NMR Analyzer v. 3.0

NMR Analysis Program

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The NMR Analyzer Help topics are as follows:

Some help contains "jump" topics which appear in solid-underlined, green text. Click the text to jump to the associated topic, then click the Back button in the Help window to return to your original help topic. Pop-up topics appear as green text with dotted underlines. Click the text to display the pop-up information, then anywhere to dismiss the pop-up box.

You can access help on individual topics through the Help menu, or if you want help on a specific command or most dialog boxes, you can press the F1 key while the command is highlighted or the box displayed.

Introduction

NMR Analyzer is a program designed for the analysis of spin systems. The user can introduce up to 7 spins, and calculate the theoretical proton NMR spectrum. The spin basis functions, spectral lines and energy levels are displayed. Advanced users can also analyze complex spin systems, as the AA'XX' or ABX systems. NMR Analyzer runs under Microsoft Windows 3.1 on 386 and 486 based computers.

Commands

The commands are organized by their appearance on the NMR Analyzer menus. Click the menu name here and see a brief description of each command.

- File menu
- Parameters menu
- Calculations menu
- Display menu
- Analysis menu
- Help menu

File menu

Use the File menu to open files, save the picture, configuration, and exit from the program.

- New
- Open
- Auto
- Save Graphic
- Save Configuration
- Exit

New

This command delete all current parameters and allow user to introduce another series of parameters, analyse a spin system or display directly the results of previously done calculations. The New command can be executed at any time.

Open

The Open command is used to load a Parameters file or an Analysis file.

Auto

The Auto command is provided to simplify the process of calculate the theoretical spectrum for a spin system. When executed, it will lead user through the parameters and calculations menu, prompting him for information, and finally it will display the spectrum.

Save graphic

Not yet implemented

The Save picture command stores in a bitmap the display in the graphic window. This can be a spectrum or a diagram. The bitmap can be modified with a painting program, like Window's Paintbrush, and included into a word processor.

Save configuration

This command stores into the file NMR.INI (placed into the Windows directory) the current frequency of the spectrometer, the name of the work files, and the work directory.

Exit

Use this command to exit program.

Parameters menu

Use the Parameters menu to introduce the number of spins (nuclei), the chemical shifts and the coupling constants.

- Parameters info
- Number of spins
- Chemical shifts
- Coupling constants
- Additional signals

Parameters info

This commands displays a dialog box allowing user introduce the title for the spectrum, and comments for the parameters file. Both title and comments will be saved in the parameters file.

Number of spins

This commands displays a dialog box requesting the number of spins. The maximun number allowed is seven.

Chemical shifts

This command displays a dialog box to introduce the chemical shifts of the considered nuclei.

Coupling constants

The Coupling constants command shows a dialog box which displays the coupling constants matrix.

Additional signals

The Additional signals command shows a dialog box to introduce data for signals which will appear in the spectrum but are not included in the calculations.

Calculations menu

Use the commands on this menu to perform calculations using the parameters introduced with the Parameters menu.

- Generate basis functions
- Generate Hamiltonian
- Diagonalize Hamiltonian
- Calculate frequencies and intensities

Generate basis functions

This command generates the spin basis functions for the considered spin system. The functions are automatically stored in the parameters file, named as the work files name with the extension .0.

Generate Hamiltonian

Choosing this command generates the Hamiltonian matrix for the spin system, using the current parameters. All calculations are automatically stored.

Diagonalize Hamiltonian

The Diagonalize Hamiltonian command diagonalizes the Hamiltonian matrix using the Givens-Householder algorithm.

Calculate frequencies and intensities

This command calculates the frequencies and intensities of the transitions between the energy levels calculated with the Diagonalize Hamiltonian command. Actually, this command generates the spectral lines which will be used by the Display spectrum command to generate the spectrum.

Display menu

Use this menu to display the theoretical spectrum, energy or Fz levels, spectral lines, and the spin basis functions.

- Spectrum
- Levels diagram
- Spectral lines
- Spin basis functions

Spectrum

This commands displays the theoretical spectrum in one of these two forms: stick plot or Lorentzian plot.

