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FRANK J. SEILER RESEARCH LABORATORY

EPRFIT: An Electron Paramagnetic Resonance Modeling and Analysis Package Version 1.10

JOSEPH A. MENAPACE

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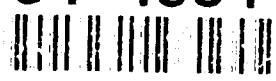
UNITED STATES AIR FORCE



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This report has been reviewed by the Technical Director and is releasable to the National Technical Information Service (NTIS). At NTIS, it will be available to the general public, including foreign nations.

This technical report has been reviewed and is approved for publication.

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EPRFIT is a computerized analysis and modeling package which simulates isotropic EPR spectra. The package performs first and second order spectral simulations of both single configuration species and exchange-broadened species containing up to 7 exchanging configurations. The program simulates spectra composed of up to 2200 individual lines and up to 14 distinct spin species with nuclear spins within the range 0 – 9.5. The various procedures within the program are accessed via a user friendly menu-based package. Data entry is conducted using a spreadsheet architecture which provides the user with easy access to data for inspection and editing. Simulation data, simulated spectra, and experimental/simulated spectrum comparison files can be retrieved and stored onto hard/floppy disk storage in either ASCII or packed formats. ASCII output provides a useful means for linking the data/spectra to other analysis packages as well as for use in printing/plotting routines. The simulated and comparison spectra can also be displayed and analyzed graphically within the program. Spectral analysis options include spectrum offsetting, panning, zooming, and peak position and intensity identification routines. These operations apply to both simulated and comparison spectra. Hardcopies of the simulation results and any combination of spectra can be printed onto Epson compatible dot matrix printers for future reference or presentation.

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EPRFIT

An Electron Paramagnetic Resonance

Modeling and Analysis Package

Version 1.10

Fall 1991

by

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INTRODUCTION

EPRFIT is a computerized analysis and modeling package which simulates isotropic EPR spectra. The package performs first and second order spectral simulations of both single configuration species and exchange-broadened species containing up to 7 exchanging configurations. The program simulates spectra composed of up to 2200 individual lines and up to 14 distinct spin species with nuclear spins within the range 0 - 9.5. The various procedures within the program are accessed via single key sequences built into a user friendly menu-based package. Data entry is conducted using a spreadsheet architecture which provides the user with easy access to data for inspection and editing. Simulation data, simulated spectra, and experimental/simulated spectrum comparison files can be retrieved and stored onto hard and floppy disk storage in either ASCII or packed formats. ASCII output provides a useful means for linking the data/spectra to other analysis packages as well as for use in printing/plotting routines such as those contained in Quattro Pro[1] and SlideWrite Plus[2]. The simulated and comparison spectra can also be displayed and analyzed graphically within the program. Spectral analysis options include spectrum offsetting, panning, zooming, and peak position and intensity identification routines. These operations apply to both simulated and comparison spectra. Hardcopies of the simulation results and any combination of spectra can be printed onto Epson[3] compatible dot matrix printers for future reference or presentation.

SYSTEM REQUIREMENTS

EPRFIT is designed for use on IBM PC-AT[4] and compatible computers operating under MS-DOS[5] 3.21 (PC-DOS[4] 3.10), or later, with at least 512 kBytes RAM. The program requires an EGA or VGA color monitor and display card to operate because of its graphics capabilities. A 360 kByte floppy disk drive minimum is required for basic program usage: at least a 20 MByte hard drive is preferred, but not necessary, to allow for fast user file storage and retrieval. The program should be used on a computer containing an 80287 or 80387 floating-point math co-processor. The hard drive and math co-processor accessories will significantly speed graphics display and spectral computation. At this point, EPRFIT will print results to either 9 or 24 pin Epson[3] compatible dot matrix printers connected to the computer through any of the first three parallel ports or the first four serial communications ports.

TECHNICAL SUPPORT

EPRFIT was written and compiled using TURBO PASCAL[1] Version 5.5. The EPRFIT code contained on the distribution disks is the executable code only. To maintain program integrity, technical support, and upgrade compatibility, the source code will not be disseminated in its entirety. Users interested in the contents of a specific procedure contained in EPRFIT can obtain a copy of the respective procedure source code by contacting the author.

Even though EPRFIT is written to handle most conceivable user and computational errors without crashing, a user may devise, or stumble across, a way to cause program failure. Furthermore, the user may have a need for a particular procedure to manipulate

spectral data, but the procedure is not available. If either of these events occur, technical support is available by contacting the author. From the author's view, the concept of technical support is two-fold. First, it gives the author feedback on program problems. These problems may be severe or subtle, but in any event, can cause the user needless headaches in attempting to use the program. Second, it gives the author the information essential to alleviate the problems. The net result of technical support is program improvement which will make the software usable in a variety of different environments and applications both in the present and in the future. When reporting program problems, write down the error code address generated, if possible. Have this error code, the program steps taken which caused the problem, and data used on hand when discussing the problem with the author. For program improvements, simply contact the author. All program improvements will be considered for implementation.

INSTALLATION

Before installing EPRFIT onto any computer system or using the program, make back-up copies of the distribution disks. Use the original distribution disks as archival media for future situations where EPRFIT must be reinstalled. For example, the original distribution disks should be used to reinstall EPRFIT should the computer media which the program is housed fails or if installing EPRFIT onto another computer system. Consult a DOS manual for the specific procedure to accomplish this task.

Hard Disk Installation

To install EPRFIT onto hard disk media on a computer system, simply create a subdirectory to house the executable code on the hard disk and change to that subdirectory. This is accomplished from the DOS prompt by typing:

MD Program_Subdirectory <Enter>
CD Program_Subdirectory <Enter>

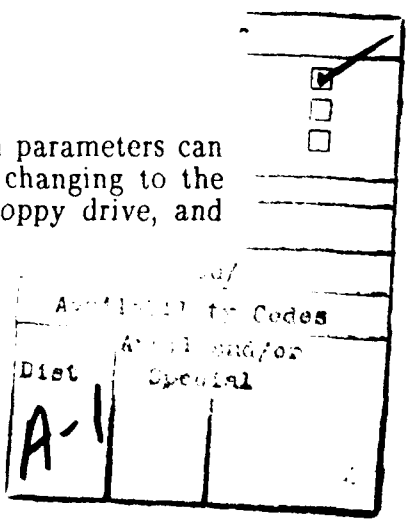
With distribution disk 1 in the A: floppy drive, the executable code is installed from the DOS prompt by typing:

COPY A:*.EXE <Enter>

If desired, subdirectories can be created on the hard disk to house the experimental spectra, simulated spectra, and simulation parameter files which are necessary for modeling and analyses. For example, to create three different subdirectories to house the experimental spectra, simulated spectra, and simulation parameter files, respectively, from the DOS prompt type:

MD Experimental_Subdirectory <Enter>
MD Simulation_Subdirectory <Enter>
MD Parameter_Subdirectory <Enter>

Example files for experimental spectra, simulated spectra, and simulation parameters can be copied to these subdirectories from the DOS prompt, if desired, by changing to the corresponding subdirectories, inserting distribution disk 2 into the A: floppy drive, and typing:



COPY A:*.ARI <Enter>
COPY A:*.ARO <Enter>
COPY A:*.SPR <Enter>

in the experimental spectra subdirectory,

COPY A:*.ASI <Enter>
COPY A:*.ASO <Enter>
COPY A:*.SPS <Enter>

in the simulated spectra subdirectory, and

COPY A:*.PRM <Enter>

in the simulation parameter subdirectory.

Floppy Disk Installation

No special installation is necessary to use EPRFIT on computer systems equipped with floppy disk drives only. To use EPRFIT on a floppy drive computer system, simply use a working disk (copy) containing the EPRFIT.EXE code. Disk changes will be necessary while running the program to accomplish any type of file operation or disk printing. Also, program start-up and file I/O operations are slower when using EPRFIT on these computer systems due to the access speed of the floppy drives.

RUNNING EPRFIT

To run EPRFIT simply type at the DOS prompt:

EPRFIT <Enter>

from the corresponding drive and subdirectory containing the program executable (EPRFIT.EXE) file.

PROGRAM STRUCTURE AND OPERATION

EPRFIT uses a menu-based option architecture to select various operations and routines. The operations and routines are accessed quickly and easily by pressing a single key corresponding to the operation or routine to be used. These keys are highlighted on the computer screen for easy identification.

