

# Interactive fitting application INFIA

## Users Manual

1998

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## 1 Introduction

Infia is a graphical, interactive program for assignment and fitting of high resolution linear molecule spectra. The program has been published in [ref.]. An example of a spectroscopic work that has been carried out using Infia is the study of some band systems of DCCBr [ref.]

## 2 System requirements

- PC system with 486/33 processor (Pentium recommended)
- 16 MB RAM (32 MB in WinNT)
- Microsoft Windows95 or WindowsNT 4.0 operating system.
- SuperVGA display with  $800 \times 600$  resolution ( $1024 \times 768$  recommended) and 256 colours (65k colours recommended).

## 3 Analysis projects and project files

It is recommended that in addition to reading this description of the project files, one looks at the corresponding example files in the demonstration project provided with the distribution package.

### 3.1 Comma Separated Value (CSV) files

Many of the files used by Infia to store analysis data to disk have *comma separated values* format and the corresponding file extension .CSV. The format of these ASCII files is:

```
fieldname1=fieldvalue1, fieldname2=fieldvalue2, ...,fieldnameN=fieldvalueN
fieldname1=fieldvalue1, fieldname2=fieldvalue2, ...,fieldnameN=fieldvalueN
fieldname1=fieldvalue1, fieldname2=fieldvalue2, ...,fieldnameN=fieldvalueN
...
```

For example, the assignment file could look like:

```
BandName=DB8b,m=-88,Type=predicted,WnObs=931.191105,WnCalc=931.181526,Weight=1.0000
BandName=DZ7b,m=-9,Type=assigned,WnObs=931.191105,WnCalc=931.190937,Weight=1.0000
BandName=DA0a,m=-111,Type=assigned,WnObs=931.205261,WnCalc=931.204861,Weight=0.1000
...
```

with each line describing the properties of a single assignment. The advantages of this file format is:

- Easy readability and understanding of the contents of the file. This implies easy conversion of the data to other formats by simple utility programs or spreadsheet applications.
- Compatibility of current file formats with future extensions. For example, if new properties "Ja" and "Jb" are later added to the assignment file format, old files without these fields remain completely readable. This is because fields of the CSV file are associated to variables of the program through the field names, not through their position in the text lines.

- **One project per band system**

It is suggested that the spectra that is to be analysed with Infia are split into separate wavenumber ranges according to band systems and that one analysis project is created for each band system. Here a 'band system' can be taken to mean simply a region of spectrum containing peaks of interest and bound by wide of spectrum that do not contain peaks of interest. Hence, bands of interest should be totally contained in the band systems and not extend from one band system to another. It is possible to create projects with wide spectrum region having multiple band systems, but this is unnecessary and only creates an additional burden for the computer memory.

### **3.2 Files that multiple projects can share**

Whereas different band systems of a molecule (or certain group of molecules) should be analysed in separate projects, these projects can have some common files and should hence be *stored in same disk directory*. The following files that can be common among different projects:

- *Molecule File*. Stores a list of molecule names (isotopic species separately) that are studied in the project, ie. molecules that are responsible for peaks in the analysed spectrum. The format of this file is comma separated values.
- *State file*. Stores a list of vibrational states that are of interest in the project. The format of this file is comma separated values.
- *Resonance File*. Stores a list of rotational and vibrational resonance elements that produce mixing of the ro-vibrational states defined in state-file. The format of this file is comma separated values.

When a new project is started, user can opt to use existing molecule, state and resonance files or create new ones.

Analysis projects of completely unrelated spectra can and should be stored in different directories.

### **3.3 Files that are unique to each project**

#### **3.3.1 Files that are needed when a new project is started (Input files)**

These files must be supplied by the user when an analysis project is started. They are ASCII files that can be easily generated from any proprietary files using simple custom program or even a standard spreadsheet.