Spectral lines

The spectral lines command shows the calculated frequencies and intensities of all or part of the possible transits.

Levels diagram

Generates a diagram of the energy levels or the Fz levels for the spin system. A dialog box allows the selection of some necessary parameters.

Spin basis functions

Display all spin basis functions used to perform calculations.

Analysis menu

Use this menu to display the theoretical spectrum, energy or Fz levels, spectral lines, and the spin basis functions.

- AB system
- AB2 system
- ABX system
- AA'XX' system

AB system

Use this command to analyse an AB system. The results of the analysis can be transfered to the main routines to calculate the theoretical spectrum.

AB_2 system

Use this command to analyse an AB_2 system. The results of the analysis can be transfered to the main routines to calculate the theoretical spectrum.

ABX system

Use this command to analyse an ABX system. The results of the analysis can be transfered to the main routines to calculate the theoretical spectrum.

AA'XX' system

Use this command to analyse the AA' or the XX' portion of an AA'XX' system. The results of the analysis can be transfered to the main routines to calculate the theoretical spectrum.

Help menu

The help menu allows access to this file. Use the different options to access differents parts of help.

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Index

Gives the user direct access to the help index.

Introduction

Gives the user direct access to the introduction of the help file.

Commands

Gives the user direct access to the information about program commands.

Procedures

Gives the user direct access to program's procedures.

Glossary

Gives the user direct access to a small glossary with basic NMR concepts.

About

Shows information about the program and copyright.

Procedures

The procedures are organized by the logical order of introduction parameters, execute calculations, and see the results. There are sections for general procedures, and analysis of complex spin systems.

How to...

Introduce spin system parameters

Execute calculations

Display results

Analyse spin systems

How to...

These section describes general procedures about some features of the program.

- Change spectrometer frequency
- Change work files name
- Delete parameters
- Execute the procedures automatically
- Introduce comments
- Introduce additional signals
- Open a file
- Save a parameters file
- Save an analysis file
- Save spectrum as bitmap
- Save diagrams as bitmap
- Save configuration
- Exit program

How to change spectrometer frequency

To change the frequency of the spectrometer, click on the Spectrometer Frequency Box and type the new frequency. This frequency will be used in all new calculations. To save this frequency as default see Save configuration.

How to change work files name

To change the name to be used for the work files, click on the Work Files Name Box, and type the new name. The name cannot be longer than 8 characters. This name will be used to save all the new files. To save this name as default see Save configuration.

How to execute the procedures automatically

You can execute automatically the needed procedures to calculate the theoretical spectrum, introducing new parameters or using parameters previously loaded. Follow the next steps:

1. If you want to execute calculations on a parameters file, choose File/Open and load the file.
2. Choose File/Auto.
3. Click Yes to erase the current parameters, or No to preserve them.
4. If you erased parameters type the new ones, else click Ok on each dialog box.
5. Click Ok to execute calculations on the current parameters. Click cancel to exit the automatic procedures.
6. Choose the spectrum parameters, and click Ok when finish.

How to delete parameters

To delete the current parameters (number of spins, chemical shifts and coupling constants), follow the next steps:

1. Choose File/New.
2. L-click OK.

The number of spins will become 1, and all data matrix will be deleted. The name on the Work Files Name Box will become UNTITLED.

How to introduce comments

To introduce comments for the parameters file, choose Parameters/Parameters info. In the Comments Text Box, introduce the desired text.

How to introduce additional signals

To introduce signals in the spectrum which will not be calculated, choose Parameters/Additional signals. The Additional Signals Dialog Box will appear. Up to six additional signals can be introduced.

1. Select the multiplicity of the signal; if none, the data for the signal will not be considered, and the text boxes for the signal will be unabled.
2. Type the chemical shift for the signal, in ppm.
3. Type the coupling constant for the signal, in Hz (if different than a singlet).
4. Type the number of protons for the signal.

Click Ok button when finish, or Cancel to exit dialog box at any moment.

