich Text Format, which allows the document to be imported directly into many word processing packages. Full read/write support for the Crystallographic Information File (CIF) is provided so that the results of the analysis can be transmitted electronically in a standardized format. Tables of all geometric information, including bond lengths, bond angles, torsion angles, non-bonded contacts, hydrogen bonding and least squares planes, may be prepared as standard text files or included in the full report.

## (5) Parameters

Crystallographic parameters (cell dimensions, space group, formula, etc.) may be viewed or modified via a set of menus. Many of these menus provide the user access to additional information via on-line databases, alleviating the need to be surrounded by numerous reference books.

## (6) HKL

A set of tools for viewing the intensity file, selecting or deselecting particular reflections, and applying corrections is provided. Several different absorption correction models are available. Reflections may also be viewed graphically, using an idealized precession photograph routine.

## (7) Utilities

Numerous convenience functions are included to make performing and analyzing crystal structures easier. These include several different methods for determining absolute configuration, TLS analysis (rigid body motion analysis), graphical representation of the least-squares refinement results, a cell reduction program and a powder simulation routine, as well as an easy way of recovering a previous state of the crystallographic model.

## (8) Graphics

With the large number of new structures being presented and published, innovative presentation graphics have become increasingly necessary to highlight important new work. **teXsan for Windows** has graphics capabilities for generating stick models, thermal ellipsoid representations, ray-traced figures and packing diagrams. The interface to ORTEP makes this popular program very easy to use and the implementation of interactive label positioning allows the user to produce figures quickly. A new program, **teXview**<sup>4</sup>, has been developed for generating high-quality molecular renderings in a number of different styles. It also features real-time rotation of thermal ellipsoids. A new Windows version of the popular **Chem-Ray** program is available as an optional graphics program.

## 3) Installation Requirements

**teXsan for Windows** runs under Windows 95 or Windows NT in VGA graphic mode and is supplied on a single CD-ROM. The software requires 25 MB free disk space for a full installation. Memory requirements are the same as for the operating system (typically 16 MB for Windows 95 and 32 MB for Windows NT).

## 4) Performance

Four cycles of full-matrix least-squares refinement of 200 parameters using 1000 reflections takes less than 15 seconds on a Pentium Pro 200 PC running either Windows NT or 95. By comparison, the same refinement takes over 45 seconds on a 180 MHz R5000 Silicon Graphics O2 and more than 70 seconds on a 100 MHz R4400 Silicon Graphics Indigo.

## 5) Licensing

The licensing policy for **teXsan for Windows** has been designed to be cost effective for licensing a large number of PC's at a single site. Licensing is controlled through the use of a Dongle plug on the parallel port of each machine. The price of a second license is 40% of list price and subsequent licenses are charged at a rate of 20% of list price. Further details may be obtained from the author at [brv@msc.com](mailto:brv@msc.com).

---

<sup>4</sup> **teXview** is a trademark of Molecular Images.