# The *Accord* Component Software Approach

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Received June 26, 1996[⊗]

*Accord* is a new, object-oriented chemistry software architecture. It promotes an evolutionary, component-based approach to delivering chemical software solutions. The *Accord* approach shifts the emphasis away from closed, proprietary systems toward an open, solution-centered model. For end-users this means more consistency across applications, lower training and support costs, and the ability to utilize *Accord's* chemical capabilities where and when required. *Accord* offers users the best of both worlds: the chemical sophistication of *Accord* combined seamlessly with the generality and power of mainstream products from the likes of Microsoft, Oracle, and Netscape.

## INTRODUCTION

In 1992 Synopsys initiated a project to develop a new software architecture that would form the cornerstone of its future chemical information products. This project was centered around one vision: Component-based software solutions would be the shape of things to come. Today, catalyzed by emerging integration standards, such as CORBA,[1] OLE,[2] and OpenDoc,[3] and the adoption of Web technologies, such as Java,[4] component-based solutions are increasingly being used by the chemical research community.

The name *Accord* (harmony; agreement) was chosen for the product range derived from this research project to emphasize the desire to complement software from horizontal system vendors, providing value-added chemical capabilities where and when required. The *Accord* architecture embraces the opportunities offered by emerging open, object-oriented environments and integration standards.[5] This enables users to use industry-standard software tools and delivery environments to build chemical software solutions based on *Accord*.

In early 1994, Synopsys released its first mainstream product that utilized the *Accord* chemical software architecture: *Accord* for Microsoft Excel.[6] This product was developed in association with a number of major chemical companies that recognized their need for a chemical spreadsheet environment to provide visualization, manipulation, and chemically-aware data analysis capabilities. Today, thousands of chemists worldwide use *Accord* for Excel on Mac and PC to transform raw chemical data into useful information. Synopsys has recently announced[7] a collaboration with Chemical Abstracts Service to allow chemical data accessed from SciFinder to be transferred to *Accord* for Excel for further chemical spreadsheet analysis.

"Chemical-awareness" is the key to the *Accord* approach. A container application[8] that has been *Accord*-enabled is able to perform chemically-meaningful operations on *Accord* chemistry objects, such as molecules, reactions, or substituents. *Accord* chemical objects are active and are not simply static pictures. Users can perform chemical calculations, search by substructure, sort by similarity, etc. directly within their software package of choice. Active chemical content is the key and is at the center of the *Accord* approach.

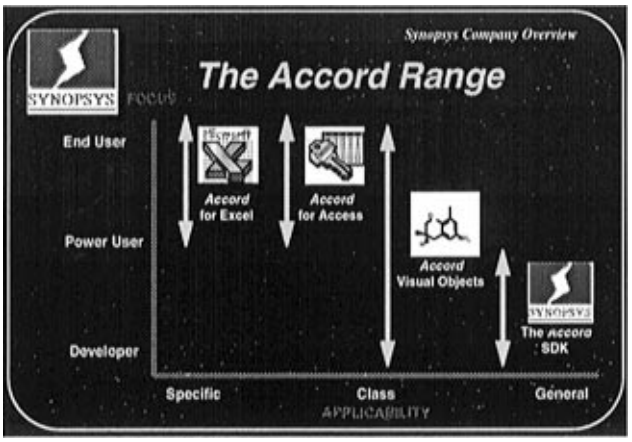


**Figure 1.**

During 1994, Synopsys provided in-house developers with access to the underlying *Accord* Application Programming Interface (API), with the release of the *Accord* Software Development Kit (SDK) on Mac and PC. Building on the success of *Accord* for Excel and the *Accord* SDK, Synopsys introduced two new *Accord*-based products in 1995: *Accord* for Microsoft Access and the *Accord* Visual Objects suite. *Accord* for Access is a fast, multiuser, chemical, relational database system. *Accord* Visual Objects brings chemical capabilities to drag-and-drop rapid application development (RAD) environments, such as Visual Basic, Delphi, and PowerBuilder.

Figure 1 shows the applicability and range of each of the products in the *Accord* desktop range. The *Accord* SDK is a developer tool which transparently integrates with most good container applications. Similarly, *Accord* Visual Objects are easy to use, programmable components with their own properties, methods, and events. *Accord* for Excel and *Accord* for Access are both add-ins designed for use within specific container applications, providing chemical spreadsheet and chemical database facilities, respectively.

## TECHNICAL APPROACH

The *Accord* architecture is open and component based. *Accord* is designed to be scalable, re-entrant, and platform independent. The software environment into which *Accord*

[⊗] Abstract published in *Advance ACS Abstracts,* January 1, 1997.

