SpectralLine Database Searching Software

OOISPECLINE-P/OOISPECLINE-U/OOISPM

A Mikropack Product

Installation and Operation Manual

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About This Manual

Document Purpose and Intended Audience

This document provides the OOISpecLine user with instructions for setting up, running and maintaining the SpectralLine Database Searching Software.

What's New in this Document

This version of the *SpectralLine Database Searching Software OOISPECLINE-P/ OOISPECLINE-U/OOISPM Installation and Operation Manual* adds our partnership agreement, and Appendix B: *Ionization States*.

Document Summary

Chapter	Description
Chapter 1: *Introduction*	Contains descriptive information about OOISpecLine's functionality.
Chapter 2: *Setup*	Contains a list of system requirements and installation instructions.
Chapter 3: *Operation*	Provides information on functions you can perform using your OOISpecLine software.
Appendix A: *Reference*	Provides a quick reference of OOISpecLine windows, commands, toolbar icons, and dialog boxes. This section also contains a list of applicable file formats, as well as a list of database sources.

Product-Related Documentation

You can access documentation for Ocean Optics products by visiting our website at **http://www.oceanoptics.com**. Select *Technical → Operating Instructions*, then choose the appropriate document from the available drop-down lists. Or, use the **Search by Model Number** field at the bottom of the web page.

Engineering-level documentation is located on our website at *Technical → Engineering Docs.*

Upgrades

Occasionally, you may find that you need Ocean Optics to make a change or an upgrade to your system. To facilitate these changes, you must first contact Customer Support and obtain a Return Merchandise Authorization (RMA) number. Please contact Ocean Optics for specific instructions when returning a product.

Chapter 1

Introduction

Overview

OOISpecLine is a high-end tool for all scientists and engineers working in the field of spectroscopy, such as astrophysics, plasma science or plasma processing. This tool makes it easy for you to do the following:

- Evaluate spectral data (i.e., find specific lines in spectra).
- Identify unknown peaks as well as atomic lines and molecular bands in spectral data. Peaks of lines and bands can be found almost instantly by scanning the extensive database for atoms and molecules and using several powerful filter functions. Much information about the lines in the evaluated spectrum is only a few mouse clicks away.
- Compare data from different measurements. All customary spectroscopic file formats can be processed directly, which allows an easy comparison of spectral data even from different data acquisition systems. Every single spectrum may be evaluated and adjusted on its own.

An extensive and detailed help file is available to supports you while you work with OOISpecLine.

Finding Peaks in Spectra

OOISpecLine makes it easy to find peaks. A powerful search algorithm searches for peaks of lines and bands in spectral data. Even difficult structures, i.e. double lines, line shoulders and complex band structures, are found easily and marked for further evaluation. For noisy data, several filter functions for data smoothing are available. You can find peaks with automatically generated parameters or with user-defined parameters for data smoothing or noise limits.

Identifying Atomic Lines and Molecular Bands

OOISpecLine saves you from the time-consuming job of scanning books and articles for atomic or ion lines and molecular bands that match the line or band in your spectra. To do this, OOISpecLine uses an extensive and up-to-date database. Almost instantly, all important information is available for a specific line without you opening a book. You can select specific elements for the identification process to avoid unnecessary hits and to shorten database-scanning time.

Database for Atoms and Molecules

The integrated database contains information about atoms, ions and molecules. This database is frequently updated and therefore always current. The database's modular structure allows you to design it to meet your unique requirements, often saving you time and money. It is also possible to obtain an extension of the database or an update of the latest data.

OOISpecLine offers a search engine for individual investigations independent from spectral data. Therefore, information about atoms, ions and molecules is at your fingertips.

Evaluating and Comparing Spectral Data

OOISpecLine offers many evaluation functions especially for spectral data, which are necessary to evaluate and process measured data. These functions include data smoothing, peak value and integral value function, and several calibration functions.

For a comparison of different spectra, up to twelve spectra can be open in one diagram even with different file formats. The spectra can be adjusted in wavelength and signal to compare the data easily.