- *Spectrum File*. This is the main input file for an analysis project. This ASCII file should have an extension SPE and format as in the following example:

```
Spectra Data File
StartWavenumber 924.99940000
EndWavenumber 989.99940000
Points 129430
Intensity List:
0.0470
0.0683
0.0885
...
```

- *Peak File*. Because Infia does not currently have peak detection / calibration abilities, separate program must be used to find the peaks in the spectrum and to construct a CSV file of the peaks:

```
Wavenumber=456.12495, Intensity=0.06072
Wavenumber=456.227757, Intensity=0.05828
Wavenumber=456.246867, Intensity=0.06917
...
```

- **Files that store data generated in the analysis project**
- *Project file*. Project files
- *Band file*. Stores properties of the bands that have been found in the analysed region of the spectrum. The format of this file is comma separated values.
- *Assignment File*. Stores the properties of peak assignments. Single spectrum peak can have many assignments. The format of this file is comma separated values.
- **Backup files**

Before saving any CSV files (states, molecules, bands, assignments, peaks), Infia copies the existing files into backup files that have BAK extension. On the unlikely event that the program crashes during a file save operation, the previous versions of the project files can be restored from these backups. To do this, copy \* .BAK to \* .CSV in the project directory.

There is no backup made of the spectrum file (name.SPE), because changes are rarely made to it. Hence it is recommended that the user keeps always a backup of the spectrum file.

## 4 Working with data tables

There are several tables in Infia that display analysis project data:

- Peak list
- Branch combination analysis results
- Band assignments
- Vibrational state parameters

- Resonances
- Bands
- Molecules

#### 4.1 Keyboard commands for tables

- Insertion of new records: **CTRL + INS**. For example, to insert new vibrational state to the Vibrational state parameters table.
- Deletion of records from table: **CTRL + DEL** key.
- Inserting TRUE for boolean fields: give **t** (as true) or **y** (as yes).
- Inserting FALSE for boolean fields: give **f** (as false) or **n** (as no).

## 5 Project management

### 5.1 Starting a new project: File / New Project

After the selection of New Project menu command:

- 1 Give name and saving location for the project file. It is a good idea to give the name of the band system as the project name (eg. `2nu4.prj`). If you have previous projects of the same molecule(s) it is highly recommended to save the new project into the same disk directory as them.
- 2 In the next dialog box, select a spectrum file for the new project. The spectrum file must be located in the project directory, if must have `.SPE` extension and it must have format described on page 4.
- 3 In the next dialog box, select a peak file for the project. The peak file must be located in the project directory, if must have `.CSV` extension and it must have format described on page 5.
- 4 In the next dialog box, select an existing **molecule file** for the project give a new file name (for example `molecules.csv`) to create a new molecule file for the project. If you have previous projects of the same molecule(s) it is highly recommended to use the existing molecule file in the same directory.
- 5 In the next dialog box, select an existing **state file** for the project give a new file name (for example `states.csv`) to create a new state file for the project. If you have previous projects of the same molecule(s) it is highly recommended to use the existing state file in the same directory.
- 6 In the next dialog box, select an existing **resonance file** for the project give a new file name (for example `resonances.csv`) to create a new resonance file for the project. If you have

previous projects of the same molecule(s) it is highly recommended to use the existing resonance file in the same directory.

## 7 Adding molecules and states to the project

The *molecule* table (viewed with Window / Molecules menu command) *state* table (viewed with Window / Vibrational state parameters menu command) should contain the molecules and their vibrational states that are of interest in the present analysis. These tables can be shared among different projects of the same molecule(s) and hence can already contain molecules and states in the beginning of a project.

