Polygen

CENTRUM
Technical Information Management System

CENTRUM[TM] is a state-of-the-art research automation system specifically designed to manage the production, communication and storage of technical information by scientists, research managers and their support personnel. *CENTRUM* allows an organization to connect existing computing resources, terminals and PC's into a single, integrated technical information management system which can link research teams, departments or multiple research sites, worldwide. Advanced network management and data security mechanisms allow reliable handling and automated archiving of valuable research data.

CENTRUM's powerful interactive scientific document composer - the heart of the *CENTRUM* system - allows researchers to prepare and share typeset quality technical documents including complex scientific graphics, with full access to the underlying data. *CENTRUM's* unique electronic mail facilities allow research documentation, together with accompanying data, to be transmitted and received throughout the network in fully editable form. *CENTRUM's* multi-window screens, accessible through existing character terminals, PC's, or next generation desktop workstations, provide a modern, graphical user interface for a company's entire research computing environment.

CENTRUM comes complete with many powerful scientific applications, including chemical structure construction, numerical analysis, and equation solving, as well as providing interactive interfaces to popular statistical analysis, chemical structure data base and molecular modelling systems. *CENTRUM* offers a full range of traditional office automation applications as well, including "desktop publishing" quality word processing, spreadsheet, drawing and paint packages and document-oriented data management. Personal calendar and system-wide resource scheduling and management facilities are also included.

CENTRUM establishes a new productivity performance standard for technical information management systems by taking full advantage of the value of an organization's existing investment in hardware and software resources. *CENTRUM's* unmatched ease-of-use insures quick and widespread acceptance by both research professionals and support personnel.

CENTRUM's unique open architecture permits the integration of your existing and future software applications and data processing systems into the *CENTRUM* environment, while maintaining a consistent user interface and network access. Full documentation and support services are available to assist application developers and system managers.

Designed for growth, a *CENTRUM* system can be cost-justified for a single project team or expanded on a modular basis to integrate scientific computing and data management resources worldwide in mixed network environments. A full range of application support and service facilities helps assure continued user satisfaction and system up-time. *CENTRUM* represents a complete and cost-effective solution to the problem of producing and communicating scientific data in a modern research organization.

FEATURES AND BENEFITS

CENTRUM can help a single research team, or an entire research department, tie together existing hardware and software resources.

CENTRUM's multi-terminal, multi-host support allows an organization to make more effective use of its existing research computing resources, increasing both professional productivity and return on investment.

- A *CENTRUM* system can be configured, and cost-justified, for an individual research team or an entire research facility - allowing a *CENTRUM* system to start small and grow to meet an expanding organization's needs over time.

- *CENTRUM* 's modular architecture and network capability permits new users, departments and sites to be added incrementally, using existing system resources.

- System management, training and support requirements are reduced and made simpler by using the standard *CENTRUM* applications environment on all hardware.

- *CENTRUM* allows centralization of systems and network management duties through its on-line registry of users, access privileges, computing and peripheral resources.

CENTRUM combines complex graphics and text to produce "intelligent" research documentation.

In a *CENTRUM* document, the research data and pictures on a page are dynamically linked to the software programs that produced the data - allowing the information content of a document to be interactively searched, analyzed and updated over time.

- *CENTRUM's* simple-to-use document composer allows researchers to prepare typeset quality literature - integrating scientific text, complex graphics and research data on-screen.

- *CENTRUM* documents accept data and graphical input from a wide variety of scientific and business application software packages.