OOISpecLine supports most customary file formats of spectroscopic data acquisition programs, such as ASCII, binary, OOIBase, DaVis, GRAMS, 4SPEC, MAPS. AvaSoft, and the SpecLine format. Processed and changed spectra can be saved as SpecLine, Excel (CSV), ASCII or binary files. For presentations several export filters are available including Windows Bitmap (BMP) format, Windows Metafile (WMF) format, and Corel Presentations (WPG) format.

OOISpecLine allows you to perform the whole evaluation of spectral data in a single program environment while eliminating file handling. You can read and evaluate spectral data, find peaks, identify lines, and then create a professional presentation of the data.

Chapter 2

Setup

System Requirements

The following are required to run the OOISpecLine software:

- IBM compatible PC with Pentium processor or equivalent and CD drive
- Operating system: Windows 98/ME or Windows NT 4.0/2000/XP
- Required free hard disk space: Approximately 30–80 Mbytes, depending on database version

Installation

Caution

Your OOISpecLine software was delivered with a hardware key. You must first install the software before plugging the hardware key to the computer.

► ***Procedure***

1. Insert the OOISpecLine CD in your CD drive.
2. Launch the setup program. The setup program leads you through the installation process. Follow the instructions and fill in the necessary information. All program files and the whole database will be copied on the hard disk of your computer. Please make sure that enough free disk space (approx. 30-80 MByte) is available.
3. Install the hardware key into the appropriate port on the computer. The OOISpecLine software will not run on a computer without this hardware key (see the following *Hardware Key* section).

Hardware Key

OOISpecLine requires a hardware key (included) to operate the software on your computer. Depending on your OOISpecLine model, you have received one of the following types of hardware keys:

- Model OOISPECLINE-U: Contains a hardware key that plugs into the computer's USB port. This hardware key can only be used with Windows 98, 2000, XP, or ME operating systems. It does *not* work with Windows 95 or NT systems.

- Model OOISPECLINE-S: Contains a hardware key that plugs into the computer's Parallel port (printer port). This hardware key is a feed-through device, allowing a computer to attach to one side of the key and a printer to be connected on the other side.

Removing OOISpecLine Software from Your Computer

► *Procedure*

To completely remove OOISpecLine software,

1. In Windows, activate the Software icon under **Control Panel**.
2. Select **OOISpecLine** in the lower list box and then click the **Add/Remove** button.

Chapter 3

Operation

Opening a Data File

► ***Procedure***

1. Select **File | Open** from the menu.
2. The **Format** drop-down list contains all file format currently supported by OOISpecLine. Choose the desired file format from the list and click **OK**.
3. If the wavelength unit of the spectra is not given in nanometers, OOISpecLine suggests a conversion of the given data. The wavelength unit nanometer is necessary for the line identification process. Please refer to the instructions in the *Converting the Wavelength Format* section.

The spectrum is displayed entirely in the diagram.

Converting the Wavelength Format

For identifying the atomic lines and molecular bands from the database the wavelength format of the spectra must be given in nanometers. If your data comes with a different format, OOISpecLine suggests a data conversion while opening the file. Of course, you can also convert the data later by selecting the menu command **Edit | Wavelength Format** or by clicking the  button in the tool bar.

In the **Wavelength Format** dialog box, you must select the wavelength format in which your data is stored. If your data is given in Angstroms or wave number, the conversion is done immediately. However, if your data is given in points or pixels, the **Wavelength Scaling** dialog box is opened. Here you must specify either wavelength values for two pixels or one wavelength value for one pixel and the dispersion value.

After you click **OK** to confirm your choice, the data is converted to nanometers.