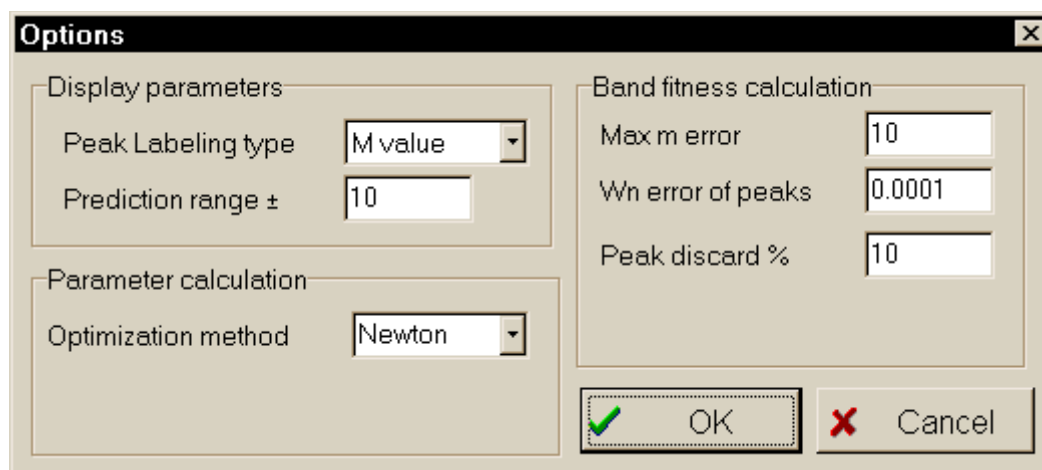
Before analysis of any band in the spectrum, the molecule producing the band must be located in the molecule table and the lower and upper vibrational states of the band in the state table. This is not a strict requirement: bands can be analysed in the beginning without assigning molecules or states for them. But at some point of the analysis the states must be added to the tables anyway, so it makes sense to add a selection of molecules and their relevant states already in the beginning of the analysis.

Note that different isotopic species should be considered different molecules. This also means that the same vibrational state of two different isotopic species should have two records in the state table, one of each isotopic species.

The user is free to choose whatever names for the vibrational states, but it is recommended that the names (1) incorporate the vibrational quantum numbers of the state in some format and (2) have all the same format.

### 5.2 Changing project options: File / Options

Options dialog box is displayed:



Meaning of settings in the options dialog:

- *Peak labeling type.* Select the text displayed in assignment labels shown in spectra for peak assignments. Choices are peak  $m$  value,  $J'$  and  $J''$  or band name.
- *Prediction range.* Defines the amount by which the assigned  $m$  range is extended for peak prediction purposes. For example, if there are peak assignments in the  $m$  range  $-55\dots60$  and the prediction range is 10, predicted wavenumbers are calculated for  $m$  range  $-65\dots70$ .
- *Optimisation method.* Defined the method to use in the non-linear least squares optimisation used for resonance fitting. Choices are Simplex (simple and unefficient, but failproof) and Newton (Gauss-Newton, efficient but needs good initial guesses)
- *Max  $m$  error.* Defines the range of  $m$  shifts that are tried in the combination difference prediction. For example. if Max  $m$  error is 10, shifts  $-10\dots+10$  are tried.
- *Wn error of peaks.* Average precision of peak center wavenumbers of the spectrum. Typically about 1/20 of the peak width. If this setting is badly incorrect, the band fitness calculation does not produce good results.
- *Peak discard %.* Percentage of worst matching peaks that are discarded before calculating the fitness value of the combination in the combination difference prediction.

### 5.3 Spectra file conversion

Spectra file conversion can convert two different spectrum formats to the .SPE format that Infia used described on page 4. The convertible formats are:

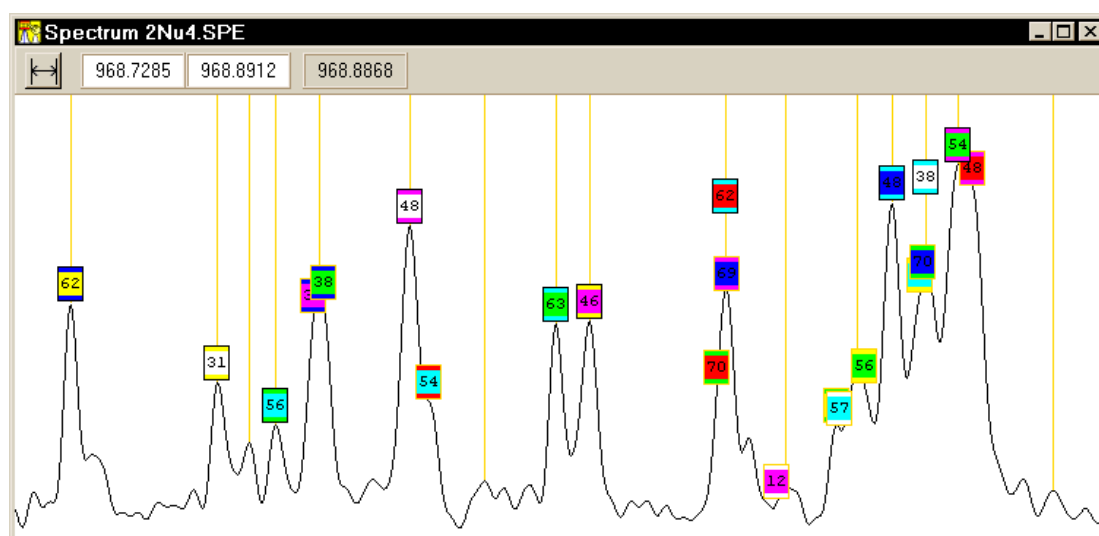
- *DIV binary format.* These are binary files with .DIV extension that are produced by certain measurement / calibration applications. They have a header of 1276 bytes followed by the spectrum point intensities as single precision (4 byte) floating point values.
- *DAT Ascii format.* This is a simple wavenumber versus intensity format looking like:

```
wavenumber1  intensity1
wavenumber2  intensity2
...
```

The special feature of this format is that the wavenumbers need not be equally spaced, ie. the steps between can vary and even be zero or negative. The data is converted to equally spaced format needed by India by interpolation (fitting 3th order polynome to 4 consequent points of data and resampling)



- **The spectrum window**



#### 5.4 Elements in the spectrum window

- **Spectrum:** the black curve
- **Detected peak positions:** yellow vertical lines
- **Assignment labels.** 62 with black border and the two colors of the bands. The text can show either the peak assigned  $m$  value or the band name (selectable from **File / Options**)
- **Prediction labels.** 56 are like assignment labels but have yellow borders. They represent the positions with predicted wavenumbers
- **Moving in the spectrum window**

See command summary for keyboard commands

## 6 Spectrum manipulation

Infia includes a number of commands for manipulation of the spectrum loaded in memory. When using these commands, two considerations must be kept in mind:

- 1 These command only affect the spectrum itself, not the peak list.
- 2 All the assignments, fits and calculations in infia are performed with the peak list only. The spectrum is displayed only for viewing pleasure.

These two considerations mean that spectrum manipulations do not affect the results of the calculations and are done for esthetic reasons only.

### **6.1 Spectra / Crop Selected Area menu command**

If the measured spectrum contains many band systems, it makes sense to slice it into smaller pieces for analysis in Infia.

Selecting a spectrum range with mouse and selecting this menu command discards all spectrum points outside the selected range.

### **6.2 Spectra / Subtract baseline menu command**

A polynome is fitted to the baseline of the spectrum and the polynome is then subtracted from all spectrum points. Helps to straighten tilted spectrum.

### **6.3 Spectra / Invert menu command**

Inversion calculates for each spectrum datapoint:

`Intensity := 1 - Intensity`

This is useful, if the measured spectrum is a transmittance spectrum having peaks downwards. The visual design of Infia assumes that the peaks are upwards.

The inversion of spectrum should not be performed if the spectrum is not yet normalised, ie. the intensities have not been scaled to 0...1 (see next paragraph)

### **6.4 Spectra / Normalize menu command**

Scales the spectrum datapoint intensities to the range 0...1. This is a requirement in Infia as all the spectrum display routines assume this intensity range. The spectrum conversion routines perform the normalisation automatically, but it must be done explicitly if the spectrum SPE data file has been prepared with some other tool.

### **6.5 Spectra / Export menu command**

With this command, one can create an wavenumber vs. intensity ASCII file of the *visible* area of the spectrum. A new resampling step can be used for the exported spectrum. The resulting file can be used to plot the spectrum with some graphing program.