Main Menu

Upon execution of EPRFIT from the DOS prompt, the **Main Menu** is displayed. This menu is the highest architectural level which directs all major simulation and analysis procedures available in EPRFIT. The **Main Menu** contains eight procedures which can be accessed by pressing the highlighted key corresponding to the procedure to be used. The procedures include:

File Manipulation
Edit / Enter Parameters from Keyboard
Initialize for New Simulation
Compute Simulation
Display Results
Print Results
Spectrum Digital Plot
ESC to Quit

File Manipulation

Pressing **F** from the **Main Menu** accesses the **File Manipulation** procedure. EPRFIT's **File Manipulation** options make it possible to store and retrieve experimental and simulated comparison spectra and simulation parameters from hard or floppy disk storage. The spectrum and parameter files used by EPRFIT are structured with unique file name extensions so that the user does not have to worry about which type of file is being manipulated. The structure also makes an unambiguous identification of file types present on the storage media which is especially useful if large numbers of data files are present. EPRFIT uses seven different file structures with unique extensions. The file structures are:

.ARI – Files with this extension contain the ASCII magnetic field/spectrum intensity values for experimental comparison spectra used for input into EPRFIT in pair format. For example, lines of data contained in these files look like:

```
3500.000  1234.763
3500.001  1234.762
3500.002  1234.735
3500.003  1231.126
    .         .
    .         .
    .         .
```

where 3500.000 and 1234.763, etc., correspond to the magnetic field and intensity values for the experimental comparison spectrum. The files contain no alpha characters and no comma delimiters. This format is selected to allow the program to accept the most generic type of spectral data file possible which is essential for compatibility with various spectrometer/computer systems as well as other data manipulation/ analysis packages. The process needed to generate an ASCII file of this structure type may vary from one spectrometer computer system to another. In general, any type of editor, word processor, or spreadsheet which reads and writes ASCII files can be used to accomplish this task. As an example of how to create such a file from a spectrum housed on a Bruker ESP300[6] spectrometer system, the following steps are used. First, the spectrum values are printed into a file on the ESP300[5] computer system. Next, KERMIT[6] is used to transport the file from the ESP300 computer system into a PC-AT[4]. A spreadsheet program, such as Quattro Pro[1] or Lotus 1-2-3[7] is then used to parse the alpha characters from the file as well as any unwanted spectral intensity values (such as

normalized or unnormalized spectral intensity values). Finally, the resulting set of spectral data pairs is written to an ASCII file with the appropriate file name extension. An ASCII file named TEST1.ARI is included on distribution disk 2 for use as an example on what the *.ARI files should look like.

.SPR – Files with this extension contain the packed representations of experimental comparison spectra contained in the *.ARI files. The data contained in these files is not readable by the user as they are in binary format. These files are used by EPRFIT to quickly and efficiently store and retrieve experimental comparison spectra from disk storage. These files are generated via translation from *.ARI files by the **ASCII Comparison Spectrum** translation procedure to save disk storage space and file manipulation time. Thus, once created, the corresponding *.ARI files can be destroyed as they take up significantly larger disk space and are inefficient for use in spectral data storage and retrieval. An example file of this type named TEST2.SPR is included on distribution disk 2 for use in learning the file manipulation procedures. TEST1.SPR can also be generated from the TEST1.ARI file included by using the **ASCII Comparison Spectrum** translation procedure in read mode.

.ARO – Files with this extension contain the ASCII magnetic field/spectrum intensity values for experimental comparison spectra used for output in pair format. For example, a few lines of data contained in these files look like:

```
3500.000  1234.763
3500.001  1234.762
3500.002  1234.735
3500.003  1231.126
   .         .
   .         .
   .         .
```

where 3500.000 and 1234.763, etc., correspond to the magnetic field and spectral intensity values for the experimental comparison spectrum. The files contain no alpha characters and no comma delimiters. These files are created when *.SPR packed experimental spectrum files are converted to ASCII format. The *.ARO files are generated for subsequent use in other data analysis/manipulation or spectrum presentation packages. An example file of this type can be generated by using the **ASCII Comparison Spectrum** translation procedure in write mode on TEST2.SPR.

.ASI – Files with this extension contain the ASCII magnetic field/spectrum intensity values for simulated comparison spectra used for input into EPRFIT in pair format. The structure of these files is the same as that used for the *.ARI files. This format is selected to allow the program to accept the most generic type of spectral simulation data file possible which is essential for compatibility with various simulation packages as well as other data manipulation/analysis packages. The process needed to generate an ASCII file of this structure type is the same as that used for

*.ARI files. An ASCII file named TEST1.ASI is included on distribution disk 2 for use as an example on what the *.ASI files should look like.

.SPS – Files with this extension contain the packed representations of simulation comparison spectra contained in the *.ASI files. The data contained in these files is not readable by the user as they are in binary format. These files are used by EPRFIT to quickly and efficiently store and retrieve simulation comparison spectra from disk storage. These files are generated via translation from *.ASI files by the **ASCII Simulation Spectrum** procedure to save disk storage space and file manipulation time. Thus, once created, the corresponding *.ASI files can be destroyed as they take up significantly larger disk space and are inefficient for use in date storage and retrieval. An example file of this type named TEST2.SPS is included on distribution disk 2 for use in learning the file manipulation procedures. TEST1.SPS can also be generated from the TEST1.ASI file included by using the **ASCII Simulation Spectrum** translation procedure in read mode.

.ASO – Files with this extension contain the ASCII magnetic field/spectrum intensity values for simulation comparison spectra used for output in pair format. The structure of these files is the same as that used for the *.ASI files. The files contain no alpha characters and no comma delimiters. These files are created when *.SPS packed simulated spectrum files are converted to ASCII format. The *.ASO files are generated for subsequent use in other data analysis/manipulation or spectrum presentation packages. An example file of this type can be generated by using the **ASCII Simulation Spectrum** translation procedure in write mode on TEST2.SPS.

.PRM – Files with this extension contain the parameters used by EPRFIT to perform EPR spectral simulations. The data contained in these files is not readable by the user as they are in binary format. The parameters are entered into EPRFIT using the **Edit / Enter Parameters from Keyboard** procedure. These files are used by EPRFIT to quickly and efficiently store and retrieve simulation parameters from disk storage. An example of this file type named TEST1.PRM is included on distribution disk 2 for use in learning about this file structure type.

The **File Manipulation** screen is set up using spreadsheet and switchboard architectures which gives the user easy access to various manipulation procedures. The **File Manipulation** screen is divided into two areas. The upper area contains the switchboard which selects the **File Manipulation** option to be performed. The lower area contains directory and file cells where the user inputs information regarding the file that is to be manipulated as well as the **Manipulate** file cell which actuates the **File Manipulation** process. The two areas of the screen are accessed by pressing **PgUp** and **PgDn** on the keyboard. Also note that a **Help** screen is present at the bottom of the **File Manipulation** screen. This screen gives the user information on what is occurring, or what is to be input, in the various areas of the screen. Pressing the **Esc** key exits the **File Manipulation** procedure.

Pressing **PgUp** after entering the **File Manipulation** screen allows the user to select the **File Manipulation** option desired. The upper screen area contains seven cells which are

used to select the proper **File Manipulation** option to perform a specific task. The cells are:

Read from Disk

This cell switches the **File Manipulation** into read mode so that a selected file is retrieved from disk storage into EPRFIT.

Write to Disk

This cell switches the **File Manipulation** into write mode so that a selected file is saved from EPRFIT onto disk storage.

ASCII Comparison Spectrum {*.ARI(O)}

This cell translates between *.ARI (*.ARO) and *.SPR files to pack or generate ASCII files for use by EPRFIT and other data analysis/manipulation packages. This cell only allows for structure translation and does not enable file usage by EPRFIT. The *.SPR files used by EPRFIT must be input using the **Packed Comparison Spectrum** procedure in read mode.

Packed Comparison Spectrum {*.SPR}

This cell saves or retrieves packed experimental comparison spectrum files to or from disk storage. This cell must be selected to retrieve or save spectra that EPRFIT uses for comparison with the spectra generated by EPRFIT's **Compute Simulation** procedure.

ASCII Simulation Spectrum {*.ASI(O)}

This cell translates between *.ASI (*.ASO) and *.SPS files to pack or generate ASCII files for use by EPRFIT and other data analysis/manipulation packages. This cell only allows for structure translation and does not enable file usage by EPRFIT. The *.SPS files used by EPRFIT must be input using the **Packed Simulation Spectrum** procedure in read mode.

Packed Simulation Spectrum {*.SPS}

This cell saves or retrieves packed simulation comparison spectrum files to or from disk storage. This cell must be selected to retrieve or save simulated spectra that EPRFIT uses for comparison with the spectra generated by EPRFIT's **Compute Simulation** procedure.

Simulation Parameters {*.PRM}

This cell saves or retrieves simulation parameter files to or from disk storage. These files contain the information which the user inputs into EPRFIT when using the **Edit / Enter Parameters from Keyboard** procedure.

Once in the upper screen area, ↑, ↓, →, ← (arrow keys), **Enter**, **Home**, and **End** change the switchboard connections between their various possibilities. Pressing the arrow keys cause cell changes in the direction of the arrows. Pressing **Enter** has the same effect as

pressing ↓. Pressing **Home** moves directly to the top of the selections. Pressing **End** moves directly to the bottom of the selections. After selection of the appropriate File **Manipulation** option and read/write function, the user must press **PgDn** and make the appropriate directory and file selections in the lower area of the screen.

The lower area of the screen contains three cells that prompt the user on which directory and file are to be manipulated as well as the cell which performs the manipulation. Once in the lower screen area, pressing ↑, ↓, →, ← (arrow keys), **Enter**, **Home**, or **End** selects the appropriate cell for use. The keys operate in the same manner as they do in the upper screen area. These cells are:

Directory

This cell allows the user to input the subdirectory (path) where the file of interest is located, or is to be located, on disk storage. The subdirectory is entered by typing the appropriate full path name, including drive name, for the subdirectory in the same manner as would be used by DOS. For example, to select a file in the EXP subdirectory existing beneath the EPRFIT subdirectory on drive C:, type:

C:\EPRFIT\EXP

Filename

This cell allows the user to input the filename for the file which is to be manipulated. No filename extensions are to be used in this cell as the EPRFIT file structure will take care of the extensions automatically. For example, to manipulate the TEST2.SPR file, simply type:

TEST2

after selecting the appropriate switchboard connections in the upper screen area.

Manipulate File

This cell performs the specific **File Manipulation** option selected. The option is processed by pressing **M** which is highlighted on the screen.