- Using *CENTRUM,* state-of-the-art graphics-based technical document processing resources can be cost-effectively distributed throughout the research organization, permitting efficient shared use of specialized peripherals and hardcopy output devices.
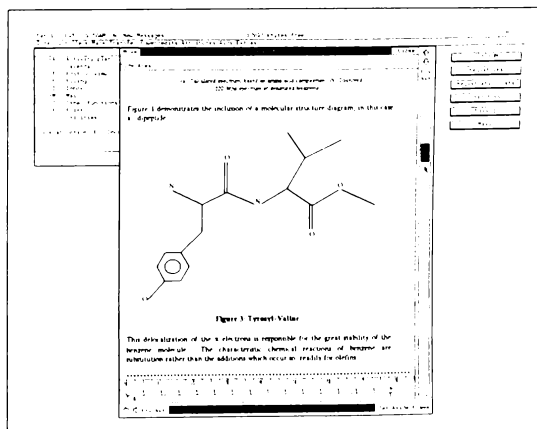

A CENTRUM document containing both text and graphics - in this case a chemical structure diagram. By pointing at the structure and clicking a mouse, a CENTRUM workstation user obtains access to a chemical structure editor or other modelling programs.

CENTRUM provides a standard, graphics-based, user interface for computing activities throughout the research organization.

CENTRUM's modern, multi-window interface employs icons and menus to provide easy-to-use, point-and-click access to documents, software applications, and research data located throughout the company.

- *CENTRUM* allows researchers to find and use software programs and data bases throughout the research computing environment without learning complicated operating system commands, file names, complex directory structures or computer procedures.

- Using *CENTRUM*, the data, software and related computing resources used to produce a document are accessible just by pointing and clicking at the desired object in the document.

- With *CENTRUM*, scientists, technical staff and administrative support personnel alike can concentrate on the content of their work, freed from many of the burdensome but important details connected with research computing and document production tasks.
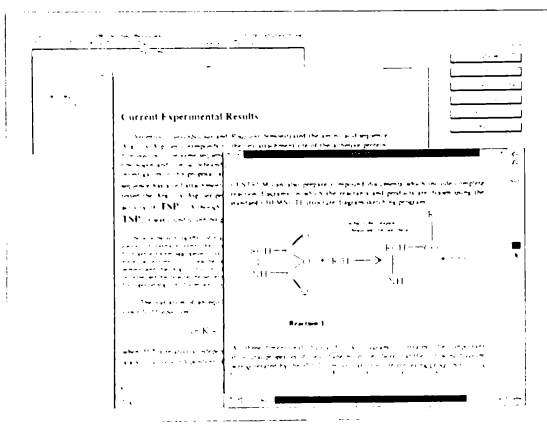
CENTRUM's multi-window user-interface permits many documents to be open at the same time, enabling users to switch rapidly between multiple documents. Electronic annotations and comments can be added for emphasis without altering underlying information.

CENTRUM links researchers, research sites and research data across the company - across the world.

CENTRUM provides a full featured document-based electronic mail facility, which can efficiently transfer graphical *CENTRUM* documents - together with their underlying data content - between *CENTRUM* users over E-mail networks, throughout the company.
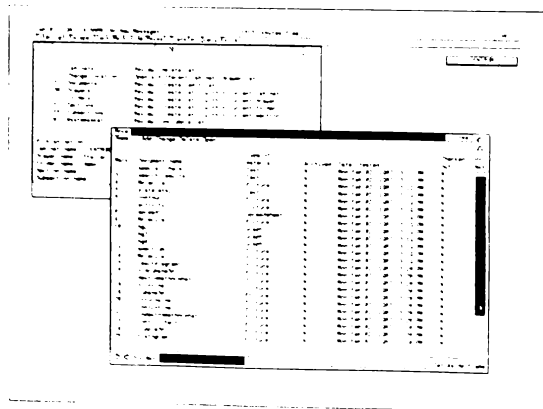
- Using *CENTRUM*, a single electronic mail transfer quickly moves a document made up of text, graphics - and its underlying data - to one or more recipients across the company or around the world, with no need to know details of network operation or complicated addressing schemes.

- All the data in a *CENTRUM* document is dynamically linked to the software used to produce it. Therefore, an E-Mail recipient or *CENTRUM* user opening a document from a shared file cabinet has full interactive access to the information content in the document - for analysis, for making annotations or comments - all without risk of alteration or damage to the original document.

CENTRUM helps locate the research and technical data needed for more effective scientific work without requiring data base experts or compromising security.

An easy-to-use "file cabinet metaphor" storage system and three-level access protection ensure that *CENTRUM* meets the most demanding document storage, retrieval and data security requirements throughout the research environment.

