

OMNIC Software: Macro Programming and Dynamic Data Exchange

Key Words

- Dynamic Data Exchange
- FT-IR Software
- Macros Programming
- Macros\Basic
- Macros\Pro
- OMNIC

Introduction

For many laboratories running routine experiments, it is imperative that the analysis steps be consistent and repeatable. In this environment, the ability to build, store, and execute automated procedures is essential. Users of OMNIC™ Spectroscopy Software Suite from Thermo Electron Corporation can create automated procedures, what we call macros, using the optional OMNIC Macros\Basic™ software or OMNIC Macros\Pro™ software packages.

Thermo's powerful OMNIC software has a graphical, intuitive user interface with pull-down menus and a customizable toolbar that greatly reduces training time. OMNIC software includes the functions necessary to perform infrared analysis, from data collection and spectral processing to file management and report generation.

Macros, external programs, and direct Dynamic Data Exchange (DDE) commands can be added to the OMNIC software interface as toolbar buttons or menu items. When saved as part of the OMNIC software configuration, they are available to the user for routine execution. This provides customized operation with an integrated look and feel, which increases the power and ease of use of the OMNIC software.

OMNIC Macros\Basic Software

A macro is a series of tasks that are joined together to form a complete multi-step experiment. Macros that set system parameters and guide the analyst through an experiment save considerable time and guarantee reproducible results, even when the experiment is performed by different operators.

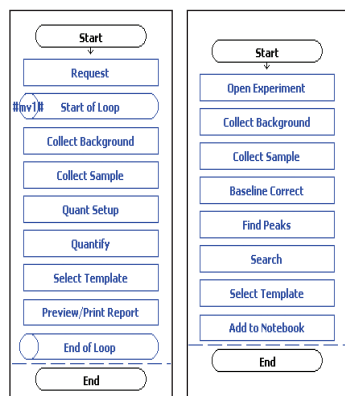


Figure 1: Two example macros written using OMNIC Macros\Basic software. The first macro scans the number of samples input by the user and for each one calculates quantitative results and outputs them in a report. The second macro sets collection parameters, scans the sample, automatically corrects the baseline, searches the result, labels the peak location on the spectrum, then stores the result in a digital laboratory notebook.

OMNIC Macros\Basic software is an intuitive programming tool. It provides a point-and-click graphical interface that allows even a novice to build and execute powerful macros as shown in Figure 1. OMNIC software's

menu commands, data collection, and processing functions can be inserted into the macro to create automated methods that launch at the click of a button. This program runs simultaneously with OMNIC software, so newly created macros can be tested as they are built to assure proper operation.

OMNIC Macros\Pro Software

Occasionally, it is necessary to utilize macro capabilities beyond those available in OMNIC Macros\Basic software. OMNIC Macros\Pro software offers advanced programming solutions, such as complex numerical analysis of spectral information and the creation of unique graphical interfaces for special analytical experiments (as shown in Figure 2).

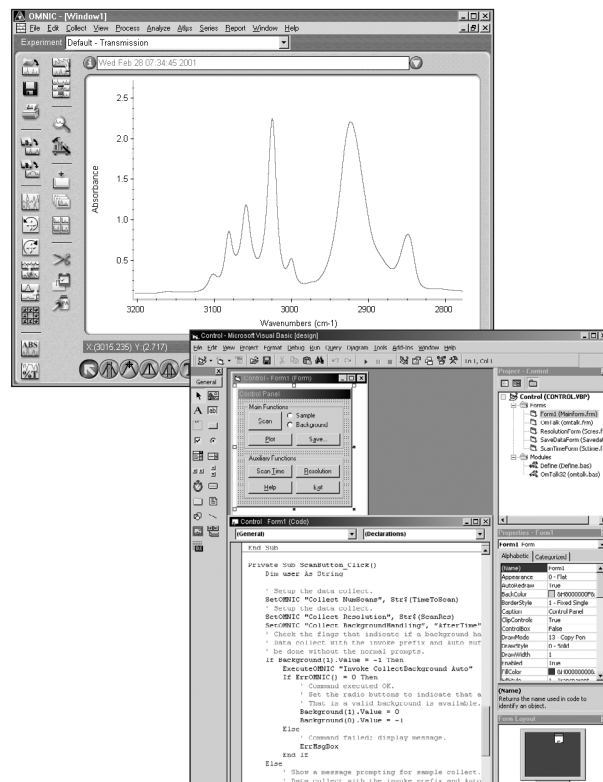


Figure 2: An example macro section using OMNIC Macros\Pro software. This section collects a background and sample, sets the display limits, and then assigns a title to the spectrum.