The directory and filename cells contain special keys which activate data editing procedures which make it easy to modify existing entries in the cells. The **Edit** mode is accessed by pressing **End** or **Back Space** while in either of these two cells. In **Edit** mode, **End** and **Home** serve dual purposes. First, they move the cursor to the end or to the beginning of the input line, respectively; and second, if pressed twice, they terminate the **Edit** mode and return to the cell movement functions the keys originally possessed. the arrow keys, → and ← , also serve dual purposes in that they cause right and left cursor movement within the input line until the beginning or end of the line is reached. At this point, further movement in these directions will exit the **Edit** mode and return the keys to their original functions. **Back Space** and **Del** allow characters to be deleted from the input line when in the **Edit** mode. **Back Space** deletes characters to the left of the cursor. **Del** deletes characters to the right of the cursor. Also, **Ins** can be pressed to select between **Insert** and **Overwrite** modes which operate on text at, or to the right, of the cursor.

Edit / Enter Parameters from KeyBoard

Pressing **E** from the **Main Menu** accesses the **Edit / Enter Parameters from KeyBoard** procedure. Parameter entry and editing is accomplished in two screens. The two screens can be alternated by pressing **PgUp** or **PgDn**. ↑, ↓, →, ← (arrow keys), **Enter**, **Home**, and **End** select the appropriate cell in these screens for input/editing. The arrow keys change the cell selects in the directions of the arrows. **Enter** operates in the same manner as the → key. **Home** moves to the top cell on the screen. **End** Moves to the last cell on the screen. The screens are set up using a spreadsheet architecture to allow the user easy access to data for inspection and manipulation. Pertinent information for the simulations is entered directly into the appropriate area on the screens by simply moving the cursor to the cell of interest and typing in the data. EPRFIT allows up to 14 different spin species to be used in the simulations with a maximum of 2200 lines for the radical being modeled. Up to 99 species of each different hyperfine splitting type with nuclear spins ranging from 0 to 9.5 can be entered as long as the total number of lines is less than, or equal to, 2200. The program allows up to 7 different configurations in the simulations to account for intramolecular exchange broadening. First and second order spectral simulations can be accomplished for both single site and exchange-broadened systems. Exchange broadening is modeled using Liouville density matrix theory as implemented by Heinzer.[8] Two types of chemical exchange are implemented in the computation: **Mutual** and **Independent**. **Mutual** exchange assumes that the populations of the different configurations, as well as the exchange rate constants, are equal. **Independent** exchange relaxes the population and rate constant constraints which allows the user the most flexibility possible in the computation.

The first parameter screen contains ten areas which require user input. **Help** corresponding to each of the areas is located in the lower portion of the screen. Pressing **ESC** will return to the **Menu Menu**. The ten areas are:

Number Different Hfs

This cell allows the user to enter the number of unique hyperfine splitting constants that are to be used in the simulation. This number corresponds to the number of spin species in the radical of interest that possess distinct nuclear spins and hyperfine splittings. The number of rows of hyperfine splittings which can be subsequently entered is dictated by this number. The number can be between 1 and 14. The default value is 1.

Number of Configurations

This cell allows the user to enter the number of configurations which contribute to an exchange-broadened spectrum. The number of columns of hyperfine splittings which can be subsequently entered is dictated by this number. The number can be between 1 and 7. The default value is 1 which corresponds to a single site.

Computation Type

This cell selects between **Manual** or **Optimize** computation types. The computation type is selected by pressing the **Space Bar** which toggles between the choices. During a **Manual** computation, the EPR spectrum is simulated using the parameters input by the user. During an **Optimized** computation,

EPRFIT will adjust the parameters entered to obtain a best fit to a comparison spectrum supplied by the user. The default type is **Manual**.

NOTE: EPRFIT Version 1.10 does not implement the **Optimize** computation procedure. EPRFIT Version 2.00 will implement a spectrum fitting routine which optimizes the parameters used in the simulation to an experimental spectrum using the Marquardt Nonlinear Regression Algorithm.[9]

Spectrum Phase

This cell selects between **Plus** and **Minus** spectrum phases for the spectrum to be simulated. The spectrum phase is selected by pressing the **Space Bar** which toggles between the choices. **Plus** spectrum phasing generates a simulated spectrum with initial positive slopes for peaks when going from low to high magnetic field. **Minus** spectrum phasing generates a simulated spectrum with initial negative slopes for peaks when going from low to high magnetic field. The default phase is **Plus**.

Sweep Limit Factor

This cell allows the user to enter the number of linewidths that EPRFIT uses to compute each line in the simulated spectrum. This feature optimizes computation time by cutting off the lineshape algorithm at a point where the line intensity is minimal. Allowed values include linewidths ranging between 1 and 99. The default value is 10 linewidths. The computation time increases with the number of linewidths.

Simulation Order

This cell selects between **First** and **Second** order spectral simulation options. The **Simulation Order** is selected by pressing the **Space Bar** which toggles between the choices. The default **Simulation Order** is **First.**

Title

This cell allows the user to enter the **Title** of the simulation as well as any pertinent information regarding the simulation being conducted. Any alphanumeric character is allowed as input in this cell. The default **Title** is none.

Equiv. Nuc.

This cell area encompasses a 14–row column which allows the user to enter the number of **Equivalent Nuclei** of each unique hyperfine splitting and nuclear nuclear spin type. The number of **Equivalent Nuclei** can range between 0 and 99. The default number is 1.

Nuc. Spin

This cell area encompasses a 14–row column which allows the user to enter the **Nuclear Spin** associated with each spin species. The **Nuclear Spin** can range from 0.0 to 9.5. The default **Nuclear Spin** is 0.0.

Configuration Hyperfine Splitting in Gauss

This cell area encompasses a 14–row by 7–column matrix which allows the user to enter the **Configuration Hyperfine Splittings in Gauss** for the spin species in each configuration contributing to the simulated spectrum. The rows correspond to the spin species and the columns correspond to the configurations. Allowed **Configuration Hyperfine Splittings** range between –9999.9 and 99999.9 Gauss to allow for positive and negative spin polarization on each spin species. The default **Configuration Hyperfine Splitting** is 0.00000.

Pressing **PgUp** or **PgDn** from the first parameter screen accesses the second parameter screen for entering and editing data. The second parameter screen contains ten areas which require user input. **Help** corresponding to each of these areas is located at the lower portion of the screen. Pressing **ESC** returns to the **Main Menu**. The ten areas include:

Exchange Type

This cell selects **Independent** or **Mutual** chemical exchange for the spectrum to be simulated. Access to the **Exchange Type** cell occurs only when the **Number of Configurations** used in the computation is greater than 1. The **Exchange Type** is selected by pressing the **Space Bar** which toggles between the available choices. **Mutual** exchange assumes that the populations of the different configurations as well as the exchange rate constants between the various configurations are equal. **Independent** exchange relaxes the population and exchange rate constant constraints which allows the user the most flexibility possible in the computation. The default **Exchange Type** is **Independent**. Different areas of screen two are accessed depending upon which **Exchange Type** is selected.

Mutual Exchange Rate Constant in Gauss

This cell is accessed only when an exchanged–broadened spectrum is being computed and if the **Exchange Type** is **Mutual**. The cell allows the user to enter the **Mutual Exchange Rate Constant**, in Gauss, for the exchange–broadened spectrum being considered. Possible values for the **Mutual Exchange Rate Constant** range from 0.0000000001 to 9999999999.9 Gauss with a default value of 1.0000000000 Gauss.

Center Field (G)

This cell allows the user to enter the magnetic field value, in Gauss, which corresponds to the **Center Field** for an EPR scan. This value is used to compute the g–value for the radical being simulated as well as the magnetic field scan center used in the graphics display. Allowed **Center Field** values range between 0.000001 and 999999.9 Gauss with a default value of 3389.975 Gauss.

Frequency (GHz)

This cell allows the user to enter the microwave **Frequency**, in GHz, corresponding to that used in an experiment for the **Center Field** used. This value is used to compute the g–value for the radical being simulated. Allowed

values for the microwave **Frequency** range between 0.000001 GHz and 999999.9 GHz with 9.500300 GHz being the default.

Sweep Width (G)

This cell allows the user to enter the **Sweep Width**, in Gauss, for the simulation. If 0.000000 is entered, EPRFIT will automatically compute the required **Sweep Width** which encompasses the entire EPR spectrum. Entering a non-zero **Sweep Width** is useful when comparing the simulated spectrum with an experimental comparison spectrum or a simulated comparison spectrum which possesses a different magnetic field dispersion. Allowed **Sweep Width** values range from 0.000000 to 999999.9 Gauss with a default of 0.000000 Gauss.

Number of Points

This cell allows the user to enter the **Number of Points** to be used to compute the simulated spectrum. Allowed values for the **Number of Points** range from 2 to 2200 points. The default value is 500 points.

Rate Constant Magnification

This cell allows the user to magnify either the **Mutual** or **Independent Exchange Rate Constants** by a constant multiplying factor. This is useful when simultaneous change of all the rate constants in a defined manner is required. Allowed **Rate Constant Magnifications** range between 0.0000000001 and 9999999999.9 with a default value of 1.0000000000. This cell can only be accessed when the **Number of Chemical Configurations** is greater than 1.

Linewidth (G)

This cell area encompasses a 7-column row which allows the user to enter the **Linewidth** associated with a single site or with each chemical configuration contributing to an exchange-broadened EPR spectrum. The **Linewidths** are entered as peak-to-peak separations of the first-derivative EPR spectral features measured in Gauss. The allowed **Linewidths** range from 0.00001 to 99999.9 Gauss. The default **Linewidth** is 1.00000 Gauss.