- *CENTRUM* documents are filed and retrieved system-wide using a familiar file folder, drawer and cabinet concept that facilitates retrieval based on keywords, author, creation date and other content-based criteria.

- The *CENTRUM* librarian function keeps track of documents and document modifications, "check-out" privileges and automatically manages multi-user access to shared documents and version control.

- Three levels of access and data security, utilizing a *CENTRUM* host's operating system, *CENTRUM* access privilege control, and optional data file encryption, assure flexible, system-wide protection and integrity of proprietary research data.

CENTRUM is an open system, designed to incorporate existing software - as well as applications developed or acquired tomorrow.

CENTRUM comes complete with all the documentation and support needed to exchange data with or interface to internally developed or popular third-party software applications and system resources into a *CENTRUM* environment - for even greater productivity savings.

- Fully documented libraries including hundreds of "C" and FORTRAN callable subroutines permit the complete integration of interactive graphics-based applications into *CENTRUM*.

- Import/Export data format translation facility allows transfer of graphical and alphanumeric data between popular software applications and *CENTRUM* documents.

- Communications gateway mechanisms allow a *CENTRUM* network to interconnect with existing network or E-Mail environments while providing common *CENTRUM* interface access.

A list of documents from a folder which are stored in a drawer of a CENTRUM file cabinet.

A range of support and service facilities helps assure continued user satisfaction.

SYSTEMS OVERVIEW

CENTRUM is backed with complete documentation, training and support.

Documentation
CENTRUM "Quick Start" Guide
CENTRUM User's Guide and Tutorial
CENTRUM Training Aids
CENTRUM Administrator's Guide
CENTRUM Application Programmer's Guide

In addition to CENTRUM documentation, two levels of on-line Help are provided; the first for context-specific help with menu commands or options, the second for direct access to on-line documentation.

Training
Both on-site and Polygen-based user training programs are available. Specialized Systems Management and Application Development training programs are also offered on a regular basis.

Support
Pre-installation site planning provides a complete configuration analysis, including a definition of required network and hardware resources. On-Site installation services are provided. Post-installation support includes software maintenance and all system updates, together with hot-line telephone support. Specialized consulting and application development services are also available at cost-effective rates.

CENTRUM is backed with complete Systems Administration and Application Development training programs.

Intelligent Document Processing

At the heart of the CENTRUM system is a sophisticated scientific document composer which allows researchers to create, integrate and edit text, complex graphics, and data to produce "compound documents". CENTRUM's document processor is targeted to the information types most frequently handled by scientists and produces typeset quality compound documents.

A key characteristic of CENTRUM compound documents is that data associated with a picture is automatically placed "behind" that graphic in the document. For example, chemical structure diagrams appearing in CENTRUM documents have atom coordinates, a connectivity table, and stereochemical indicators transparently attached to the diagram. Similarly, data plots have data tables transparently attached. To process data associated with a given picture, a CENTRUM user can simply point at the picture of interest using a mouse, and an appropriate application program will automatically be invoked. For instance, by pointing at a chemical structure diagram a user can invoke a program to search for structurally related compounds in a structure database or a molecular modelling program to perform calculations on the structure.

Data remains "attached" to the pictures in a document when the document is electronically mailed, filed to a disk, or backed up to magnetic tape. Further, if the underlying scientific data changes, the relevant pictures are automatically updated. This feature allows scientists to share research data network-wide, simply by electronically mailing CENTRUM documents containing text, graphical pictures, and underlying scientific data. The recipients of electronically mailed CENTRUM documents can edit or analyze underlying data as conveniently as the document's on-line author. In those situations where it is inappropriate to send underlying data, the sender can mail only textual and pictorial aspects of the documents. Project teams or departments can store data within CENTRUM documents, making it easy to revise reports or perform data analysis many months or even years later.

