

Commercial Announcements

CELLS Calculated Electron Lattice Structures

For users of the Intellect 200 System, CELLS is an iterative FORTRAN application package providing the crystallographer with a method of producing electron microscope images from a postulated central lattice structure for comparison of these images with images obtained from the microscope.

CELLS contains all necessary software components to do an on-line investigation of an unknown material by: 1) plotting the projected structure ... 2) modifying coordinates with graphics cursor ... 3) plotting a theoretical diffraction pattern with the spots scaled to calculated intensities ... 4) calculating Fourier coefficients of the projected potential and diffracted beams for a variable stacking sequence multi-slice calculation and ... 5) displaying theoretical micrograph.

Micro Consultants Ltd., Kenley Lane, Kenley, Surrey CR2 5YR England Tel 01-668-4151

ChemLibrary for Egg Users

ChemLibrary, provided by Elsevier Scientific Software, is a database containing chemical structures (organic, inorganic, biochemical) such as cycloalkanes, amino acids and sugars, which may easily be incorporated into working text.

ChemLibrary also provides many common structure skeletons which may be edited to include hetero atoms or functional groups. With ChemLibrary the Egg users may create customized structures to be added to a library of prebuilt structures.

Elsevier Scientific Software
Attn: K. Foley
POB 330 A.H. Amsterdam
The Netherlands
Tel (020) 5862828

Elsevier Scientific Software
3-28-1 Yushima, Bunkyo-ku
Tokyo 11, Japan
Tel (3) 8360810

Elsevier Scientific Software
(JIC) Atten: J. Tagler
52 Vanderbilt Ave.,
New York, N.Y. 10017 U.S.A.
(Tel) 212 916-1250

Chem Text Chemist's Personal Software Series

Designed for the IBM personal computer standard, Chem Text integrates text with chemical structures, reaction diagrams, equations, flowsheet or other images. With Chem Text the user "draws" images with a mouse; there is no sequence that need be followed and images are not constructed from fixed elements. Chem Text software provides the "chemistry" needed to assemble a molecular or a reaction sequence: atoms, bonds, stereochemical bonds, isotopes, charge and valence. Chemical templates may be used to help generate clear accurate drawings. Previously created images may be modified and graphics from other programs may be imported.

Molecular Design Ltd.
2132 Farallon Drive
San Leandro, California
U.S.A. 94577
Tel 415 895-1313

Molecular Design MDL AG
Wallstrasse 8
CH-4002 Basel, Switzerland
Tel 41/61/232929

The Clearinghouse A Program Catalog for Digital Users

A forum for instructional computing information, "The Clearinghouse" is a catalog which includes software descriptions, tools and utilities. Terminal based software descriptions range from biology, medicine, physics, mathematics and language instruction to statistics and teacher education. Over 100 programs are described.

Iowa State University

ISU Mail Center

Attention: The Computation Center

104 Atanasoff Hall

Ames, Iowa 50010-9907 U.S.A.

Tel 515 294-0323 (Note: A description of your software interest is requested) Bitnet GMBLM@ISUMVS

EQUIS Environmental Quality Information Software (for the smaller laboratory)

A microcomputer based Environmental Quality Information Software, EQUIS, is a complete data management system for the regulatory environment where demonstration of acceptable quality levels (e.g., for drinking water, sewage, waste disposal) is required.

EQUIS provides 1) Sample and data tracing ... This function logs in samples with indication of tests to be done, notation of current status and analysis ... data tracing associates analytical results with each logged in sample ... 2) Method quality control ... allows definition of QC samples to be analyzed concurrently with unknown samples ... allows monitoring of QC sample data (e.g. method sensitivity, linear range) ... 3) Reporting ... this provides for summarization of all discrete data in the Laboratory.

The Perkin Elmer Corporation

Attention: Mary Anne MacLean

Marketing Specialist

761 Main Ave.,

Norwalk, Connecticut 06859-001 U.S.A.

Tel 203 727-1000

Mathematical Function Library for FORTRAN, ULI

United Laboratories' Mathematical Function Library provides: 1) Extensive coverage of special functions used in the physical sciences ... 2) A detailed description of each function's computational technique ... 3) High accuracy, fully tested material ... 4) User friendly documentation ... 5) Optional FORTRAN source or assembler code profiles.