OMNIC Macros\Pro software features many essential characteristics for a macro development environment with complete access to the OMNIC software parameters and commands. It runs in a multi-tasking mode, is capable of sophisticated numerical data analysis, and provides an intuitive means for developing graphical user interfaces without resorting to the complexities of a standard programming language. OMNIC Macros\Pro software accomplishes this using Microsoft® Visual Basic™ programming language and Dynamic Data Exchange (DDE).

Dynamic Data Exchange

One of the major advantages of the Windows® environment is multi-tasking, where more than one application can be running at the same time. In this environment it is possible for programs to communicate with each other. One program can send data to the other and execute commands in a remote manner. This type of interaction between Windows-based programs is called Dynamic Data Exchange (DDE).

DDE is the form of inter-process communications (IPC) used by Microsoft Windows programs to support the exchange of commands and parameters between two applications. This communication consists of a conversation that is similar to a conversation between two people. A DDE conversation establishes a temporary or permanent link between two Windows applications and acts as a conduit for the exchange of information between the connected applications. The exchanged data can be information that is copied from one application to the other, or commands for the other application to process.

In a DDE conversation, the application initiating the conversation is known as the destination application. The application responding to the conversation is called the source application. This terminology at first may seem backward, but keep in mind that the application that initiates the conversation is usually requesting some information to be sent to it (the destination of the information) by the responding application (the source of the information). An application may be involved in several conversations at the same time.

To initiate a DDE conversation, the destination application sends a message to the Windows operating system defining the source application that it wants to communicate with and a topic for the conversation. The topic defines the subject of the conversation and usually relates to some unit of source application data. For Microsoft Excel, this is a file with a .XLS or .XLC extension; for Word, a file with a .DOC or .DOT extension; and, for OMNIC software, the extension is .SPA or .SPG.

Windows applications that support DDE "listen" for conversations that refer to them. When a source application receives a request concerning a topic that it recognizes, it responds by starting a conversation. Once the conversation starts, the topic cannot be changed unless the current conversation is ended and a new one is initiated.

During a DDE conversation, the source and destination applications can exchange information in a bi-directional manner. Items consist of data or commands that are meaningful to both the source and destination applications. The item can be changed by either the source or the destination during any given conversation.

Not all software programs running in the Windows environment have the ability to interact with other programs through DDE. Special code in the program is required for this sharing of information. Some programs support simple data transfers via DDE while others, such as Excel, offer extensive capabilities. OMNIC software provides an environment that is rich in DDE support, providing for a high level of interaction between it and other DDE supported applications.

Visual Basic & OMNIC Macros\Pro Software Programming

There are many Windows compatible programming environments that can be used with OMNIC software via DDE. High level Windows compatible languages such as Microsoft Visual C++ and JAVA can be used to create advanced macros that will interact with OMNIC software. Thermo has chosen Microsoft Visual Basic as the programming environment to include in the OMNIC Macros\Pro software package. Visual Basic is a straightforward program that allows easy access to OMNIC software through DDE. OMNIC software now also supports the new visual Basic.NET environment.

The OMNIC Macros\Pro software package consists of three distinct parts. The first part is the information about DDE that is needed to set OMNIC software's parameters, issue commands, and retrieve results. This information is presented in the manual section on OMNIC software and DDE. It is very universal and provides all of the information needed to control OMNIC software from Visual Basic or any Windows programming environment, supporting the full range of DDE capabilities. The second part is a copy of Microsoft Visual Basic programming software, which allows the construction of sophisticated graphical user interfaces using point-and-click programming. Numerical analysis is easily coded using an easy-to-learn language whose syntax is based on the original BASIC computer language. The final part of the OMNIC Macros\Pro software package consists of example Visual Basic programs that illustrate powerful macros creations and interact with OMNIC software using DDE. Each macro is thoroughly explained and editable, allowing the creation of new macros by modifying the examples provided.

Assistance in preparing Macros\Pro applications is available in the Help feature of OMNIC software and through the customs solution group. Essentially, OMNIC software represents a fully customizable operating platform integrated with the Windows DDE environment.

In addition to these offices, Thermo Electron Corporation maintains a network of representative organizations throughout the world.

Australia
+61 2 9898 1244
Austria
+43 1 333 50340
Belgium
+32 2 482 30 30
Canada
+1 800 532 4752
China
+86 10 5850 3588
France
+33 1 60 92 48 00
Germany
+49 6103 4080
Italy
+39 02 950 591
Japan
+81 45 453 9100
Netherlands
+31 76 587 98 88
Nordic
+46 8 556 468 00
South Africa
+27 11 570 1840
Spain
+34 91 657 4930
Switzerland
+41 61 48784 00
UK
+44 1442 233555
USA
+1 800 532 4752

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