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CENTRUM's intelligent document processor is a true What-You-See-Is-What-You-Get (WYSIWYG) system - the appearance of the document on the screen matches what will appear in hardcopy form. The document processor contains many features which facilitate typeset quality output including multiple font styles and sizes, full justification, automatic hyphenation, on-screen page breaks, 80,000 word spelling checker (with user-extendable dictionary), on-screen super/subscripts, boldfacing, italics, underscoring, headers and footers. *CENTRUM* also offers additional facilities including full footnote handling, table of contents generation, and index generation.

CENTRUM's document processor incorporates a "format template" facility which fully describes the formatting details of a document. These templates automatically adjust memos, progress reports, or other technical documents according to a predefined format as text is entered. This feature promotes consistency between reports produced by different groups or departments and allows scientists and technical support personnel to concentrate on the substance of the document rather than matters of form.

Information Types

CENTRUM's document composer can incorporate a wide range of scientific information types, including the following:

- Scientific graphs, including XY-plots, polar plots, histograms, bar charts, 3-D function plots, 3-D surface plots, and contour maps
- Chemical structure diagrams
- Three-dimensional molecular models, represented in skeleton, ball-and-stick, or space-filled form
- Reaction diagrams
- Strip charts, generated from UV, IR, or NMR spectroscopy datasets
- Mathematical equations and general formulae
- Spreadsheets or data tables
- Technical illustrations, diagrams, or charts
- Forms, such as those used in entering data for mailing lists or phone directories
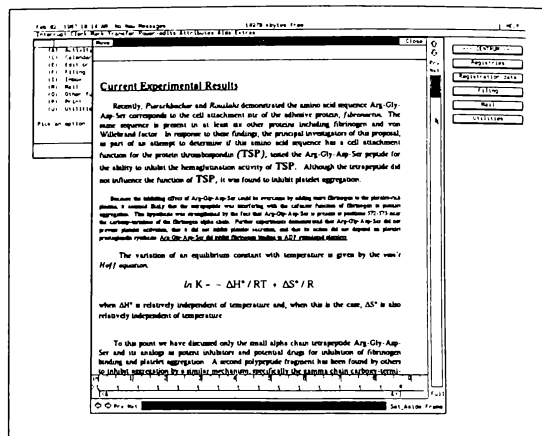
CENTRUM's document processor produces typeset quality output including scientific fonts and full text justification.

CENTRUM's document processor can also incorporate tabular and graphical output from a variety of third-party software packages without special formatting or complicated cut-and-paste procedures. For example, a scientist can use a single *CENTRUM* command to directly absorb the tables and graphs from an interactive RS/1 session and automatically size and position them into a report page. Later, the data can be extracted from the document and resubmitted to RS/1 for further analysis. No cut-and-paste operations or application program file format conversions are required.

CENTRUM's presentation graphics application can be used to add annotations (arrows, boxes, circles, and textual captions) on top of spreadsheets, chemical structure diagrams, scientific graphs or any other graphical pictures in a *CENTRUM* document. This capability is an effective way to add comments, make observations, or highlight a particular part of a picture. Annotations to a document can then be sent along with the original via electronic mail. Because these electronic comments do not disturb the underlying contents of the picture, a clean copy of the document is always available for further editing.
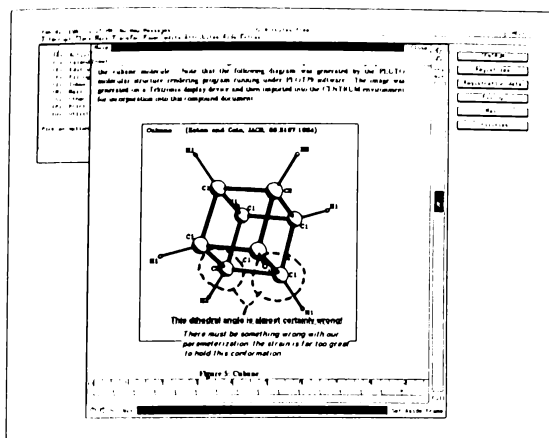
A three-dimensional molecular model and text combined in a CENTRUM document. A molecular mechanics program remains linked to this document allowing users full access to underlying data.