How to open a file

To open a parameters file or an analysis file, you can use several methods for specifying a filename:

You can enter a path and filename in the File Name Box.
You can specify a drive and directory and then select a name from the list.

Shortcut: You can double-click the filename in the list box to open the file without clicking the Ok button.

You can specify one of the two following formats to restrict the types of files displayed in the Files box:

NMR = Parameter
DAT = Analysis

After selecting a filename click the Ok button. If you want to cancel the operation, click Cancel button.

How to save a parameters file

To save a parameters file, you must choose Calculations/Generate basis functions. This will automatically generate the necessary parameters and will store the results into a file, which will be named as the Work Files Name with the NMR extension.

How to save an analysis file

To save a file containing data for spin system analysis you must click Save data in the currently opened Analysis Dialog Box. This will automatically store the data into a file, which will be named as the Work Files Name with the DAT extension.

How to save spectrum as bitmap

Not yet implemented

To save the spectrum in the Graphic Box in bitmap format, follow the next steps:

1. Type the filename of the spectrum in the Work File Name Box.
2. Choose Display/Spectrum.
3. When the spectrum has been displayed, choose File/Save graphic.

How to save diagrams as bitmap

Not yet implemented

To save the spectrum in the Graphic Box in bitmap format, follow the next steps:

1. Type the filename of the spectrum in the Work File Name Box.
2. Choose Display/Energy levels.
3. Select energy levels or Fz levels.
4. When the diagram has been displayed, choose File/Save graphic.

How to save configuration

To save the currents frequency, work files name and directory as defaults, choose File/Save configuration. The new configuration will be saved in the RMN.INI file. The configuration file is automatically read in when the program is loaded.

How to exit program

To exit program, follow the next steps:

1. Choose File/Exit.
2. Confirm exit by clicking Ok button.

Introduce spin system parameters

These procedures describe how to introduce the parameters needed to calculate the theoretical spectrum.

- Introduce number of spins (nuclei)
- Introduce chemical shifts
- Introduce coupling constants

Introduce number of spins (nuclei)

To introduce the number of spins, follow the next steps:

1. Choose Parameters/Number of spins. The number of nuclei dialog box will be displayed.
2. Type in the text box the number of spins.
3. Clik the Ok button.

Warning: the number of spins includes all nuclei in a group. So, for example, the number of nuclei in the ethyl group is five, though the three protons in the methyl are chemically equivalent, and the two protons in the methylen are chemically equivalent.

Optional: the parameters can be loaded instead typing them; see How to open a file.

Introduce chemical shifts

To introduce the chemical shifts necessary to characterize the spin system, follow the next steps:

1. Choose Parameters/Chemical shifts. The chemical shifts dialog box will be displayed.
2. Type in the boxes the chemical shifts (they can be disordered).
3. Click the Ok button to accept.

Optional: the parameters can be loaded instead typing them; see How to open a file.

Introduce coupling constants

If the spin system needs to be characterized with coupling constants, follow the next steps:

1. Choose Parameters/Coupling constants. The coupling constants matrix dialog box will be displayed.
2. Type in the boxes the coupling constants (they can be disordered).

The text boxes of the row n *represents the coupling constants of the nucleus* n *with the another nuclei. Since the coupling constant of the nucleus* i *with the nucleus* j*, is the same of the nucleus* j *with the nucleus* i*, the coupling constants matrix is simmetrical*. *The program makes this matrix simmetrical automatically.*

3. Click the Ok button to accept.

Optional: the parameters can be loaded instead typing them; see How to open a file.

Execute calculations

After the introduction of the parameters, user must execute calculations on them to obtain the results. To do that, follow the next steps:

1. Choose Calculations/Generate basis functions. This will generate the spin basis functions for the spin system. You can now display the spin basis functions. See Display spin basis functions.
2. Generate Hamiltonian. This will generate the Hamiltonian matrix for the spin system.
3. Diagonalize Hamiltonian. The program will diagonalize the Hamiltonian matrix using a Givens-Householder algorithm.
4. Calculate frequencies and intensities.

See Also:

How to execute the procedures automatically.