Adjusting the Wavelength in Spectral Data

Often the wavelength must be adjusted, because the wavelength scaling of the measurement is not correct or different spectra can only be compared if the wavelength scales match exactly. With OOISpecLine, you can adjust the wavelength by one of the following methods:

1. Select the menu command **Edit | Scaling** or click the  button to open the **Scaling** dialog box, which is available for all displayed spectra. You can shift, stretch or compress the spectra in wavelength and signal. The reference point for stretching and compressing the wavelength is always the smallest data value. This dialog box remains available until you close it.
2. If the line cursor function is activated, you can change the wavelength at the position of the line cursor with the menu command **Edit | Adjust Wavelength**. Execute this command twice to change the value again, resulting in an adjustment of the dispersion of the spectra. A detailed description of this function is given in the **Adjust Wavelength at Line Cursor** dialog box.

Smoothing Data

OOISpecLine offers several filter functions to smooth noisy data. The **Edit | Smooth Data** menu command or the  button opens the **Data Smoothing**, dialog box in which you can select an appropriate filter function:

- The Fourier filter (according to the Wiener method) is a low-pass filter, which lets through low frequencies up to a specified limit and cuts off all frequencies above the limit. The filter function is a superposition of two functions, which are extracted from the signal range and the noise range of the data. This filter is applied best to data with white noise.
- The polynomial filter (according to the Savatzky-Golay method) calculates a weighted average value with the specified polynomial order for a data point from the neighboring points. The smoothed data is displayed as a new spectrum in the diagram and in the **File List** dialog box, and is labeled “smoothed”.

Comparing Spectral Data

For a comparison of spectral data, up to twelve different spectra can be opened and adjusted in a single diagram window. These spectra can be in different formats.

The **File | Overlay File** menu command or the  button in the tool bar opens a new spectrum and displays it in the already existing diagram window.

To select a spectrum for evaluation, check the corresponding file name in the dialog **File List** dialog box. All functions are available for all spectra.

The **File | Close Overlay File** menu command or the  button in the tool bar closes the selected spectrum and the entry in the **File List** dialog box is deleted. If you press the **Del** key in the **File List** dialog box, the file is also closed.

Arithmetic of Spectra

For comparing spectra, it is often very helpful to combine different spectra by arithmetic functions (+, -. *, /). If at least two spectra are overlaid in the diagram window, you can open the **Combine Spectra** dialog box by selecting the **Edit | Arithmetic of Spectra** menu command or by clicking the  button in the tool bar.

Select the spectra to combine from the file lists, and then select the operation. You can choose between addition, subtraction, multiplication and division.

The calculated data is displayed as a new spectrum in the diagram and in the **File List** and is labeled according to the operation.

Integrals

Integrals of lines and band structures are very important for evaluating spectral data. **OOISpecLine** offers an appropriate function that is very easy to use. Select the **Edit | Integral** menu command or click the  button. The Integral dialog box opens and two dashed, vertical lines are displayed. The lines indicate the limits of the integral. You can move these lines with the mouse or with the keyboard using the **L** (left) or **R** (right) key in combination with the arrow keys. Specific integral limits can be specified in the dialog box. The integral value and the limits are displayed in the dialog box.

Identify Spectrum

Before you can identify the spectrum you must first activate the line identification mode by selecting the menu command **Identification | Open Line Identification** menu command or by pressing the  button in the tool bar. The dialog **Line Identification** dialog box is displayed. Select the **Identify Spectrum** option.

Identify Spectrum is split into two processes, which can be carried out independently:

- Peak finding – searches the spectrum for peaks. Use the **Find Peaks** register to perform functions such as smoothing noisy data or evaluating only a part of the spectrum. After searching for peaks, the lines and band structures found are marked.
- Line identification – searches for each peak in the database for entries. Use the Identify Lines register to select the atoms and molecules, which should be search in the database, and to specify the hit interval. After the line identification process has executed, the identified lines and band structures are labeled in the diagram

You can find detailed information about these functions under the specific key words.

Start the peak finding and/or line identification processes by pressing the **Start** button in the dialog **Line Identification** dialog box. Change the parameters for these processes by pressing the **Options** button to open the **Options: Identify Spectrum** dialog box.

A compilation of the parameters and actions are displayed **Line Identification** dialog box, as well as the number of peaks found and identified.