Applications

CENTRUM enables the researcher to access scientific software applications without leaving the document composer. The application programs used to produce the contents of each picture in a document are linked to the document. Pointing at a particular picture on the screen and clicking with a mouse automatically brings up a menu of appropriate application programs which can be used to process the contents of the picture. For example, clicking on a chemical structure diagram can produce a menu which allows a scientist to select from a structure sketching program, a structure viewing program, an annotation editor, and molecular mechanics programs.

A selected application appears in a "pop-up" window which temporarily overlays the user's current document. When the scientist has finished using the application program, a simple point-and-click on the "Close" icon on the window's border informs *CENTRUM* to shut down that application, remove the pop-up window, and return to the document. The picture in the document is automatically updated to reflect any changes that were made to its underlying data. These important features mean that a *CENTRUM* user does

not need to know operating system commands, file names, or directory structures in order to use scientific applications from within *CENTRUM's* document processor.

A large and growing library of integrated application programs is available to process objects placed in *CENTRUM* documents. *CENTRUM* users can also incorporate their own proprietary applications. General facilities include applications for electronic spreadsheets, business graphics, a graphics editor, personal databases, calendar/personal time management, and activity planning/project management. *CENTRUM* also offers many scientific applications for technical document preparation, chemistry specific tasks and remote system access including:

- A molecule editor application which supports 2-D molecular sketching, rapid conversion to 3-D models and interactive 3-D display and manipulation.
- A chemical reaction editor which composes chemical equations and reaction diagrams using scientific fonts and symbols.
- A molecular structure comparison application which superimposes one molecular structure upon another according to a least squares minimization of distances between designated matching "atom pairs".
- A simple-to-use interface to third party applications like RS/1, and popular chemical structure and reaction data bases - allowing data to be directly incorporated into *CENTRUM* documents.
- A scientific graphing application which prepares publication quality scientific plots from data contained in spreadsheets and data tables.
- A linear regression/curve fitting application adept at performing regression and curve fitting operations on discrete datasets contained in data tables.
- A descriptive statistics application which calculates mean, variance, and standard deviation, among others, on discrete datasets contained in data tables.
- Interfaces to various molecular mechanics or molecular orbital applications including QCPE programs such as MM2 and MNDO, as well as Polygen proprietary products such as CHARMm and HYDRA.

• Virtual terminal emulation (VT-100, VT-220, VT-240, Tektronix 4010/4014/4015) with the ability to log-in to remote hosts connected over a network. This capability allows scientists to run interactive sessions with mainframe application programs and databases from within CENTRUM's operating environment.

The graphical output of all these applications, together with the underlying data, can be inserted directly into CENTRUM compound documents.

User Interface

CENTRUM's graphical, multi-window screens combined with a modern icon-based user interface make it easy for scientists with any level of computer experience to enjoy CENTRUM's power and benefits. All CENTRUM applications utilize the same user-interface, eliminating the need to learn a new set of procedures for each program. After logging on, there is typically no need for a CENTRUM user to leave the CENTRUM operating environment during the course of the workday.
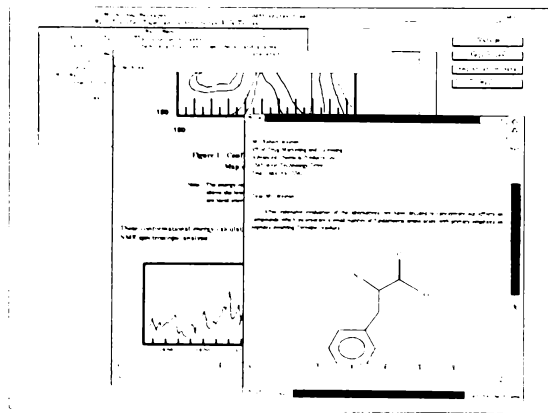
CENTRUM's simple, "desktop metaphor" user interface provides consistancy across many applications. Quick access to application icons, in the upper right corner of the screen, and the main menu, shown in the upper left corner, is always available. Multiple documents and applications can be open on-screen at the same time.