Population

This cell area encompasses a 7-column row which allows the user to enter the **Population** associated with each chemical configuration contributing to an exchange-broadened EPR spectrum. This cell area is only accessible when **Independent** exchange is considered as the configuration **Populations** are taken to be equal under **Mutual** exchange. Allowed **Populations** range from 0.00001 to 1.00000 with a default value of 1.00000 for single site computations or a default value that depends upon the number of configurations selected by **Mutual** exchange. The **Populations** are normalized to unity after leaving the second parameter screen.

Rate Constants Between Configurations in Gauss

This cell area encompasses a 6-row by 7-column matrix which allows the user

to enter the **Independent** exchange **Rate Constants Between Configurations** contributing to an exchange–broadened EPR spectrum. This area is only accessible when **Independent** exchange is considered. Exchange **Rate Constants** are entered, in Gauss, into the upper triangular portion of this matrix. Allowed **Independent Rate Constants** range between 0.00000001 and 99999999.9 Gauss with the default value of 1.00000000 Gauss.

Cells in the **Edit / Enter Parameters from Keyboard** screens that require any user input besides the **Space Bar** contain special keys which activate data editing procedures. These keys make it easy to modify existing entries in the cells. The **Edit** mode is accessed by pressing **End** or **Back Space** while in any cell requiring user input. In **Edit** mode, **End** and **Home** serve dual purposes. First, they move to the cursor to the end or to the beginning of the input line, respectively. Second, if pressed twice, they terminate the **Edit** mode and return the to cell movement functions that the keys originally possessed. The arrow keys, → and ←, also serve dual purposes in that they cause right and left cursor movement within the input line until the beginning or end of the line is reached. At this point, further movement will exit the **Edit** mode and return the keys to their original functions. **Back Space** and **Del** in **Edit** mode allow characters to be deleted from the input line. **Back Space** deletes characters to the left of the cursor. **Del** deletes characters to the right of the cursor. Also, **Ins** can be pressed to select between **Insert** and **Overwrite** modes which operate on text at, or to the right, of the cursor.

Initialize for New Simulation

Pressing **I** from the **Main Menu** accesses the **Initialize for New Simulation** procedure. The **Initialize for New Simulation** procedure returns EPRFIT to the state present when the program was initially executed from the DOS prompt. All simulation and comparison information resident in computer memory is destroyed during this operation. Thus, EPRFIT will prompt the user to confirm access to the procedure. All data and spectra required for future use must be saved using the **File Manipulation** procedure prior to completing the **Initialization** process. The **Initialization** procedure is useful when the user wants to start a new simulation from scratch and desires a clean workspace.

Compute Simulation

Pressing **C** from the **Main Menu** accesses the **Compute Simulation** procedure. The **Compute Simulation** procedure performs the spectral simulation for EPRFIT based upon the simulation parameters entered. While this procedure is executing, EPRFIT reports computational milestones on a status board thus making it possible to monitor the progress the program is making in simulating a spectrum. As the computation proceeds, each milestone changes color and a progress report of line processing is updated.

Display Results

Pressing **D** from the **Main Menu** accesses the **Display Results** procedure. EPRFIT has the capability to display either the computational results of the simulation or to graphically display the spectra for analysis and comparison. The **Display Results** menu contains two procedures which select either the computational results or the spectral graphics for display. These procedures are accessed by pressing **R** to display the computation results or **S** to graphically view spectra. Pressing **Esc** will return the program to the **Main Menu**.

Results Screen

Pressing **R** from the **Display Results** menu accesses the **Results Screen** procedure. The **Results Screen** displays information pertaining to the simulation type utilized as well as pertinent information about the simulation generated by the computation. The center of the simulated spectrum is reported which is based upon the g-value, scan **Center Field**, and microwave **Frequency** determined from the computation. The largest unnormalized peak height and spectrum width are reported to allow the user to obtain information about the spectral intensity and magnetic field dispersion for comparison with other spectra. The number of lines contained in the simulated spectrum reported correspond to the actual number of lines present based upon the simulation order. This number may, or may not, correspond to the number of observed lines. The T_2 relaxation time is reported for the different configurations based upon the **Linewidths** used. The number of relaxation times reported depends upon the number of configurations used to perform the simulation. The intramolecular **Exchange Rate Constants** are reported in Hz between each configuration if an exchange-broadened spectrum is being modeled. The number and uniqueness of the **Exchange Rate Constants** reported depends upon the **Exchange Type** used, if any, and upon the **Number of Configurations** contributing the exchange-broadened spectrum.

Spectrum Display

Pressing **S** from the **Display Results** menu accesses the **Spectrum Display** procedure. EPRFIT is capable of graphically displaying simulated and comparison spectra on the computer screen. Either a simulated spectrum, comparison spectrum, or both can be displayed. The individual spectra as well as pertinent information pertaining to them are color coded on the graphics display for easy identification. Through unique palette manipulation techniques, individual spectra display changes can be accomplished using a single keystroke. Changes are seen on the screen immediately. Data parsing algorithms select only the data needed for display at the current dispersion settings, so no time is wasted plotting spectra whose resolution is greater than that of the screen. An extensive **Help** menu can be called if the user needs to determine what specific actions are available in various sections of the program. All routines used in the graphics display use real math; thus, the representations possess the accuracy of the experiment, or of the simulation, and not the screen. The user can manipulate individual spectra or both simulated and comparison spectra simultaneously in all analysis routines.

NOTE: EPRFIT Version 2.00 will incorporate algorithms which will enable the user to perform spectrum smoothing, baseline correction, peak peaking, differentiation, integration, addition, and subtraction.

Upon entering the **Spectrum Display** procedure, EPRFIT enters graphics mode and presents the **Main Display**. The upper portion of the display shows the **Title** of the simulation, the spectra, and the magnetic field and intensity dispersions. The simulation spectrum and its pertinent data are colored yellow. The comparison spectrum and its pertinent data are colored blue. In the lower area of the display, the magnetic **Field Increment** and **Intensity Increment** values are shown. These values correspond to the increments EPRFIT is

currently using when any type of spectral manipulation is being conducted. The type of spectrum displayed and the spectrum which is currently selected for manipulation is also presented. **Help** for the available options in this display, as well as all other displays, can be accessed by pressing **H** which is highlighted in the center of the display's lower area. After pressing **H**, the **Help** screen appears in the lower area of the screen display. It is highly recommended that the user activate the **Help** screen until a firm grasp of the various manipulation procedures is attained. Pressing **H** a second time turns the **Help** screen off.

The **Main Display** is the highest architectural level which directs all graphical manipulation and analysis routines available in EPRFIT. The **Main Display** contains eight procedures which can be accessed by pressing the highlighted keys on the **Help** screen which correspond to the procedure to be used. These keys are active even when the **Help** screen is on or off. The **Main Display** procedures are:

OffSet

Pressing **O** from the **Main Display** accesses the **OffSet** procedure. The **OffSet** procedure makes it possible for the user to **OffSet** displayed spectra with respect to one another without changing their respective magnetic field and intensity values. This routine makes it possible to obtain the g-value of a simulated radical by comparing the simulated spectrum to an experimental spectrum. This routine also makes baseline **OffSet** corrections easy: either the simulated spectrum or the comparison spectrum can be **Offset** so that comparisons can be made. The utilization of real math allows the user to **OffSet** the spectra with a high degree of accuracy. **OffSetting** can be done on **Zoomed** and **Panned** spectra. **OffSetting** is easily accomplished by selecting a point in the spectrum with a cross-hair and relocating it to a new position. Small **OffSets** can be accomplished using the arrow keys.

↑, ↓, →, ←, *Home, PgUp, End, PgDn – OffSet Moves*

These keys, which are located on the ten-key pad, **OffSet** selected spectra by the current magnetic **Field** and **Intensity Increment** values. The keys provide for movement in eight compass directions. The arrow key, ↑, **OffSets** the selected spectra up. The arrow key, ↓, **OffSets** the selected spectra down. The arrow key, →, **OffSets** the selected spectra right. The arrow key, ←, **OffSets** the selected spectra left. **Home OffSets** the selected spectra up and left. **PgUp OffSets** the selected spectra up and right. **End OffSets** the selected spectra down and left. **PgDn OffSets** the selected spectra down and right.

–, + – *Adjust Size Increment*

Pressing – decreases the selected magnetic **Field Increment** or **Intensity Increment** by one unit corresponding to the most significant digit in the increment. Pressing + increases the selected magnetic **Field Increment** or **Intensity Increment** by one unit corresponding to the most significant digit in the increment.

Change Line Style

Pressing **C** changes the line style used to display the spectra. The **Change Line Style** procedure selects between **Line Overlay** or **Exclusive Or** to draw the spectra. These two line styles can be used as a guide for the closeness of a fit when both the simulated and experimental spectra are considered. With **Line Overlay**, points of the comparison spectrum coinciding with those of the simulation are erased. With **Exclusive Or**, points of the comparison spectrum coinciding with those of the simulation are set to a different color. This effect is most easily observed if only one of the spectra is visually displayed by selection with the **F1 – Spectra to Display** key.

*/, * – Adjust Size Increment by Decade*

Pressing **/** decreases the selected magnetic **Field Increment** or **Intensity Increment** by one order of magnitude. Pressing * increases the selected magnetic **Field Increment** or **Intensity Increment** by one order of magnitude.