S0095-2338(96)00083-2 CCC: $14.00 

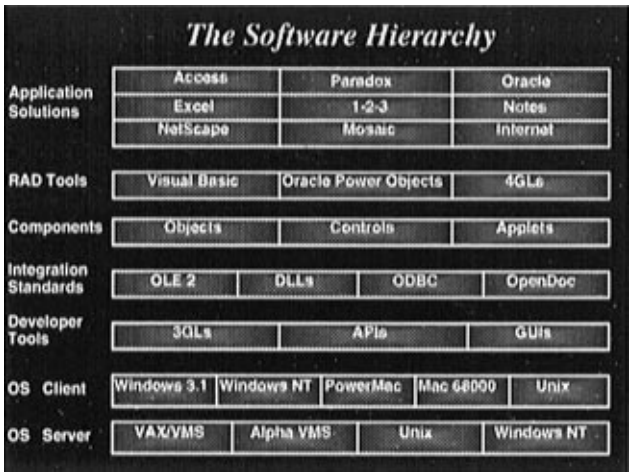


**Figure 2.**

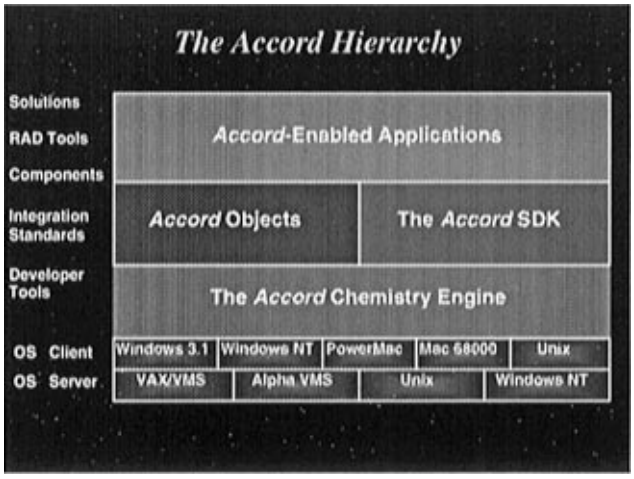


**Figure 3.**

fits is shown in Figure 2. At the bottom of the hierarchy are the basic operating systems and, at each subsequent level, specific technologies and standards become relevant and deployment choices have to be made.

## THE *ACCORD* CHEMISTRY ENGINE

At the heart of the system is the *Accord* Chemistry Engine. This is the cornerstone of all *Accord*-based products and provides the chemical processing framework of the system. On top of the *Accord* Engine are layered the *Accord* SDK, *Accord* Visual Objects, and specific add-in applications, such as *Accord* for Excel. Figure 3 overlays the *Accord* product range on the software hierarchy shown in Figure 2.

Because the *Accord* Chemistry Engine is based on an up-to-date software design there are no inherent constraints on physical storage or memory usage. For instance, there are no limits on the size of molecules, reactions, or chemical databases. Similarly, its implementation is scalable and open, allowing the software to be easily ported and utilized, as appropriate, to handle the chemical information processing and storage needs of users on their platform of choice.

All *Accord*-enabled applications are based on the same core *Accord* Chemistry Engine. This means that new chemical representation enhancements, such as support for reactions, new calculations, and format converters are inherited by all *Accord*-enabled products and solutions. The strong object-oriented design of *Accord* also ensures that new features are assimilated into the production systems with minimum perturbation to existing applications.

## *ACCORD* CHEMISTRY OBJECTS

Central to the *Accord* architecture are *Accord* Chemistry Objects. An *Accord*-enabled application solution instantiates and utilizes these objects programmatically via calls to the *Accord* API. *Accord* Objects have properties that describe them and methods that can be used to manipulate them. For example, a method could be invoked to cut the contents of a Chemistry Object to the clipboard or an application could display a molecule's molecular weight property.

## OLE 2 SUPPORT

*Accord* Visual Objects provide a higher-level OLE automation interface to the *Accord* Chemistry Object and additional support for event handling. *Accord* Visual Objects can be included in any OLE-enabled container application. Within Visual Basic, the *Accord* VBX provides a rich set of chemical properties, methods, and events. Similarly, the *Accord* ActiveX Control can be used within a growing number of 32-bit visual development environments. *Accord* Visual Objects can be linked to other "data aware" controls to manipulate and store chemistry in a variety of database repositories, including Oracle and Access.

The *Accord* Chemistry Viewer is an applet designed to allow in-plane visualization and manipulation of chemistry in container applications. A version of the *Accord* Chemistry Viewer is available free on the Internet to view chemistry stored in WWW pages or as MIME[9] attachments to e-mail documents. The full commercial version of the *Accord* Chemistry Viewer supports chemically-aware cut and paste to chemical editors, such as ChemDraw and ISIS/Draw, and is OLE-enabled.

## *ACCORD* CHEMICAL DATABASES

*Accord* provides a native database persistence model for storing, indexing, and retrieving chemical objects. *Accord* chemical databases provide fast, efficient mechanisms for searching by exact, substructure, or chemical similarity.