CENTRUM employs a "desktop metaphor" so that the screen looks like a conventional office desk. This is coupled with a multi-windowing facility in which the windows represent pieces of paper on the desktop; they can be moved, resized, and overlapped as needed. Multiple applications can appear and be run on the desktop at one time. An application that is not being used can be reduced to a smaller icon and placed at the side of the desktop, where it remains dormant. Later, recalling the application is as simple as clicking on the icon to return it to its original size.

All operations in CENTRUM are menu-driven. Many of the menu items have keyboard equivalents which by-pass the menus to accomodate more experienced users. On-screen pointing and marking is accomplished using a mouse, although most operations can be performed using keystrokes as well, for added flexibility.

Electronic Mail

CENTRUM's intelligent document processor is completely integrated into a powerful electronic mail system. Without leaving the document processor, a scientist can issue a single command to mail an entire compound document - text, graphics, and underlying data - to any designated user, or users, in the CENTRUM networked environment. There is no need to send multiple mail files, some with text, others with graphics, and still others containing data. A simple mail operation moves all the material over the network as a single document.

Receiving mail is just as easy. An "inbox" is maintained for each CENTRUM user. When a new document arrives, an alert message is displayed on the recipient's CENTRUM screen. Arriving mail can be edited using CENTRUM's document processor, analyzed using underlying data, forwarded to other users, deleted from the "inbox", and/or filed away for later reference.

The sender does not need to know anything about the structure of the network in order to activate CENTRUM's electronic mail capabilities. CENTRUM assists with facilities for organizing the users on the network into manageable units, for example on the basis of department or

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project team. Further, an on-line data base of each department's users, computers and peripherals is maintained. This allows electronic mail to be sent between users - across multiple sites - even around the world - simply by addressing the mail to a given user in a specific department. *CENTRUM* examines the network data bases to determine what computer the recipient is currently working on, and automatically routes mailed documents to the appropriate "inbox" and computer.

CENTRUM's electronic mail system can also be interconnected to third-party mail networks such as that found in DEC's ALL-IN-1 system. Subject to ALL-IN-1 document limitations, *CENTRUM* documents can be mailed to ALL-IN-1 users and ALL-IN-1 documents can be mailed to *CENTRUM* users. In addition, *CENTRUM* users can electronically mail documents over an existing ALL-IN-1 mail network to other *CENTRUM* users.

appropriate password is supplied; keeping the password secret ensures that unauthorized users will not be able to decrypt sensitive documents.

Organizations can also establish shared file cabinets, where multiple users can keep documents of common interest. Documents can be checked-in and checked-out of the shared cabinet, as in a conventional lending library. A "librarian" program keeps track of which documents are checked out, so that two users cannot simultaneously check out the same document with "write-privilege". Relevant users are automatically notified when a shared document has been revised.

Electronically searching *CENTRUM's* file cabinets based on author, creation date, and/or keywords or other textual information contained in a "header" record allows rapid access to documents of interest.

Document Filing and Security

CENTRUM documents are stored in a hierarchical file system using a "file cabinet metaphor". The cabinets contain drawers, folders, sections, and subsections. Storing *CENTRUM* documents in these cabinets eliminates the need for researchers to deal with specific computer data files and directory structures.

Each *CENTRUM* user is equipped with a "private" file cabinet for personal document storage. No other *CENTRUM* user can see or manipulate the contents of a private cabinet. Document security is assured with a three-level mechanism. At the lowest level, the *CENTRUM* host's operating system provides standard file protection/access rights which prevent unauthorized users from gaining access to private documents at the operating system level. Within *CENTRUM*, the file cabinets are organized in such a way that users cannot utilize menus or commands to see others' private cabinets. At the third level of security, *CENTRUM* documents can be optionally encrypted using a "trapdoor" data encryption algorithm. Encrypted documents can only be accessed if an