Ctrl[Home] – Reset OffSet

Pressing **Ctrl** and **Home** simultaneously returns the spectral **OffSet** to the position where it is located when the **OffSet** procedure is initially accessed. Any **OffSets** accomplished in prior **OffSet** procedure accesses are conserved.

Ins – Select Cursor OffSet

Pressing **Ins** accesses the **Cursor OffSet** procedure. The **Cursor OffSet** procedure makes it possible for the user to **OffSet** selected spectra by using a cross-hair. In addition to the normal graphics display present in this procedure, a cross-hair appears in the spectrum which can be used to select a point in the spectrum to anchor and to position the **OffSet**. The magnetic field and intensity corresponding to the cross-hair anchor is reported in the lower left area of the display. The magnetic field and intensity for the **OffSet** position is reported in the lower right area of the display. The **OffSet** magnetic field and intensity are reported in the lower center of the display. **OffSets** are accomplished in two steps. First the cross-hair is moved to the point in the spectrum area which is to be **OffSet** (anchor). The position is updated using the **Enter** key. The cross-hair is then moved to the point in the spectrum area where the selected point is to be located. Pressing **Enter** performs the **OffSet**. The anchor cross-hair is colored red and the offset cross-hair is colored green for easy identification.

↑, ↓, →, ←, Home, PgUp, End, PgDn – OffSet Target Moves

These keys, which are located on the ten-key pad, move the cross-hair by the current magnetic **Field Increment** and **Intensity Increment** values. The keys provide for movement in eight compass directions. The arrow key, ↑, moves the cross-hair up. The arrow

key, ↓, moves the cross-hair down. The arrow key, →, moves the cross-hair right. The arrow key, ←, moves the cross-hair left. **Home** moves the cross-hair up and left. **PgUp** moves the cross-hair up and right. **End** moves the cross-hair down and left. **PgDn** moves the cross-hair down and right. All movement in the vertical or horizontal direction stops when the spectrum graph limits are reached.

-, + - Adjust Size Increment

Pressing - decreases the selected magnetic **Field Increment** or **Intensity Increment** by one unit corresponding to the most significant digit in the increment. Pressing + increases the selected magnetic **Field Increment** or **Intensity Increment** by one unit corresponding to the most significant digit in the increment.

Change Line Style

Pressing **C** changes the line style used to display the spectra. The **Change Line Style** procedure selects between **Line Overlay** or **Exclusive Or** to draw the spectra. These two line styles can be used as a guide for the closeness of a fit when both the simulated and experimental spectra are considered. With **Line Overlay**, points of the comparison spectrum coinciding with those of the simulation are erased. With **Exclusive Or**, points of the comparison spectrum coinciding with those of the simulation are set to a different color. This effect is most easily observed if only one of the spectra is visually displayed by selection with the **F1 - Spectra to Display** key.

*/, * - Adjust Size Increment by Decade*

Pressing / decreases the selected magnetic **Field Increment** or **Intensity Increment** by one order of magnitude. Pressing * increases the selected magnetic **Field Increment** or **Intensity Increment** by one order of magnitude.

Ctrl[Home] - Reset OffSet

Pressing **Ctrl** and **Home** simultaneously returns the cross-hair to the position where it is located when the **Cursor Offset** procedure is initially accessed. The cross-hair also returns to the red anchor cross-hair type. Any **OffSets** accomplished in prior **OffSet** procedure accesses are conserved.

Enter - Update Cursor OffSet

Pressing **Enter** can cause two responses. If the anchor cursor is being manipulated, **Enter** selects the current position as the anchor point and retrieves the green **OffSet** cursor. If the **OffSet** cursor is present, pressing **Enter** performs the spectrum **OffSet**.

Del – Select Increment

Pressing **Del** selects between the magnetic **Field Increment** and the **Intensity Increment**. The active increment is highlighted on the screen for easy identification. This procedure is used when the user needs to adjust the increments during an analysis.

Esc – Exit

Pressing **Esc** causes EPRFIT to exit the **Cursor OffSet** procedure and returns to the **OffSet** procedure display. Unfinished **OffSets** are not conducted unless the **Enter** key has been pressed when the green **OffSet** cross-hair is visible to update the process before exiting.

F1 – Spectra to Display

Pressing **F1** selects between the three types of spectra that can be displayed in EPRFIT. The three possibilities include: **Simulation, Experiment,** and **All**. When the **Simulation** spectrum is selected, only the simulated spectrum will appear on the screen (if a computation has been conducted). When the **Experiment** spectrum is selected, only the experimental or simulated comparison spectrum will appear on the screen if the corresponding file was read into the program from the **File Manipulation** procedure. The **All** selection displays both the simulation and comparison spectra. The spectra as well as any information pertinent to them is color coded on the screen for easy identification.

Field Center

Pressing **F** centers the selected spectra in the graphics display. This procedure resets the spectral **OffSets** for selected spectra to zero. This procedure does not affect spectral **Zooms** or **Pans**.

F2 – Spectra to Manipulate

Pressing **F2** selects manipulation of the **Simulated, Experimental**, or **All** spectra. When this key is pressed, any subsequent spectral manipulation procedures will apply to the selected spectrum or spectra. The manipulate spectra area of the screen is updated to show which spectrum manipulation is active so the user can easily identify which spectrum, or spectra, will be affected by subsequent manipulation.

Del – Select Increment

Pressing **Del** selects between the magnetic **Field Increment** and the **Intensity Increment**. The active increment is highlighted on the screen for easy identification. This procedure is used when the user needs to adjust the increments during an analysis.

Esc – Exit

Pressing **Esc** causes EPRFIT to exit the **OffSet** procedure and returns the program to the **Main Display**.

F1 – Spectra to Display

Pressing **F1** selects between the three types of spectra that can be displayed in EPRFIT. The three possibilities include: **Simulation, Experiment,** and **All**. When the **Simulation** spectrum is selected, only the simulated spectrum will appear on the screen (if a computation has been conducted). When the **Experiment** spectrum is selected, only the experimental or simulated comparison spectrum will appear on the screen if the corresponding file was read into the program from the **File Manipulation** procedure. The **All** selection displays both the simulation and comparison spectra. The spectra as well as any information pertinent to them is color coded on the screen for easy identification.

Field Center

Pressing **F** centers the selected spectra in the graphics display. This procedure resets the spectral **OffSets** for selected spectra to zero. This procedure does not affect spectral **Zooms** or **Pans**.

F2 – Spectra to Manipulate

Pressing **F2** selects manipulation of the **Simulated, Experimental**, or **All** spectra. When this key is pressed, any subsequent spectral manipulation procedures will apply to the selected spectrum or spectra. The manipulate spectra area of the screen is updated to show which spectrum manipulation is active so the user can easily identify which spectrum, or spectra, will be affected by subsequent manipulation.

Zoom

Pressing **Z** from the **Main Display** accesses the **Zoom** procedure. The **Zoom** procedure allows the user to **Zoom** in on a selected area of a spectrum. **Zooming** is easily accomplished by framing the desired area using the arrow keys. This routine also makes it possible for the user to adjust the spectral dispersion for either the simulated or comparison spectrum with a single keystroke so that both spectra possess the same dispersion in the magnetic field direction. The real math used in the **Zooming** algorithm gives **Zooming** accuracy limited by the data used and not by the screen resolution. **Zooming** can be conducted in both the field and intensity directions. Individual spectra can be manipulated, or both can be **Zoomed** simultaneously.

In addition to the normal graphics display, a colored frame appears in the spectrum area which is used to select the area of the screen to be **Zoomed**. The active sides of the frame which can be moved are colored red. The inactive frame sides are colored blue. The frame's left and top side magnetic field and intensity values are reported in the left lower area of the display. The frame's right and top side magnetic field and intensity values are reported in the right

lower area of the display. The differences between the right and left side values and the top and bottom sides values is reported in the lower center area. Depending upon the spectra selected for display and the spectra selected for manipulation, these reports may, or, may not, be present. Furthermore, they are colored the same color as the corresponding spectra for easy identification of which spectrum is being operated on.

↑, ↓, →, ←, Home, PgUp, End, PgDn – Adjust Window Size

These keys, which are located on the ten-key pad, allow the active frame sides to be moved. The keys provide for movement in eight compass directions in increments dictated by the magnetic **Field Increment** and **Intensity Increment** values. The arrow key, ↑, moves the active frame sides up. The arrow key, ↓, moves the active frame sides down. The arrow key, →, moves the active frame sides right. The arrow key, ←, moves the active frame sides left. **Home** moves the active frame sides up and left. **PgUp** moves the active frame sides up and right. **End** moves the active frame sides down and left. **PgDn** moves the active frame sides down and right. All movement in the vertical or horizontal direction stops when the spectrum graph limits are reached.

Shift [↑, ↓, →, ←, Home, PgUp, End, PgDn] – Translate Window

These keys, which are located on the ten-key pad, allow concerted movement of both active and inactive frame sides. Access to these key operations is accomplished by pressing **Shift** in combination with the desired key. The keys provide for movement in eight compass directions in increments dictated by the magnetic **Field Increment** and **Intensity Increment** values. **Shift** ↑ moves the frame up. **Shift** ↓ moves the frame down. **Shift** → moves the frame right. **Shift** ← moves the frame left. **Shift Home** moves the frame up and left. **Shift PgUp** moves the frame up and right. **Shift End** moves the frame down and left. **Shift PgDn** moves the frame down and right. All movement on the vertical or horizontal direction stops when the spectrum graph limits are reached.