Adding and Deleting Peaks

If you want to select peaks for the line identification process on your own or if some peaks were not marked by the peak finding process (due to noisy data, for example) you can add or delete peaks for line identification easily.

Select the **Identification | Add Line** menu command or click the  button to change the mouse pointer to a cross in the diagram window. Move the mouse pointer to the specific wavelength using the mouse or the arrow keys. The current position of the mouse pointer is displayed in the right corner of the Status bar at the bottom of the window. Pressing the left mouse button adds a marking for the line identification process.

To delete a peak for the line identification process, select the specific peak with the left mouse button. The peak is selected if a dashed rectangle is displayed around the marking. To delete the peak select the **Identification | Delete Line** menu command or click the  button in the menu bar.

Display Line Positions from Database

As an alternative to the identification of the spectrum, you can display the line positions from the database in the spectrum. This allows you to have a quick overview of possible atomic lines or molecular bands.

Before you can display the line positions from the database you must activate the Line Identification mode by selecting the menu command **Identification | Open Line Identification** menu command or by clicking the  button in the tool bar. The **Line Identification** dialog box is displayed from which you select the **Display line positions from database** option.

Start the process by clicking the **Start** button in the **Line Identification** dialog box.

You can change the parameters for a database search by clicking the **Options** button to open the **Options: Display Line Positions From Database** dialog box. Then select the atoms and molecules, which should be search in the database. You can find detailed information about these functions under the specific key words.

Saving and Loading Configurations

For your convenience, you can save and load configurations of identification processes and database searches. In the **Options: Identify Spectrum** and **Options: Display Line Positions From Database** dialog boxes, you can save the actual settings using the button **Save configuration...** button. Or, you can load a previously stored configuration using the **Load configuration...** button.

Getting Information about Lines

To obtain detailed information for a specific line, you must first select this line by clicking on it. The line is selected if a dashed rectangle is displayed around the marking. Selecting **Identification | Line Info** menu command or clicking the  button in the tool bar displays all available information for the selected line in the **Line Information** window.

Saving Data

Evaluated and changed spectra can be saved in its current form as a SpecLine, an Excel (CSV) file, an ASCII file, or a binary file by selecting the **File | Save as...** menu item or by pressing the  button in the tool bar. Specify the format and file name in the **Save as** dialog box.

In the Excel (CSV), ASCII and binary formats, only spectral data is saved, whereas in the SpecLine format, the data from the spectrum identification and database search is saved as well.

For presentations, the entire diagram can be exported in several graphic formats.

The **File | Export...** menu command exports the diagram in a graphic format. You specify this format and the file name in the **Export as Graphic File** dialog box.

To copy the entire diagram to the clipboard in bitmap format, select the **Edit | Copy to Clipboard** menu command or click the  button in the tool bar.

Database Search

OOISpecLine's database search capability enables you to search individually for atomic lines and molecular bands in the database independent of spectral data.

► *Procedure*

To search the database,

1. Select the **Database | Open...** menu command or click the  button in the tool bar. The **Database Search** dialog box appears. Here you can change the parameters for the searching process.
2. Select the desired elements from the periodic table and the molecule list.
3. Check the **Neutrals** and **Ions** options and specify the wavelength and intensity range for the searching process.
4. Click **OK**. The line search process starts. All lines found are listed in the **Database** window with information about line strength, energy levels, transition, and quantum numbers.

Appendix A

Reference

Overview

This appendix is intended to be used as a quick reference for OOISpecLine windows and commands.