CENTRUM's powerful electronic mail system enables users to send documents containing complex graphics and text as well as underlying data, when needed, across multiple sites - even around the world.
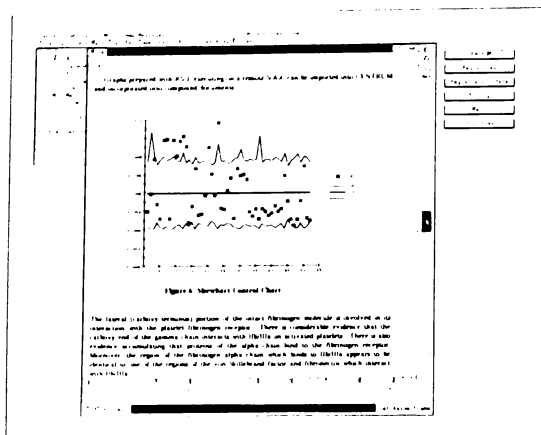
Graphs and tables produced with RS/1 on a remote VAX host, can be input easily into CENTRUM and included in a compound document. Data can also be exported from CENTRUM into RS/1 for further analysis.
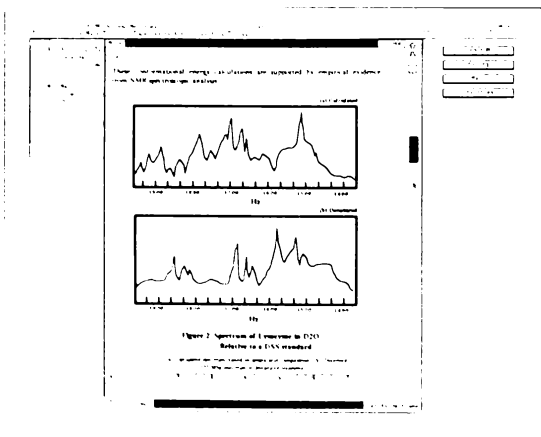
Data acquired from laboratory instruments, such as Nuclear Magnetic Resonance (NMR) spectroscopic data shown here, can also be easily input into CENTRUM and included in CENTRUM documents.

Import/Export of External Data Files

CENTRUM can import data from, and export data to, a variety of popular external systems. These might include chemical structures and reactions from structure and synthetic database systems running on a remote or local VAX host. Data can also be imported from or exported to RS/1 tables and graphs, DEC ALL-IN-1 documents and spreadsheets, Lotus 1-2-3 spreadsheets, as well as ASCII files. CENTRUM's applications can then process this data and/or include the results in a compound document. For example, data acquired from laboratory instrumentation can be written to intermediate files, transported to a CENTRUM host computer and then imported into the CENTRUM system for inclusion in documents or for processing by a data analysis application. New chemical structures can be constructed using CENTRUM's Molecule Editor, placed into compound documents, and then automatically added to a remote chemical structure database.

Open Architecture/Extensibility

Designed to accomodate future growth, CENTRUM provides an open architecture for customers to add their own applications to the system. By following straightforward, well documented procedures, customers can integrate existing and future applications into CENTRUM. To assist in this activity, Polygen makes available linkable object libraries which customers can combine with their own applications to enable the applications to perform input/ouput in a CENTRUM-compatible manner. These libraries contain several hundred "C" and FORTRAN callable subroutines whose calling parameters are fully documented. In addition, great flexibility exists for defining the data structures of new document objects according to customer requirements so that new types can be added as needed.

CENTRUM functions both as an integrated technical information management system and as an attractive development environment for the effective integration of a company's hardware and software resources - now and in the future.

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CENTRUM SYSTEM CONFIGURATIONS

CENTRUM is available on a wide variety of hardware, from PC's and workstations to superminicomputers. *CENTRUM* runs on DEC VAX computers and workstations, personal computers and DEC VTxxx series terminals. *CENTRUM's* advanced networking facilities allow research teams, departments, or multiple research sites to conveniently share data between many types of hardware. Figures 1 through 3 illustrate typical *CENTRUM* hardware configurations.

On a workstation, such as the DEC VAXstation 2000, *CENTRUM* takes full advantage of the workstation's high-resolution bit-mapped display, large memory capacity, fast central processor, built-in Ethernet communications hardware, and mouse pointing device. *CENTRUM* provides an icon-based user interface, powerful networking and E-Mail services, and high quality, fully formatted, scientific document composition facilities.