–, + – Adjust Size Increment

Pressing – decreases the selected magnetic **Field Increment** or **Intensity Increment** by one unit corresponding to the most significant digit in the increment. Pressing + increases the selected magnetic **Field Increment** or **Intensity Increment** by one unit corresponding to the most significant digit in the increment.

Equalize Magnetic Fields

Pressing **E** equalizes the magnetic field dispersion between the simulated and comparison spectra. The magnetic fields are adjusted to the values corresponding to the spectrum with the smallest magnetic field dispersion.

*/, * – Adjust Size Increment by Decade*

Pressing **/** decreases the selected magnetic **Field Increment** or **Intensity**

Increment by one order of magnitude. Pressing * increases the selected magnetic **Field Increment** or **Intensity Increment** by one order of magnitude.

Ctrl[Home] – Reset Window

Pressing **Ctrl** and **Home** simultaneously resets the frame to the position where it is located when the **Zoom** procedure last updated the spectra.

Ins – Select Window Sides

Pressing **Ins** selects which frame sides are to be activated. The active frame sides are colored red and the inactive frame sides are colored blue.

Change Line Style

Pressing **C** changes the line style used to display the spectra. The **Change Line Style** procedure selects between **Line Overlay** or **Exclusive Or** to draw the spectra. These two line styles can be used as a guide for the closeness of a fit when both the simulated and experimental spectra are considered. With **Line Overlay**, points of the comparison spectrum coinciding with those of the simulation are erased. With **Exclusive Or**, points of the comparison spectrum coinciding with those of the simulation are set to a different color. This effect is most easily observed if only one of the spectra is visually displayed by selection with the **F1 – Spectra to Display** key.

Del – Select Increment

Pressing **Del** selects between the magnetic **Field Increment** and the **Intensity Increment**. The active increment is highlighted on the screen for easy identification. This procedure is used when the user needs to adjust the increments during an analysis.

F1 – Spectra to Display

Pressing **F1** selects between the three types of spectra that can be displayed in EPRFIT. The three possibilities include: **Simulation, Experiment,** and **All**. When the **Simulation** spectrum is selected, only the simulated spectrum will appear on the screen (if a computation has been conducted). When the **Experiment** spectrum is selected, only the experimental or simulated comparison spectrum will appear on the screen if the corresponding file was read into the program from the **File Manipulation** procedure. The **All** selection displays both the simulation and comparison spectra. The spectra as well as any information pertinent to them is color coded on the screen for easy identification.

Unzoom

Pressing **U** returns the spectral magnetic field and intensity dispersions to their maximum values for the spectrum selected. This procedure is useful for initializing the **Zoom** display or if a full spectrum display is desired.

Field Center

Pressing **F** centers the selected spectra in the graphics display. This procedure causes the selected spectral scan centers to be placed at the center of the spectrum display area. The process does not affect spectral **OffSets and Pans**.

Esc – Exit

Pressing the **Esc** key causes EPRFIT to exit the **Zoom** procedure and return to the **Main Display**.

Enter – Update

Pressing **Enter** performs the **Zoom** operation. This procedure **Zooms** in on the area selected within the frame and displays that screen area as a full graphics display.

F2 – Spectra to Manipulate

Pressing **F2** selects manipulation of the **Simulated, Experimental**, or **All** spectra. When this key is pressed, any subsequent spectral manipulation procedures will apply to the selected spectrum or spectra. The manipulate spectra area of the screen is updated to show which spectrum manipulation is active so the user can easily identify which spectrum, or spectra, will be affected by subsequent manipulation.

Spectral Analysis

Pressing **S** from the **Main Display** accesses the **Spectral Analysis** procedure. The **Spectral Analysis** procedure makes it possible for the user to accurately measure the peak positions and intensities of either the simulated or experimental spectra graphically. Measurements are conducted using a set of cross-hairs which when placed in a particular spectral area reports the field and intensity for that area. The cross-hairs are operated using the arrow keys. EPRFIT also incorporates a hopping routine which moves the cross-hairs in the field or intensity directions in increments set by the differences between them. This is useful in determining relative peak intensity, in identifying peaks which are associated through hyperfine splitting, and in measuring linewidth variations across spectra.

In addition to the normal graphics display, a set of cross-hairs appear in the spectrum area which can be used to determine peak positions and intensities. The magnetic field and intensity for the left cross-hair center is reported in the left lower area of the display. The magnetic field and the intensity corresponding to the right cross-hair center is reported in the lower right area of the display. The difference between the cross-hair magnetic field positions and intensities is reported in the center lower area of the display. Depending upon the spectra selected for display and the spectra selected for manipulation, these reports may, or may not, be present. Furthermore, they are colored the same color as their corresponding spectrum for easy identification of which spectrum is being operated on. Since the screen has two

cross-hairs, EPRFIT provided for individual movement of each. The active cross-hair which can be moved is colored red. The inactive cross-hair is colored blue.

↑, ↓, →, ←, Home, PgUp, End, PgDn – Cursor Movement

These keys, which are located on the ten-key pad, allow individual cross-hair movement. The keys provide movement in eight compass directions in increments dictated by the magnetic **Field Increment** and **Intensity Increment** values. The arrow key, ↑, moves the active cross-hair up. The arrow key, ↓, moves the active cross-hair down. The arrow key, →, moves the active cross-hair right. The arrow key, ←, moves the active cross-hair left. **Home** moves the active cross-hair up and left. **PgUp** moves the active cross-hair up and right. **End** moves the active cross-hair down and left. **PgDn** moves the active cross-hair down and right. All movement on the vertical or horizontal direction stops when the spectrum graph limits are reached.

Shift [↑, ↓, →, ←, Home, PgUp, End, PgDn] – Translate Cursors

These keys, which are located on the ten-key pad, allow concerted movement of both active and inactive cross-hairs. Access to these key operations is accomplished by pressing **Shift** in combination with the desired key. The keys provide movement in eight compass directions in increments dictated by the magnetic **Field Increment** and **Intensity Increment** values. **Shift** ↑ moves the cross-hairs up. **Shift** ↓ moves the cross-hairs down. **Shift** → moves the cross-hairs right. **Shift** ← moves the cross-hairs left. **Shift Home** moves the cross-hairs up and left. **Shift PgUp** moves the cross-hairs up and right. **Shift End** moves the cross-hairs down and left. **Shift PgDn** moves the cross-hairs down and right. All movement on the vertical or horizontal direction stops when the spectrum graph limits are reached.

–, + – Adjust Size Increment

Pressing – decreases the selected magnetic **Field Increment** or **Intensity Increment** by one unit corresponding to the most significant digit in the increment. Pressing + increases the selected magnetic **Field Increment** or **Intensity Increment** by one unit corresponding to the most significant digit in the increment.

Change Line Style

Pressing **C** changes the line style used to display the spectra. The **Change Line Style** procedure selects between **Line Overlay** or **Exclusive Or** to draw the spectra. These two line styles can be used as a guide for the closeness of a fit when both the simulated and experimental spectra are considered. With **Line Overlay**, points of the comparison spectrum coinciding with those of the simulation are erased. With **Exclusive Or**, points of the comparison spectrum coinciding with those of the simulation are set to a different color. This effect is most easily observed if only one of the

spectra is visually displayed by selection with the **F1 – Spectra to Display** key.

*/, * – Adjust Size Increment by Decade*

Pressing **/** decreases the selected magnetic **Field Increment** or **Intensity Increment** by one order of magnitude. Pressing ***** increases the selected magnetic **Field Increment** or **Intensity Increment** by one order of magnitude.

Ctrl[Home] – Reset Cross-Hairs

Pressing **Ctrl** and **Home** simultaneously resets both cross-hairs to the positions where they are located when the **Spectral Analysis** procedure is initially accessed.

Ins – Select Cross-Hair

Pressing **Ins** selects which cross-hair is to be activated. The active cross-hair is colored red and the inactive cross-hair is colored blue.

Del – Select Increment

Pressing **Del** selects between the **Field Increment** and the **Intensity Increment**. The active increment is highlighted on the screen for easy identification. This procedure is used when the user needs to adjust the increments during an analysis.

Esc – Exit

Pressing **Esc** causes EPRFIT to exit the **Spectral Analysis** procedure and return to the **Main Display**.

F1 – Spectra to Display

Pressing **F1** selects between the three types of spectra that can be displayed in EPRFIT. The three possibilities include: **Simulation, Experiment,** and **All**. When the **Simulation** spectrum is selected, only the simulated spectrum will appear on the screen (if a computation has been conducted). When the **Experiment** spectrum is selected, only the experimental or simulated comparison spectrum will appear on the screen if the corresponding file was read into the program from the **File Manipulation** procedure. The **All** selection displays both the simulation and comparison spectra. The spectra as well as any information pertinent to them is color coded on the screen for easy identification.

U/D – Hop Up / Down

Pressing **U** causes the cross-hairs to move up by the difference between the intensity values for each of the cross-hairs. Pressing **D** causes the cross-hairs to move down by the difference between the intensity values for each of the cross-hairs.

L/R – Hop Left / Right

Pressing **L** causes the cross-hairs to move left by the difference between the magnetic field values for each of the cross-hairs. Pressing **R** causes the cross-hairs to move right by the difference between the magnetic field values for each of the cross-hairs.