The underlying database or file system used must conform to the *Accord* chemical database gateway specification and new database drivers can be defined without change to the core *Accord* Chemistry Engine. New database drivers can be added as required, which allows almost any industry-standard RDBMS or file system to act as a repository for *Accord* Chemistry Objects. Similarly, custom database drivers can be written that are optimized for specific delivery environments, such as CD-ROM.

*Accord* chemical databases can be accessed directly from the *Accord* API or via SQL using the *Accord* ODBC driver. This means users can utilize *Accord's* chemical database capabilities from within any environment that can call the *Accord* SDK or that can act as an ODBC client. For example, from within Visual Basic either chemical database access mechanism can be utilized.

Because *Accord's* chemical database capability is based on proven relational database technology, chemical searching is fast and reliable. Using up-to-date chemical indexing mechanisms, *Accord* performs substructure searches in

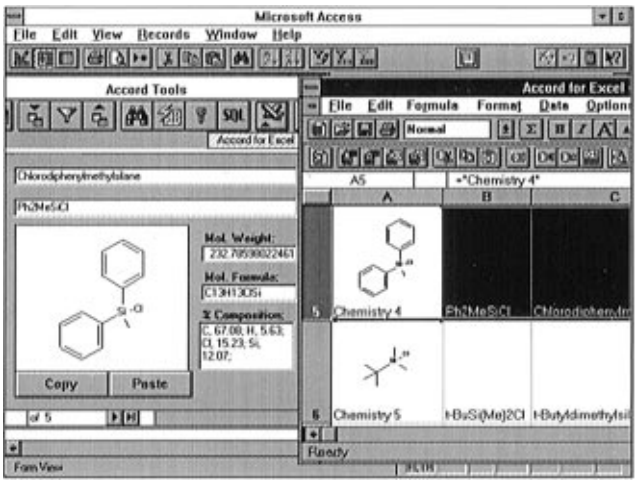


**Figure 4.**

seconds on a standard desktop PC. Because the chemical searching is supported via SQL, chemical query terms can be easily combined with numeric and text queries.

## *ACCORD* ADD-INS

Generally, an *Accord*-enabled application is written in the macro or scripting language of a container application. It may be necessary to write certain functions in C/C++ for performance reasons, and these functions may also make calls to the *Accord* API. This means that the bulk of the software development can be done via simple point-and-click operations with code modules being developed for more complex tasks.

An *Accord* application may be configured as an "add-in", which means the user can easily activate the *Accord* application using the GUI tools provided by the container applications. *Accord* for Access and *Accord* for Excel are both add-ins, providing chemical database and chemical spreadsheet capabilities, respectively. Figure 4 shows how hit sets can be transferred from *Accord* for Access to *Accord* for Excel for further spreadsheet analysis.

## FUTURE DIRECTIONS

*Accord* forms the cornerstone of Synopsys' future chemical information strategy. Development of *Accord* is currently focused in the following areas:

- Advanced Chemical Representation Issues
- Additional Platform and 32-Bit Support
- Distributed Processing and Upsizing

## CONCLUSION

*Accord* is a set of chemically-aware software components, based around a common vision. *Accord* provides chemically-aware depiction, searching, calculation, and data manipulation facilities within industry-standard container applications, such as Access, Excel, Netscape, Oracle, and Visual Basic. The *Accord* approach is fully consistent with the shift toward open, component software solutions catalyzed by the Internet, OLE, and OpenDoc.

Basing a chemical information solution on *Accord* puts the user in control. Developers can make the software choices that best suit their application, using *Accord* chemistry components where and when required. The *Accord* architecture is open, modular, and scalable to meet the chemical information processing needs of users. Synopsys is currently extending *Accord* to support a wider range of chemical entities, such as organometallics, and to migrate the software architecture to additional client and server platforms.

## REFERENCES AND NOTES

(1) For more information on the Common Object Request Broker Architecture (CORBA) contact Object Management Group, Inc. Framingham Corporate Center, 492 Old Connecticut Path, Framingham, MA 01701, U.S.A.
(2) OLE 2 Programmer's Reference, Microsoft Press, 1994.
(3) For more details on the OpenDoc specification contact Apple Computer, Inc. (http://www.apple.com/).
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(5) Hagadone, T. R. Capturing Chemical Structure Information on a Relational Database System: The Chemical Software Component Approach. *J. Chem. Inf. Comput. Sci.* **1995**, *35*, 879−884.
(6) Hopkinson, G. A. Desktop Chemical Data Analysis: Meeting the Needs of Discovery Scientists. Proceedings of the 1994 International Chemical Information Conference, Annecy, France, 1994; pp 129−134.
(7) For more information visit the Synopsys World-Wide Web Site at http://www.synopsys.co.uk/.
(8) A container application is the host environment for an object. Container applications provide persistent storage for the object, an environment for display and user interaction.
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CI960083W