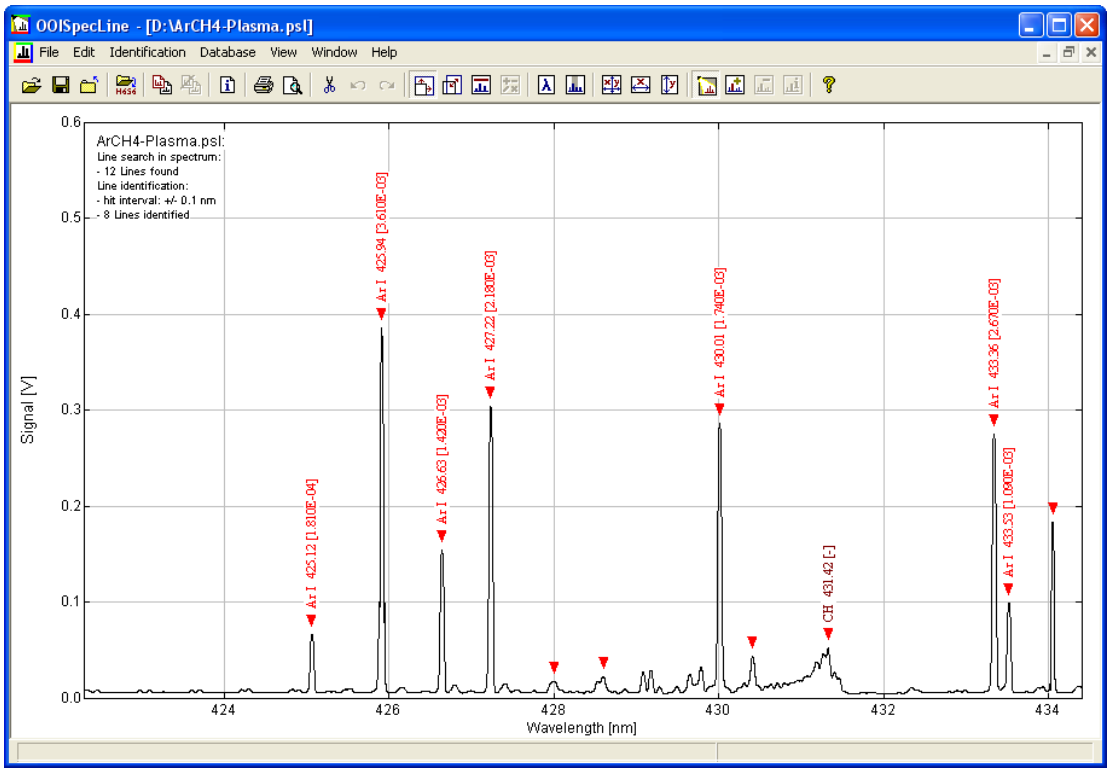
OOISpecLine Windows

The main OOISpecLine windows consist of the following:

- *Diagram Window*
- *Line Information Window*
- *Database Window*

Diagram Window

The Diagram window is the main window of OOISpecLine in which the spectral data is graphically displayed. Here, you can start the peak finding and line identification processes and evaluate spectral data using the evaluation functions.



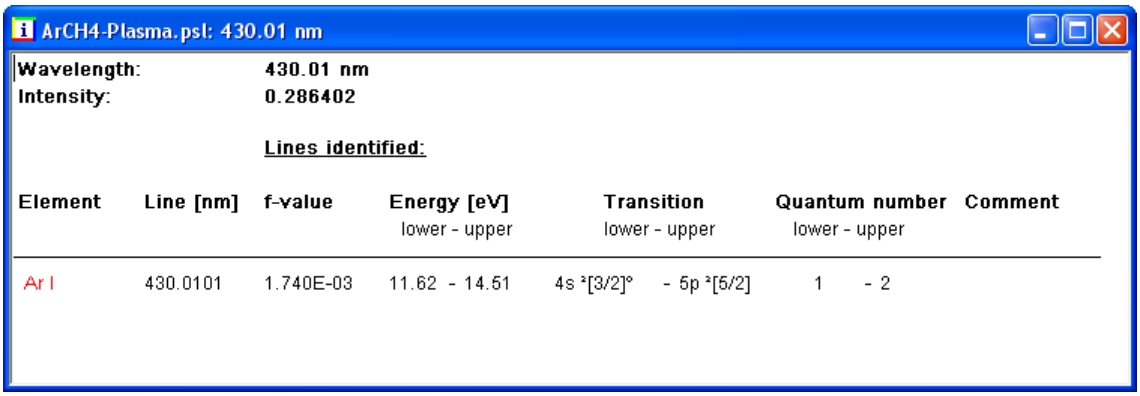
You can open as many Diagram windows as you like. In each Diagram window, up to twelve spectra (even with different file formats) can be opened, displayed and evaluated.