F2 – Spectra to Manipulate

Pressing **F2** selects manipulation of the **Simulated** or **Experimental** spectra. When this key is pressed, any subsequent spectral manipulation procedures will apply to the selected spectrum. The manipulate spectra area of the screen is updated to show which spectrum manipulation is active so the user can easily identify which spectrum will be affected by subsequent manipulation.

Pan

Pressing **P** from the **Main Display** accesses the **Pan** procedure. The **Pan** procedure makes **Panning** through **Zoomed** or **OffSet** spectra easy by selecting a point with a cross-hair and relocating it to a new position. Small **Pans** can be accomplished using the arrow keys. **Panning** can be conducted in both the field and intensity directions. Individual, or all, spectra can be manipulated simultaneously. This routine is useful in checking and comparing various regions of the spectra. Real math operations make this routine highly accurate.

↑, ↓, →, ←, Home, PgUp, End, PgDn – Panning Moves

These keys, which are located on the ten-key pad, **Pan** selected spectra by the current magnetic **Field Increment** and **Intensity Increment** values. The keys provide for movement in eight compass directions. The arrow key, ↑, **Pans** the selected spectra up. The arrow key, ↓, **Pans** the selected spectra down. The arrow key, →, **Pans** the selected spectra right. The arrow key, ←, **Pans** the selected spectra left. **Home Pans** the selected spectra up and left. **PgUp Pans** the selected spectra up and right. **End Pans** the selected spectra down and left. **PgDn Pans** the selected spectra down and right.

–, + – Adjust Size Increment

Pressing – decreases the selected magnetic **Field Increment** or **Intensity Increment** by one unit corresponding to the most significant digit in the increment. Pressing the + key increases the selected magnetic **Field Increment** or **Intensity Increment** by one unit corresponding to the most significant digit in the increment.

Change Line Style

Pressing **C** changes the line style used to display the spectra. The **Change Line Style** procedure selects between **Line Overlay** or **Exclusive Or** to draw the spectra. These two line styles can be used as a guide for the closeness of a fit when both the simulated and experimental spectra are considered.

With **Line Overlay**, points of the comparison spectrum coinciding with those of the simulation are erased. With **Exclusive Or**, points of the comparison spectrum coinciding with those of the simulation are set to a different color. This effect is most easily observed if only one of the spectra is visually displayed by selection with the **F1 – Spectra to Display** key.

*/, * – Adjust Size Increment by Decade*

Pressing **/** decreases the selected magnetic **Field Increment** or **Intensity Increment** by one order of magnitude. Pressing ***** increases the selected magnetic **Field Increment** or **Intensity Increment** by one order of magnitude.

Ctrl[Home] – Reset Pan

Pressing **Ctrl** and **Home** simultaneously returns the spectral **Panning** to the position where it is located when the **Pan** procedure is initially accessed.

Ins – Select Cursor Pan

Pressing **Ins** accesses the **Cursor Pan** procedure. The **Cursor Pan** procedure makes it possible for the user to **Pan** selected spectra by using a cross-hair. In addition to the normal graphics display present in this procedure, a cross-hair appears in the spectrum which can be used to select a point in the spectrum to anchor and to position the **Pan**. The magnetic field and intensity corresponding to the cross-hair anchor is reported in the lower left area of the display. The magnetic field and intensity for the **Pan** position is reported in the lower right area of the display. The **Pan** magnetic field and intensity are reported in the lower center of the display. **Panning** is accomplished in two steps. First the cross-hair is moved to the point in the spectral area which is to be **Panned** (anchor). The position is updated using the **Enter** key. The cross-hair is then moved to the point in the spectral area where the selected point is to be located. Pressing **Enter** performs the **Pan**. The anchor cross-hair is colored red and the offset cross-hair is colored green for easy identification.

↑, ↓, →, ←, Home, PgUp, End, PgDn – Panning Target Moves

These keys, which are located on the ten-key pad, move the cross-hair by the magnetic **Field Increment** and **Intensity Increment** values. The keys provide for movement in eight compass directions. The arrow key, ↑, moves the cross-hair up. The arrow key, ↓, moves the cross-hair down. The arrow key, →, moves the cross-hair right. The arrow key, ←, moves the cross-hair left. **Home** moves the cross-hair up and left. **PgUp** moves the cross-hair up and right. **End** moves the cross-hair down and left. **PgDn** moves the cross-hair down and right. All movement in the vertical or horizontal direction stops when the spectrum graph limits are reached

-, + – Adjust Size Increment

Pressing - decreases the selected magnetic **Field Increment** or **Intensity Increment** by one unit corresponding to the most significant digit in the increment. Pressing + increases the selected magnetic **Field Increment** or **Intensity Increment** by one unit corresponding to the most significant digit in the increment.

Change Line Style

Pressing **C** changes the line style used to display the spectra. The **Change Line Style** procedure selects between **Line Overlay** or **Exclusive Or** to draw the spectra. These two line styles can be used as a guide for the closeness of a fit when both the simulated and experimental spectra are considered. With **Line Overlay**, points of the comparison spectrum coinciding with those of the simulation are erased. With **Exclusive Or**, points of the comparison spectrum coinciding with those of the simulation are set to a different color. This effect is most easily observed if only one of the spectra is visually displayed by selection with the **F1 – Spectra to Display** key.

*/, * – Adjust Size Increment by Decade*

Pressing / decreases the selected magnetic **Field Increment** or **Intensity Increment** by one order of magnitude. Pressing * increases the selected magnetic **Field Increment** or **Intensity Increment** by one order of magnitude.

Ctrl[Home] – Reset Cross-Hair

Pressing **Ctrl** and **Home** simultaneously returns the cross-hair to the position where it is located when the **Cursor Pan** procedure is initially accessed. The cross-hair also returns to the red anchor cross-hair type.

Enter – Update Cursor Panning

Pressing **Enter** can cause two responses. If the anchor cursor is being manipulated, **Enter** selects the current position as the anchor point and retrieves the green **Pan** cursor. If the **Pan** cursor is present, pressing **Enter** performs the spectrum **Panning**.

Del – Select Increment

Pressing **Del** selects between the magnetic **Field Increment** and the **Intensity Increment**. The active increment is highlighted on the screen for easy identification. This procedure is used when the user needs to adjust the increments during an analysis.

Esc – Exit

Pressing **Esc** causes EPRFIT to exit the **Cursor Pan** procedure and returns to the **Pan** procedure display. Unfinished **Pans** are not conducted unless the **Enter** key has been pressed when the green **Pan** cross-hair is visible to update the process before exiting.

F1 – Spectra to Display

Pressing **F1** selects between the three types of spectra that can be displayed in EPRFIT. The three possibilities include: **Simulation, Experiment,** and **All**. When the **Simulation** spectrum is selected, only the simulated spectrum will appear on the screen (if a computation has been conducted). When the **Experiment** spectrum is selected, only the experimental or simulated comparison spectrum will appear on the screen if the corresponding file was read into the program from the **File Manipulation** procedure. The **All** selection displays both the simulation and comparison spectra. The spectra as well as any information pertinent to them is color coded on the screen for easy identification.

Field Center

Pressing **F** centers the selected spectra in the graphics display. This procedure resets the **Pan** settings for a selected spectrum to zero. This process does not affect spectral **OffSets** and **Zooms**.

F2 – Spectra to Manipulate

Pressing **F2** selects manipulation of the **Simulated, Experimental**, or **All** spectra. When this key is pressed, any subsequent spectral manipulation procedures will apply to the selected spectrum or spectra. The manipulate spectra area of the screen updates to show which spectrum manipulation is active so the user can easily identify which spectrum, or spectra, will be affected by subsequent manipulation.

Del – Select Increment

Pressing **Del** selects between the magnetic **Field Increment** and the **Intensity Increment**. The active increment is highlighted on the screen for easy identification. This procedure is used when the user needs to adjust the increments during an analysis.

Esc – Exit

Pressing **Esc** causes EPRFIT to exit the **Pan** procedure and returns the program to the **Main Display**.

F1 – Spectra to Display

Pressing **F1** selects between the three types of spectra that can be

displayed in EPRFIT. The three possibilities include: **Simulation, Experiment,** and **All**. When the **Simulation** spectrum is selected, only the simulated spectrum will appear on the screen (if a computation has been conducted). When the **Experiment** spectrum is selected, only the experimental or simulated comparison spectrum will appear on the screen if the corresponding file was read into the program from the **File Manipulation** procedure. The **All** selection displays both the simulation and comparison spectra. The spectra as well as any information pertinent to them is color coded on the screen for easy identification.

Field Center

Pressing **F** centers the selected spectra in the graphics display. This procedure resets the **Pan** settings for a selected spectrum to zero. This process does not affect spectral **OffSets** and **Zooms**.

F2 – Spectra to Manipulate

Pressing **F2** selects manipulation of the **Simulated, Experimental**, or **All** spectra. When this key is pressed, any subsequent spectral manipulation procedures will apply to the selected spectrum or spectra. The manipulate spectra area of the screen updates to show which spectrum manipulation is active so the user can easily identify which spectrum, or spectra, will be affected by subsequent manipulation.

Initialize Graphics Parameters

Pressing **I** accesses the **Initialize Graphics Parameters** procedure. The **Initialize Graphics Parameters** procedure returns the EPRFIT graphics display to its default state which is present at the time of program execution. All graphics parameters are reset to their default values. No confirmation prompt for the **Initialization** is given, so BE CAREFUL. The simulation parameters, however, are maintained so that further work can be done. The **Initialize Graphics Parameters** procedure is useful when the user wants to return the graphics display to its original form.