Display results

This section describes the necessary steps to display the spectrum and other results of the calculations.

- Display a spectrum
- Display spectral lines
- Display energy levels
- Display Fz levels
- Display spin basis functions

Display a spectrum

There are two manners of display a theoretical spectrum.

A. If it was previously calculated:

1. Type in the Work Files Name Box the name of the files for that spin system.
2. Choose Display/Spectrum.
3. Set parameters, and click the Ok button.

B. Execute the necessary procedures from the beginning. See Procedures.

See Also:

Spectrum parameters dialog box.

Display energy levels

There are two manners of display a diagram of energy levels.

A. If it was previously calculated:

1. Type in the Work Files Name Box the name of the files for that spin system.
2. Choose Display/Levels diagram.
3. Set parameters, and click the Ok button.

B. Execute the necessary procedures from the beginning. See Procedures.

See Also:

Diagram parameters dialog box.

Display Fz levels

There are two manners of display a diagram of Fz levels.

A. If it was previously calculated:

1. Type in the Work Files Name Box the name of the files for that spin system.
2. Choose Display/Levels diagram.
3. Set parameters, and click the Ok button.

B. Execute the necessary procedures from the beginning. See Procedures.

See Also:

Diagram parameters dialog box.

Display spectral lines

There are two manners of display the spectral lines.

A. If they were previously calculated:

1. Type in the Work Files Name Box the name of the files for that spin system.
2. Choose Display/Spectral lines.
3. Set parameters, and click the Ok button.

B. Execute the necessary procedures from the beginning. See Procedures.

See Also:

Spectral lines dialog box.

Display spin basis functions

There are two manners of display the spin basis functions.

A. If they were previously calculated:

1. Type in the Work Files Name Box the name of the files for that spin system.
2. Choose Display/Spin basis functions.

B. You can also display the spin basis functions inmediately after generating them, by choosing Display/Spin basis functions. See Execute calculations.

See Also:

Spin basis functions dialog box.

Analyse spin systems

This section describes the necessary steps to analyse complex spin systems.Click the desired spin system for more information.

Analyse AB spin systems

Analyse AB$_2$ spin systems

Analyse ABX spin systems

Analyse AA'XX' spin systems

Analyse AB spin system

Follow the next steps to analyse the data of the AB spin system:

1. Type in the Spectrometer Frequency Box the work frequency.
2. Type in the Work Files Name Box the desired name.
3. Choose Analyse/AB spin system. The AB system analysis dialog box will be displayed.
4. Type in the text boxes all four characteristic frequencies. They can be disordered.
5. Click Analyse to display results. This will also transfer the chemical shifts and coupling constant to the main routines, allowing the calculation of the theoretical spectrum. See Execute calculations.
6. If you want to save the frequencies of the spin system in a file, Click Save data; the work frequency and spin system frequencies will be saved in a file, using the work files name as file name, and the extension DAT.
7. Click Cancel to close the dialog box.

Optional: Analysis data can be loaded instead typing them; see How to open a file.

Analyse AB_2 spin system

Follow the next steps to analyse the data of the AB_2 spin system:

1. Type in the Spectrometer Frequency Box the work frequency.
2. Type in the Work Files Name Box the desired name.
3. Choose Analyse/AB_2 spin system. The AB_2 system analysis dialog box will be displayed.
4. Type in the text boxes all eight characteristic frequencies. They can be disordered.
5. Click Analyse to display results. This will also transfer the chemical shifts and coupling constant to the main routines, allowing the calculation of the theoretical spectrum. See Execute calculations.
6. If you want to save the frequencies of the spin system in a file, Click Save data; the work frequency and spin system frequencies will be saved in a file, using the work files name as file name, and the extension DAT.
7. Click Cancel to close the dialog box.

Optional: Analysis data can be loaded instead typing them; see How to open a file.