The diagram consists of a frame with title and axis labels. The spectra are displayed in color or black and white. In addition, a grid of lines and a legend with specific information can be inserted.

Lines and band structures found by the peak finding process are marked with a red triangle. If they are identified, they are also labeled with the element name and wavelength. These marked and identified atomic lines and molecular bands can be selected with the left mouse button. The currently selected line is indicated by a frame around the marking and label.

Line Information Window

The Line Information window displays all identified lines of atoms and ions and all molecular bands for the selected line. On top the wavelength and intensity of the selected line from the spectra is given followed by the *Lines identified* table, in which each row contains specific information from the database:



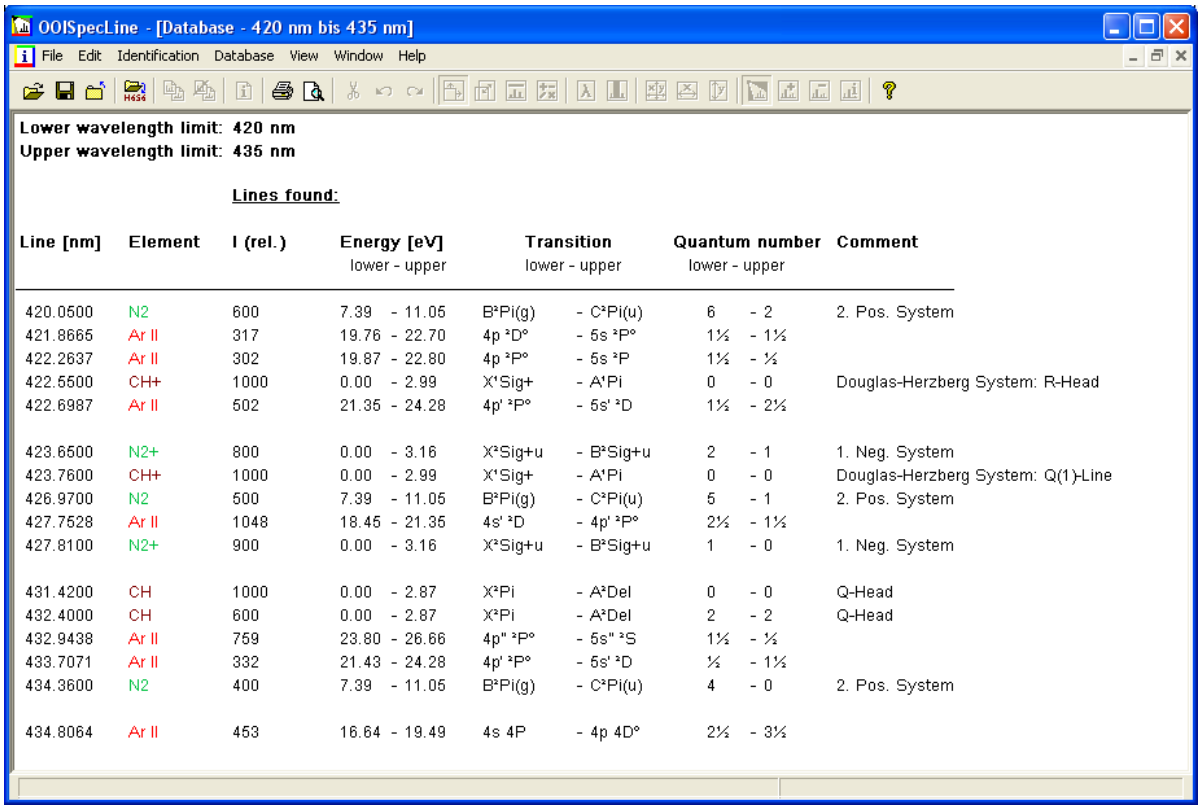
Field	Description
Element	Lists the element name and ionization state in spectroscopic notation for each identified line or band. The color of the entry corresponds to the color of the element in the diagram window.
Line (nm)	This is the exact wavelength of the identified line or band from the database. If several lines or bands of the same element were found, the strongest line is marked with an asterisk (*). Only this line is displayed in the diagram window.
Line Strength (f-value)	Depending on your selection the line strength is displayed in relative units, in f-values (oscillator strength) or A_{ik}-values (transition probabilities). The line strength in relative units is related to the f-value of the atomic line. A relative line strength of 1000 corresponds to an f-value of 1. If no data is available for an element, the relative line strengths are normalized to the strongest line or band that is set to 1000.
Energy (eV)	The energy in electron volt (eV) of the lower level (left column) and of the upper level (right column) involved in the transition.
Transition	The notation of the transition with the lower electronic state (left column) and the upper electronic state (right column).
Quantum number	The quantum numbers of the lower level (left column) and of the upper level (right column) involved in the transition. For atoms the quantum number J, and for molecules the vibrational quantum number v is given.
Comment	Additional information concerning the transition. Information (especially for molecules) regarding band heads and rotational branches are given in this column.