## **7 Making assignments**

Assignments to the selected band can be made in three ways

### 7.1.1 Making assignments in spectrum window

- 1 In the spectrum view, click the desired peak with the right mouse button.
- 2 In the pop-up menu, select either *Automatically assign...* or *Manually assign...* In the manual assignment the peak  $m$  quantum number is asked from the user. In the automatic assignment the peak  $m$  is taken from the nearest predicted peak.

### 3 Making assignments in the assignment table

In the assignment table of the band, predictions can be converted into assignments to the nearest spectrum peak. Also, assignments that are considered bad can be converted to predictions or deleted altogether (with **CTRL+DEL** key).

Go to the *type* field of the assignment. Type letter 'a' or 'p' to the field for assignment or prediction respectively.

### 7.1.2 Making assignments in the Loomis-Wood view

To assign a peak to the selected band, hold **CTRL** and click the peak with mouse.

To remove assignment of a peak, hold **SHIFT** and click the peak with mouse.

## 8 Working with spectrum peaks

### 8.1 Peaks / Add peak menu command (CTRL + P)

### 8.2 Peaks / Delete selected peaks menu command

### 8.3 Peaks / Recalc peak intensities menu command

This procedure iterates through all spectrum peaks and sets their intensities to the spectrum intensity at the wavenumber they are located at. This is useful if the peak detection routine that has been used does not calculate intensities or calculates them incorrectly.

In most cases the usage of this method for peak intensity determination is recommended. However, note that Infia assumes that peak intensities range from 0 to 1. Hence normalisation (and possible inversion) of the spectrum is necessary before recalculating peak intensities.

## 9 View options

## 10 Band operations

The type of a band (viewed in the *type*-column of the Band table) can be: *P*, *R*, *PR* or *Q*. Hence in Infia, the term "band" does not have strictly the same meaning as it has in spectroscopy. In infia, band can mean a single *P*, *Q* or *R* branch, or a combination of *P* and *R* branches.

Note, that it is possible to have a *PR* band that only has assignments from *P* or *R* branch. This is useful when the spectrum is so simple that correct assignments can be done directly and combination difference analysis is not required. *P* and *R* type bands are meant for use in combination difference analysis.

Some menu commands in the Band menu apply only to certain subset of the four types of bands in Infia. Unavailable commands are gray and can not be chosen.

### 10.1 Operations for all types of bands

#### 10.1.1 Band / Polynome prediction menu command (F8)

Polynome prediction can be used to fit fourth order polynome to any type of band and use the fit results to calculate predicted wavenumbers. No parameter values are calculated.

#### 10.1.2 Band / Shift *m* values menu command

Shifts all the *m* assignments in a band by fixed integer amount.

#### 10.1.3 Band / Duplicate

Makes an exact copy of the band and its assignments. Sometimes when assignment of a band is somewhat unclear it is useful to work with a duplicate of a band. If it turns out that the assignments have been incorrect from some point onward, one can delete the duplicate and start again from the original (other way is to reload the project without saving changes first.)

#### 10.1.4 Band / Automatic Colors menu command

Sets the band label colors of all bands in the band table to some predefined values.

### 10.2 Parameter calculation

Parameter calculation is only available for *PR* and *Q* bands. For these types, the program assumes that the *m* assignments and lower state assignment are correct.

### 10.2.1 Band / Calculate params (All free) menu command (Shift + F8)

Fits a fourth (or sixth) order polynomial to the peak wavenumbers of a *PR* band and uses the resulting coefficients to calculate lower and upper state rotational parameters. If *H* parameters of upper or lower states are not fixed to zero, sixth order fit is used. Results are shown in the script window (viewable with menu command **Window / Script window**). In the script text, the new parameter values are compared to the old ones in the state table in terms of value and accuracy.

### 10.2.2 Band / Calculate params (Lower fixed) menu command (Ctrl + F8)

Reduces the peak wavenumbers of a *Q* or *PR* band using known lower state parameters and then fits a second order polynome to the reduced wavenumbers. This gives the upper state parameters of the band usually with a higher accuracy than in the free polynomial fit.