Analyse ABX spin system

Follow the next steps to analyse the data of the ABX spin system:

1. Type in the Spectrometer Frequency Box the work frequency.
2. Type in the Work Files Name Box the desired name.
3. Choose Analyse/ABX spin system. The ABX system analysis dialog box will be displayed.
4. Type in the text boxes all eight characteristic frequencies for the AB portion of the spectrum and all six frequencies of the X portion. You must also assign four of the AB frequencies to one of the two seudoquartets, by clicking the check boxes.
5. Click Analyse to display results. This will also transfer the chemical shifts and coupling constant to the main routines, allowing the calculation of the theoretical spectrum. See Execute calculations.
6. If you want to save the frequencies of the spin system in a file, Click Save data; the work frequency and spin system frequencies will be saved in a file, using the work files name as file name, and the extension DAT.
7. Click Cancel to close the dialog box.

Optional: Analysis data can be loaded instead typing them; see How to open a file.

Analyse AA'XX' spin system

Follow the next steps to analyse the data of the AA'XX' spin system:

1. Type in the Spectrometer Frequency Box the work frequency.
2. Type in the Work Files Name Box the desired name.
3. Choose Analyse/AA'XX' spin system. The AA'XX' system analysis dialog box will be displayed.
4. Type in the text boxes all ten characteristic frequencies. They can be disordered.
5. Click Analyse to display results. This will also transfer the chemical shifts and coupling constant to the main routines, allowing the calculation of the theoretical spectrum. See Execute calculations.
6. If you want to save the frequencies of the spin system in a file, Click Save data; the work frequency and spin system frequencies will be saved in a file, using the work files name as file name, and the extension DAT.
7. Click Cancel to close the dialog box.

Optional: Analysis data can be loaded instead typing them; see How to open a file.

Glossary

Click the word to display its definition.   All terms defined in this glossary are also available through the Help Search feature.

- AA'XX' spin system
- AB spin system
- AB_2 spin system
- ABX spin system
- AX spin system
- Chemical equivalence
- Chemical shifts
- Coupling constants
- Doublet
- Eigenfunction
- Eigenvalue
- Energy levels
- Fz levels
- Hamiltonian
- Magnetic equivalence
- Multiplet
- Multiplicity
- Quartet
- Singlet
- Spectral lines
- Spin basis functions
- Spin notation
- Triplet

AA'XX' spin system

A system formed by four nuclei, characterized by only two resonance frequencies and four coupling constants. We encounter AA'XX systems in molecules such as *para*-disubstituted benzenes, furan, and 1,2-difluoroethylene.

AB spin system

A system formed by two nuclei, characterized by two resonance frequencies and one coupling constant, as the AX system. Because of the small ratio $\Delta\delta/J$, the inner lines become bigger and the outer lines become smaller.Then, a distorted AX spectrum is observed. This is commonly known as *roof efect.*

AB**2** spin system

A system formed by three nuclei, observed in compounds that possess a two-fold axis of symmetry such as 2,6-dimethylpyridine and 1,2,3-trichlorobenzene.

ABX spin system

A system formed by three nuclei, in which the A and B nuclei have similar chemical shifts, and the X nucleus has a very different shift. The X nucleus in such systems is said to be weakly coupled and the A and B nuclei are said to be strongly coupled. The 1,2,4-trichlorobenzene is an example of the ABX system.

AX spin system

The more simple system of coupled nuclei; is characterized by two resonance frequencies and a coupling constant. Two doublets are observed, and the coupling constant can be measured directly. This is a very common spin system.

Chemical equivalence

The nuclei with the same resonance frequency are called *isochronous*. They are usually chemically equivalent, that is, they have identical chemical environments. Two nuclei can be is isochronous and have two very diferent chemical environments. The chemical equivalence is a necessary condition for the magnetic equivalence.

Chemical shifts

The resonance position of a a given nucleus as a distance from a standard, commonly Tetramethylsilane (TMS). This values as reported in a δ scale, which is independent of the field of the magnet, and expressed in *parts per million* or ppm.

Coupling constants

This parameter expresses the magnitude of the splitting in a NMR signal, caused by the coupling of the spins of nonequivalent vicinal nuclei. It is known as J, and expressed in Hz. The value of J depends on the molecular stereochemistry and the number of bonds between the coupled protons, among othe factors.