CENTRUM can also operate on popular personal computers such as IBM PC/XT's, PC/AT's, or DEC VAXmates which have been equipped with a high-resolution display and connected to a VAX-based *CENTRUM* server. *CENTRUM* uses the same graphical user-interface on the PC's as it does on more powerful workstations. Multiple PC's can be connected to a single *CENTRUM* server computer; the PC's perform all graphics operations locally, while the server executes all non-graphics *CENTRUM* operations for the PC's. The server computer can be a VAX superminicomputer, such as VAX 7xx or 8xxx series, or desktop VAX workstations.

CENTRUM also supports alphanumeric terminals, such as DEC VT-100's, VT-220's, and graphics terminals like DEC VT-240's, connected over RS-232C serial lines to a *CENTRUM* server. *CENTRUM's* user interface on character-only terminals is similar to that available on the PC's and desktop workstations.

CENTRUM supports a wide variety of hard copy output devices including laser and dot matrix printers as well as HPGL-compatible plotters. Full support is provided for all leading laser printer page description languages such as Adobe's *PostScript*, Imagen's imPRESS, and Hewlett Packard's PCL.
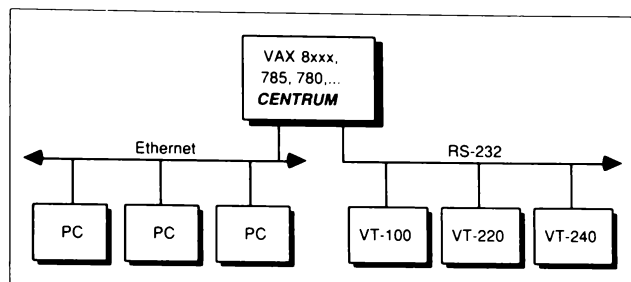

Figure 1. A typical centralized configuration: a large central timesharing CENTRUM server supporting many PC and terminal users.
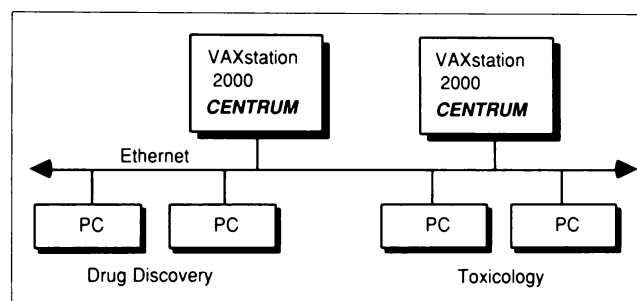

Figure 2. A typical distributed configuration: users are divided into groups; each is supported by CENTRUM server workstations.
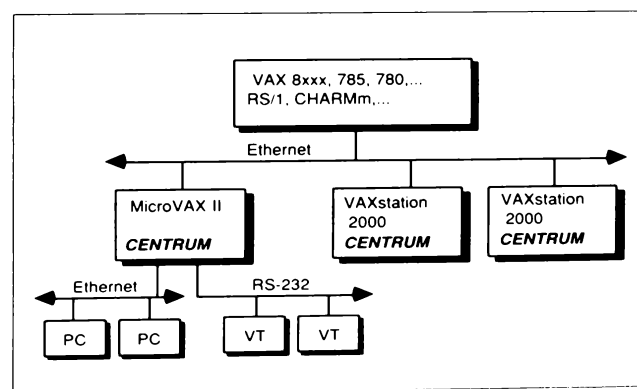

Figure 3. A typical hybrid configuration: a CENTRUM server supports a group of PC's and terminals while CENTRUM workstations are directly linked to the network. The central VAX superminicomputer provides all users with access to statistical and modelling applications via the CENTRUM network.

CENTRUM

Polygen Corporation, operating in the USA, Europe, and Japan, is a leading supplier of molecular modelling, simulation, and technical information management systems for the pharmaceutical and chemical industries.

Polygen