### 10.2.3 Band / Transfer results menu command (F9)

When band parameters are calculated with the free polynomial fit or reduced wavenumber fit, the resulting new parameters are stored in temporary state objects of the band. If the parameters resulting from the calculation are considered better (usually in terms of their standard error) than previous parameters in the state table or if there are no previously determined values, the resulting parameters can be copied with this command to the state table.

### 10.2.4 Prediction with known parameters

Assume, that one has analysed the ground state bands of the  $\nu_5$  band system,  $\nu_5$  band system and  $\nu_4 + \nu_5$  band system of some molecule (it *does* make sense to analyse first the strong ground state bands from all measured band systems and only then proceed to analyse the weaker hot bands). This analysis yield the parameters for the  $\nu_5$ ,  $\nu_4$  and  $\nu_4 + \nu_5$  vibrational states. This means that we can fully predict the positions of peaks in the  $\nu_4 + \nu_5 \leftarrow \nu_5$  hot band in the  $\nu_4$  band system and  $\nu_4 + \nu_5 \leftarrow \nu_4$  band in the  $\nu_5$  band system. Prediction with known parameters –command does just that.

To use prediction with known parameters:

- 1 Open the project that should have the new band
- 2 Make a new band record and set its molecule and lower and upper states to the states whose parameters are known.
- 3 Choose Prediction with known parameters.

- 4 Give maximum  $m$  value to include in the prediction (predicted peaks will be calculated in the range  $-\text{MaxM} \dots +\text{MaxM}$ )
- 5 When the predicted peaks appear, check them and convert them to assignments where appropriate.

## 6 **Branch combination**

Branch combination works for P and R type bands (Check from the band table that the type of the band is correct) with some peaks assigned in the respective branch with preliminary  $m$  assignments. To find the correct lower state,  $m$  assignments and peaks from the opposing branch do following:

- 1 Check in the state table, that all states you want to try as the lower state for the band have TRUE in the *Use* field and that all the others have FALSE.
- 2 Estimate, how big error you might have in the  $m$  assignments and set in the File / Options dialog box the *Max M Error* value accordingly. Also check the values of other *Band Fitness Calculation* options.
- 3 Choose the Band → P/R Branch → Predict Opposing (or F7)
- 4 Wait some seconds as Infia tries all combinations of  $m$  shifts and lower states and predicts peaks from the other branch.
- 5 Branch Combination Analysis Results –window is displayed. It shows the fitness values of all combinations sorted best first. Select any combination and inspect the *opposing* –type peaks in the assignment window.
- 6 When correct combination (usually the first one) has been chosen, select menu command Band → P/R Branch → Merge Opposing to convert the opposing peaks to assignments. This also changes the type of the band to PR, sets the correct molecule and lower state and performs the correct  $m$  shift for the original assignments.

## 7 **Resonance calculations**

## 11 **Loomis-Wood view**

### 11.1 **Drawing loomis-Wood view**

See Command Summary for **Creating Loomis-Wood views**


## 11.2 Working with assignments in Loomis-Wood view

See Command summary **Working with Assignments**

## 12 Command Summary (only often used commands)

### 12.1 Viewing the spectrum

To use these commands, the spectrum window must be active (to make it active, click its title bar with mouse or selected **Window / Spectrum** menu command)

If you want to...	How to do it
View the whole spectrum	Click  with mouse
Zoom a range of the spectrum	Select the range by dragging with mouse and press <b>Page Down</b>
Increase the level of magnification	Press <b>Page Down</b>
Decrease the level of magnification	Press <b>Page Up</b>
Move (scroll) the spectrum left or right	Press ← or →
Increase or decrease the vertical magnification	Press ↑ or ↓
Show or hide <b>peak marker</b> lines	Press <b>F5</b>
Show or hide <b>predicted peak</b> labels	Press <b>F4</b>
Show or hide <b>assignment labels</b> of other bands than the selected band	Press <b>F3</b>