Doublet

A characteristic signal caused by the splitting of the single signal because a non-equivalent nucleus (a proton) attached to the same carbon or to adjacent carbon atom. The signal appears as two sharp singlets and the magnitude of the splitting is expressed as the coupling constant, J.

Eigenfunction

The spin system as a whole can exist only in certain states, the *stationary states* or *eigenstates*. Each eigenstate is characterized by a *wave function* or *eigenfunction*, wich is normally constructed as a linear combination of spin basis functions.

Eigenvalue

The energy of an *eigenstate*. The *eigenvalues* are solutions of the Schrödinger equation, and they are determined by the interaction between the nuclei and the external magnetic field, as well as by the spin-spin interaction of the nuclei with one another.

Energy levels

The energy levels of a spin system are calculated by aplying the Schrödinger equation to the considered nuclei. These energy values are therefore eigenvalues and give the energy for an eigenstate characterized by a *wave function* or eigenfunction.

Fz levels

The product functions for a spin system are characterized by the total spin, the sum of the magnetic quantum numbers of the individual nuclei. Fz is defined as an operator, which conmutes with the Hamiltonian operator. This allows factorize the Hamiltonian matrix into submatrices. The Fz levels are characterized by the same total spin. For the AX spin system, the values of the Fz operator are -1, 0 and 1.

Hamiltonian

The Hamiltonian operator gives the value of the energy (eigenvalue) of a wave function which is an eigenfunction. When applied to a spin system, a Hamiltonian matrix is obtained, which can be factorized in submatrices by results of the Fz operator.

Magnetic equivalence

Two nuclei are magnetically equivalent when they are chemically equivalent and have only one characteristic spin-spin interaction with the nuclei of a neighbouring group. The chemical equivalence is a necessary condition for magnetic equivalence.

Multiplet

A NMR signal is said to be a multiplet when its hyperfine structure (the couplings), cannot be easily resolved. This situation comes normally from the magnetic non-equivalence of the coupled nuclei and the so called *second order rules*. The analysis of some multiplets requires a theoretical treatment.

Multiplicity

For nuclei with spin quantum number $I = ½$ the multiplicity of the splitting equals n + 1 where n is the number of nuclei in the neighbouring group. This is one of the *first order rules*.

Quartet

A signal with the relative intensities 1:3:3:1. This signal comes from the coupling of a proton with three other equivalent protons in the neighbouring group. A typical case is the splitting of the methylene protons signal in the ethyl radical.

Singlet

The NMR simplest signal. It consists on a sharp signal. and is therefore characterized only by a resonance frequencie. Two or more protons chemically equivalent give a signal like this.

Spectral lines

These are the lines observed in a NMR spectrum. Spectral lines represent transits between energy levels of different Fz value. A theoretical spectrum can have many lines, but only the observed lines are spectral lines.

Spin basis functions

Basis functions are those which serve as basis for a linear combination. In this case, the linear combination gives an eigenfunction of the spin system. The spin basis functions for a two spin system, are αα, αβ, βα and ββ, where the second and third functions have the same value of Fz. Since the eigenfunction must have only one Fz value, only that two functions must be conbined to give the eigenfunction with Fz zero.

Spin notation

The spin notation serves to abreviate the description of complex spin systems. The notation uses shift letters to denote nuclei; AB means two nuclei, with their corresponding chemical shifts, which are very close; AX means two nuclei with very different chemical shifts. If two nuclei with the same chemical shift are magnetically non-equivalent, the spin notation denotes them as AA'... The AA'XX' spin system, is therefore a four nuclei system, with two very different chemical shifts, and all four nuclei are magnetically non-equivalent.

Triplet

A signal with the relative intensities 1:2:1. This signal comes from the coupling of a proton with two other equivalent protons in the neighbouring group. A typical case is the splitting of the methyl protons signal in the ethyl radical.

Parameters file

This file stores the basic parameters for calculate a spectrum: the frequency of the spectrometer, the number of spins, their chemical shifts and their coupling constants. The file stores also the spin basis functions for the spin system.