The Mathematical Library contains over 125 special functions. Most functions have an accuracy exceeding 12 digits; optional fast routines available for selected functions.

John Wiley & Sons

Attn: Joan Coleman

605 3rd Ave.,

New York, N.Y. 10158-1012 U.S.A.

NAG Numerical Algorithms Group Fortran Libraries
NAG provides three Libraries of mathematical and statistical Fortran routines for developing application programs: NAG Fortran Library ... NAG Fortran Workstation Library ... NAG Fortran PC50 Library. Together with the Graphical Supplement to the NAG Fortran Library, these provide immediate access to 764 tested state of the art numerical algorithms implemented on PC's for solving computationally intensive problems.

Each Library is organized into chapters, each devoted to a mathematical or statistical area. NAG Fortran Library contains 688 routines: for linear algebra; differentiation and integration; approximation and optimization; statistics; functions and transforms and utilities. NAG Workstation Library provides 172 routines, covering the principal areas of mathematics and statistics selected from the Fortran Library. NAG PC50 Library includes 50 user level routines from the Fortran Library.

Numerical Algorithms Group
1101 31st St., Suite 100
Downers Grove, Illinois
60515-1263
Tel 312 971-2337

SuperStructure – for Chemical Structure Graphics
SuperStructure allows rapid drawing of chemical structures – from simple to complex, as selected from on screen menus. Modes of operation include ENTRY/EDIT of chemical structures and EDIT of chemical structures transmitted from host. The program supports creation of structures of complex compounds with up to 255 atoms ... charged and isotypically labeled atoms ... screens of pre-drawn common ring systems and acrylic fragments, plus user defined and saved moieties ... all bonds ... translation, rotation, mirroring, deletion and copying of whole molecules moieties and fragments. (Hardware requires use of the Sun Flex Touch Pen*).

SuperStructure comes in two versions:

1) SuperStructure. This version includes communications protocol using standard ASCII characters to transmit structures to and from user's host.

2) SuperStructure/CIS. This is a question only system designed to work with the CIS.

*Registered trademark of Sun Flex Touch Pen.

Fein-Marquart Associates, Inc.,
7215 York Road,
Baltimore, Maryland 21212 U.S.A.
Tel 301 821-5980

Commercial Announcements: CD-ROM

CD-ROM edition: 1987 Registry of Mass Spectral Data
World's largest mass spectral database, available for PC's. More than 123,000 mass spectra. PPM/STIRS search software ... direct access to chemical names and synonyms for all compounds ... displayable source data ... CAS registry numbers.

CD-ROM edition: Kirk-Othmer Encyclopedia of Chemical Technology
Over 1200 articles ... access to all cited and general references ... abstracts for all articles ... searchable index, cross-references to printed edition of the encyclopedia ... all tables fully searchable, displayable. Rapid indexing and retrieval.

CD-ROM edition: Encyclopedia of Polymer Science and Engineering
Contains 19 volumes of articles, together with 100 new topics, including natural and synthetic polymers ... plastics, fibers and elastomers. Plus expanded coverage in CAD/CAM robotics and composites. Rapid indexing and retrieval.

For information on any of the above CD-ROM editions contact the appropriate John Wiley office, as listed in the next column.

John Wiley & Sons
Attn: Joan Coleman
605 3rd Ave.,
New York, N.Y. 10158-1012 U.S.A.

John Wiley & Sons (SEA) Pte. Ltd.
37 Jalan Pemimpin
Block B. #05-04 Union Industrial Bldg.
Singapore 2057
Telephone: 2561147

Jacaranda Wiley Ltd.
G.P.O. Box 859
Brisbane, Queensland 4001
Australia
Telephone: 369-9755

John Wiley & Sons Ltd.
Baffins Lane, Chichester
Sussex PO 19 1UD England
Telephone: (0243) 779777

John Wiley & Sons Canada Ltd.
22 Worcester Road
Rexdale Ontario M9W 1L1, Canada
Telephone: (416) 675-3580