F1 – Spectra to Display

Pressing **F1** toggles between the three types of spectra that can be displayed in EPRFIT. The three possibilities include: **Simulation, Experiment,** and **All**. When the **Simulation** spectrum is selected, only the simulated spectrum will appear on the screen (if a computation has been conducted). When the **Experiment** spectrum is selected, only the experimental or simulated comparison spectrum will appear on the screen if the corresponding file was read into the program from the **File Manipulation** procedure. The **All** selection displays both the simulation and comparison spectra. The spectra as well as any information pertinent to them is color coded on the screen for easy identification.

ESC – Exit

Pressing **Esc** causes EPRFIT to exit graphics mode and return to the

Display Results screen. All graphics parameters are conserved until an **Initialization** procedure is called or until EPRFIT is terminated. This allows the user to leave and enter the graphics display without having to re-enter the graphics parameters.

Change line Style

Pressing **C** changes the line style used to display the spectra. The **Change Line Style** procedure allows the user to select **Line Overlay** or **Exclusive Or** to draw the spectra. These two line styles can be used as a guide for the closeness of a fit when both the simulated and experimental spectra are considered. With **Line Overlay**, points of the comparison spectrum coinciding with those of the simulation are erased. With **Exclusive Or**, points of the comparison spectrum coinciding with those of the simulation are set to a different color. This effect is most easily observed if only one of the spectra is visually displayed by selection with the **F1 – Spectra to Display** key.

Print Results

Pressing **P** from the **Main Menu** accesses the **Print Results** procedure. EPRFIT's print options make it possible to output the simulation parameters and results as well as simulated and comparison spectra onto 9 or 24 pin Epson[3] and HP[10] laserjet compatible printers. Printing can be accomplished to printers connected to the computer through either of three parallel ports (LPT1, LPT2, LPT3) or through either of four serial ports (COM1, COM2, COM3, COM4). If a printer is not readily available, the print output can be sent to a file which can be copied onto a disk and taken to a printer in another area.

The **Print Results** screen is set up using spreadsheet and switchboard architectures which gives the user easy access to various printing options. The print options screen is divided into two areas. The upper area contains the switchboard which selects the printing option to be performed. The lower area contains directory and file cells where the user enters information regarding the file that is to be used to house the print output file, if necessary, as well as the Print Data cell which actuates the desired printing operation. The two areas of the screen are accessed by pressing **PgUp** and **PgDn** on the keyboard. Also note that a **Help** screen is present at the bottom of the print option screen. This screen gives the user information on what is occurring, or what is to be input, in the various areas of the screen. Pressing **Esc** exits the **Print Results** procedure and returns the program the **Main Menu**.

Pressing **PgUp** after entering the **Print Results** screen allows the user to select the printing option desired. The upper screen area contains fifteen cells which are used to select the proper printing option to perform a specific task. The cells are:

Computation

This cell selects the simulation parameters and computation results for printing.

Spectrum

This cell selects a graphical display of the spectra for printing. The output format is dictated by the graphics settings used in the **Spectrum Display** graphics procedures.

Dot Matrix Printer

This cell selects the print output to be directed onto a 9 or 24 pin Epson[3] compatible dot matrix printer.

Laser Printer

This cell selects the print output to be directed onto a HP[10] compatible laser printer. This routine, however, will not be available until the release of EPRFIT version 2.00. EPRFIT Version 2.00 will implement routines to output the parameters, results, and spectra onto HP[10] compatible laserjet printers for very high quality hardcopies.

LPT1

This cell selects the printer connected to the computer via the LPT1 parallel port.

LPT2

This cell selects the printer connected to the computer via the LPT2 parallel port.

LPT3

This cell selects the printer connected to the computer via the LPT3 parallel port.

COM1

This cell selects the printer connected to the computer via the COM1 serial communications port. This port is initialized by EPRFIT to possess a 9600 baud rate, no parity, 8 bit data length, and 1 stop bit length. Any printer connected to this port must possess these setting for the routines to operate properly.

COM2

This cell selects the printer connected to the computer via the COM2 serial communications port. This port is initialized by EPRFIT to possess a 9600 baud rate, no parity, 8 bit data length, and 1 stop bit length. Any printer connected to this port must possess these setting for the routines to operate properly.

COM3

This cell selects the printer connected to the computer via the COM3 serial communications port. This port is initialized by EPRFIT to possess a 9600 baud rate, no parity, 8 bit data length, and 1 stop bit length. Any printer connected to this port must possess these setting for the routines to operate properly.

COM4

This cell selects the printer connected to the computer via the COM4 serial communications port. This port is initialized by EPRFIT to possess a 9600 baud rate, no parity, 8 bit data length, and 1 stop bit length. Any printer connected to this port must possess these setting for the routines to operate properly.

File

This cell selects an option for which the print output is directed to a file located in disk storage. This file will have a *.PRN extension after the print procedure is invoked. These files can be very large; therefore, they should be generated on a hard disk or high capacity floppy disk. To print a *.PRN file on a printer at a later time, the following command must be typed in at the DOS prompt:

COPY Print_Filename.PRN /B LPT1:

Any valid port name can be substituted for **LPT1** in the above example. **DO NOT** use the DOS PRINT command to output the files to a printer. The *.PRN files contain binary print code which may cause unpredictable responses from the printer.

Landscape

This cell selects a landscape presentation format for the print output on the printer. At this point, only graphic representations for the spectra can be displayed in this format. The simulation parameters and computation results are printed in portrait presentation format only.

Portrait

This cell selects a portrait presentation format for the print output on the selected printer.

Gray Scale

This cell selects a gray scale and landscape presentation format for the print output on the printer. This presentation format uses gray scaling which allows the different colors used in the graphics display to be discerned on the print output. At this point, only graphic representations for the spectra can be displayed in this format. The simulation parameters and computation results are printed in portrait presentation format only.

Once in the upper screen area, ↑, ↓, →, ← (arrow keys), **Home** , **Enter**, and **End** change the switchboard connections between their various possibilities. The **Arrow** keys cause cell changes in the direction of the arrows. **Enter** functions in the same manner as ↓. **Home** moves directly to the top of the selections, while **End** moves to the bottom of the selections. After selection of the appropriate print option procedure, the user must press **PgDn** and make directory and file selections, if necessary, in the lower area of the screen.

The lower area of the screen contains three cells that prompt the user on which directory and filename are to be used for print file output, if desired, as well as the cell which performs the printing of the data. Once in the lower screen area, ↑, ↓, →, ← (arrow keys), **Home**, **Enter**, and **End** select the appropriate cell for use. The keys operate in the same manner as they do in the upper screen area. These cells are:

Directory

This cell allows the user to input the subdirectory (path) where the print file is to be located in disk storage. The subdirectory is entered by typing the appropriate full path name, including drive name, for the subdirectory in the same manner as would be used by DOS. For example, to select a file in the EXP subdirectory existing beneath the EPRFIT subdirectory on drive C:, type:

C:\EPRFIT\EXP

Filename

This cell allows the user to input the filename for the print file which is to be constructed. No filename extensions are to be used in this cell as the EPRFIT file structure will take care of the extensions automatically. The print files will possess a *.PRN file name extension for easy identification. For example to generate a TEST2.PRN file, simply type:

TEST2

after selecting the appropriate switchboard connections in the upper screen area. These files can be very large; therefore, they should be generated on a hard disk or high capacity floppy disk. To print a *.PRN file on a printer at a later time, the following command must be typed in at the DOS prompt:

COPY Print_Filename.PRN /B LPT1:

Any valid port name can be substituted for **LPT1** in the above example. **DO NOT** use the DOS PRINT command to output the files to a printer. The *.PRN files contain binary print code which may cause unpredictable responses from the printer.

Print Data

This cell performs the specific print option selected. The option is accessed by pressing **P** which is highlighted on the screen.

The directory and filename cells contain special keys which activate data editing procedures which make it easy to modify existing entries in the cells. The **Edit** mode is accessed by pressing **End** or **Back Space** while in either of these two cells. In **Edit** mode, **End** and **Home** serve dual purposes. First, they move to the cursor to the end or the beginning of the input line, respectively; and second, if pressed twice, they terminate the **Edit** mode and return to the cell movement functions they originally possessed. The arrow keys, → and ←, also serve dual purposes in that they cause right and left cursor movement within the input line until the beginning or end of the line is reached. At this point, further movement in these directions will exit the **Edit** mode and return the keys to their

original functions. **Back Space** and **Del** allow characters to be deleted from the input line when in the **Edit** mode. **Back Space** deletes characters to the left of the cursor. **Del** deletes characters to the right of the cursor. Also, **Ins** can be pressed to select between **Insert** and **Overwrite** modes which operate on text at, or to the right, of the cursor.

Spectrum Digital Plot

The **Spectrum Digital Plot** procedure outputs the simulated and comparison spectra to an HP[10] compatible (HPGL format) plotter. This procedure will not implemented until EPRFIT Version 2.00 is released.

Esc to Exit

The **Esc to Exit** procedure terminates EPRFIT and returns the computer to DOS. All information resident in memory must be stored before exiting or else it will be lost. EPRFIT prompts the user to confirm exit to ensure that all pertinent information is appropriately saved.

REFERENCES

1. Trademark or registered trademark of Borland International, Inc., or Borland/Analytica, Inc.

2. Trademark of Advanced Graphics Software, Inc.

3. Registered trademark of the Seiko Epson Corporation.

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