Analysis file

This file stores the type of the spin system to be analized and the needed frequencies. It stores also the frequency of the spectrometer and, in the case of the AA'XX' spin system, the seudoquartet's assignation.

Spectrum parameters dialog box

This dialog box sets the parameters to display spectrum:

Maximun shift: this is the maximun chemical shift of the spectrum. Use the horizontal scroll bar to sets the maximun shift, or type it into the text box. The maximun chemical shift is 15.

Minimun shift: this is the minimun chemical shift of the spectrum. Use the horizontal scroll bar to sets the minimun shift, or type it into the text box. The minimun chemical shift is 0.

Title: type in this text box the title of the spectrum. It will be displayed in the Graphic Box.

Type of plot: click option button to display spectrum as stick plot (faster, but very schematic) or as Lorentzian plot (slower).

Display range: click this check box to see in the spectrum the frequency of spectrometer, the range of chemical shifts, and the resolution.

Linewidth: this scroll bar is enabled only when the Lorentzian plot button is on. Sets the linewidth for the Lorentzian plot. Allowed values are between 0 and 1.

Scale factor: this scroll bar sets the height of the peaks. Use it to scale plot in the y axis.

When all parameters are set, click Ok button. to display spectrum. Click Cancel at any time to exit the dialog box.

Diagram parameters dialog box

This dialog box sets the parameters to display diagrams:

Diagram type: click option button to display energy levels diagram or Fz levels diagram.

See transits: click the check box to see the transits between levels. When checked, it activates the intensity scroll bars.

Minimun intensity: sets the minimun intensity of the transits to be displayed. If both intensities are equal to zero, then all transits will be displayed. This scroll bar is enabled only when the See transits check box is checked. The minimun intensity is the same as in the Spectral lines dialog box.

Maximun intensity: sets the maximun intensity of the transits to be displayed. If both intensities are equal to zero, then all transits will be displayed. This scroll bar is enabled only when the See transits check box is checked. The maximun intensity is the same as in the Spectral lines dialog box.

When all parameters are set, click Ok button to display diagram. Click Cancel at any time to exit the dialog box.

Spectral lines dialog box

This dialog box displays the spectral lines for the spin system. They can be displayed by intensity or transition numbers.

Intensities: click option button to display lines by their intensities.

Transition index: click option button to display lines by their transition index.

Initial level: if the transition index option button is on, type in this text box the number of the starting level for the transition.

Final level: if the transition index option button is on, type in this text box the number of the finishing level for the transition.

Minimun intensity: sets the minimun intensity of the transits to be displayed. If both intensities are equal to zero, then all transits will be displayed. This scroll bar is enabled only when the intensities option button is on. The minimun intensity is the same as in the Diagram parameters dialog box.

Maximun intensity: sets the maximun intensity of the transits to be displayed. If both intensities are equal to zero, then all transits will be displayed. This scroll bar is enabled only when the intensities option button is on. The maximun intensity is the same as in the Diagram parameters dialog box.

When all parameters are set, click Ok button to display spectral lines. Click Cancel at any time to exit the dialog box.

Spin basis functions dialog box

This dialog box displays the spin basis functions for the spin system.

Next: click this button to see the next group of basis functions. They are grouped by the same value of Fz.

Previous: click this button to see the previous group of basis functions.

When the group of basis functions has the maximun or minimum allowed value or Fz (it means, when the only function displayed is ααα.... or βββ...) click Previous or Next button will display an error message and close the dialog box. Click Cancel button at any time will have the same effect.

Bibliography

If you are interested in the basis of the Nuclear Magnetic Resonance, these two books were extensively used in the making of this program. Some aspects, like the quantum mechanical principles, and the analysis of complex spin systems are well treated. See also references cited therein:

NMR Spectroscopy. An introduction. Günther, Harald. John Wiley & Sons, 1980.

Nuclear Magnetic Resonance. Basic principles. Atta-ur-Rahman. Springer-Verlag, New York, 1986.