### 12.2 Making and removing assignments

If you want to...	How to do it
Assign a peak <u>in spectrum window</u> to selected band with <u>definite</u> <i>m</i> number	<ol style="list-style-type: none"><li>1. <b>Click</b> the peak with right mousebutton</li><li>2. From the pop-up menu, select <b>Manually assign to...</b></li><li>3. Give the <i>m</i>-assignment</li></ol>
Assign a peak <u>in spectrum window</u> to selected band with automatic <i>m</i> assignment	<ol style="list-style-type: none"><li>1. <b>Click</b> the peak with right mousebutton</li><li>2. From the pop-up menu, select <b>Automatically</b></li></ol>

	assign to...
Assign a predicted peak <u>in assignment table</u>	In the <b>Type</b> column of the assignment table, press <b>a</b> (for "assignment") and <b>Enter</b> or or ↓
Assign a peak to selected band <u>in Loomis-Wood window</u>	Hold <b>CTRL</b> and <b>click</b> at the peak
Remove an assignment <u>in the assignment table</u>	In the <b>Type</b> column of the assignment table, press <b>p</b> (for "predicted") and <b>Enter</b> or or ↓
Remove an assignment of selected band in the <u>Loomis-Wood window</u>	Holt <b>Shift</b> and <b>click</b> the peak

### 12.3 Calculating predicted peaks and spectrum parameters

All the calculation commands apply to **Selected Band**. You can select a band from the **Band Table** viewable with **Window / Bands**.

If you want to...	How to do it
Calculate <b>predicted wavenumbers</b> with a polynome fit.	Press <b>F8</b> or select menu command <b>Band / Polynome prediction</b> .
Calculate parameters of the <b>upper and lower</b> vibrational state of the band.	Press <b>Shift + F8</b> or select menu command <b>Band / Calculate Params (All Free)</b>
Calculate parameters of the <b>upper state</b> while fixing the parameters of lower state.	Press <b>CTRL + F8</b> or select menu command <b>Band / Calculate Params (Lower Fixed)</b>
<b>See the results</b> of a parameter calculation	Select <b>Windows / Script Window</b> menu command
<b>Transfer the results</b> of the most recent calculation into the state table.	Press <b>F9</b> or select menu command <b>Band / Transfer results</b>

### 12.4 Making Combination difference analysis

If you want to...	How to do it
<b>Define</b> what <b>lower states</b> will be tried in the combination difference analysis	<ol style="list-style-type: none"> <li>1. Go to <b>State Table</b> with <b>Window / Vibrational state parameters</b> menu command</li> <li>2. In the <b>Use</b> column, set <b>True</b> to the states to include in the analysis by pressing <b>T</b> and <b>Enter</b> in the corresponding position. Set <b>False</b> with <b>F</b></li> </ol>



	and <b>Enter</b> to other states.
<b>Define</b> options for the analysis	Select <b>File / Options</b> and set <b>Band Fitness Calculation</b> options
<b>Make</b> combination difference analysis	Press <b>F7</b> or select <b>Band / P/R Branch / Predict opposing</b> menu command
<b>Construct a PR-Band</b> based on selected combination	<b>Band / P/R Branch / Merge Opposing</b> menu command

### 12.5 Working with Loomis-Wood views

If you want to...	How to do it
Define the size of the Loomis-Wood image to be <b>Full Screen size</b> .	<ol style="list-style-type: none"> <li>1. Select <b>Window / Loomis-Wood Plot</b></li> <li>2. <b>Maximize</b> the size of the Loomis-Wood window</li> <li>3. Select <b>Loomis-Wood / Loomis Parameters</b> menu command and press <b>Get Window Size</b> button.</li> </ol>
<b>Draw a Loomis-Wood image</b> with the selected band straightened.	Press <b>CTRL+W</b> or select <b>Loomis-Wood / Draw Loomis Wood</b> menu command.
<b>Zoom</b> to a part of a Loomis-Wood image	<b>Drag</b> the desired square from the Loomis-Wood image with holding <b>Right mouse button</b>
<b>View</b> a region around a peak in the <b>spectrum window</b>	<b>Click</b> on the peak
Make and remove assignments	See " <i>Making and removing assignments</i> " command summary.