Note

The table can be printed and copied to the clipboard for further processing in other programs. The table can also be saved as an RTF or an ASCII file.

Database Window

The Database window lists all atomic and ion lines as well as molecular bands found in the database for the given search parameters. On top the wavelength interval is given followed by the *Lines found* table containing information about the lines:



Field	Description
Wavelength	Displays the exact wavelength of the identified line or band.
Line (nm)	This is the exact wavelength of the identified line or band from the database. If several lines or bands of the same element were found, the strongest line is marked with an asterisk (*). Only this line is displayed in the diagram window.
Element	Lists the element name and ionization state in spectroscopic notation for each identified line or band. The color of the entry corresponds to the color of the element in the element in the selection list of the search engine dialog box.
Line Strength: I (rel.)	Depending on your selection the line strength is displayed in relative units, in f-values (oscillator strength) or A_{ik}-values (transition probabilities). The line strength in relative units is related to the f-value of the atomic line. A relative line strength of 1000 corresponds to an f-value of 1. If no data is available for an element, the relative line strengths are normalized to the strongest line or band that is set to 1000.

Field	Description
Energy (eV)	The energy in electron volt (eV) of the lower level (left column) and of the upper level (right column) involved in the transition.
Transition	The notation of the transition with the lower electronic state (left column) and the upper electronic state (right column).
Quantum number	The quantum numbers of the lower level (left column) and of the upper level (right column) involved in the transition. For atoms the quantum number J, and for molecules the vibrational quantum number v is given.
Comment	Additional information concerning the transition. Information (especially for molecules) regarding band heads and rotational branches are given in this column.

Note

The table can be saved as an Excel (CSV), an RTF or an ASCII file. The table can also be printed and copied to the clipboard for further processing in other programs.

Menu Commands

Menu	Command	Icon	Description
File	File | Open		Opens a data file in a new Diagram window.
	File | Close		Closes the active Diagram window with all spectra.
	File | Save As		Saves data as follows, depending on the active window: • Diagram window: The selected spectrum is saved with all changes as a SpecLine, a binary or an ASCII file. • Line information window: The list containing the line information is saved as an RTF or an ASCII file. • Database window: The list containing the line information is saved as an Excel (CSV), an RTF or an ASCII file.
	File | File Info		Displays information about the files appearing in the active Diagram window (such as the file names, the wavelength and signal range, and the number of data points).

Menu	Command	Icon	Description
File (Cont'd)	File | Overlay File		Opens a data file in the active Diagram window. Up to 12 data files (even with different file formats) can be opened, evaluated and processed in one Diagram window.
	File | Close Overlay File		Closes the selected spectrum without closing the Diagram window. Use the *File List* dialog box to select a spectrum.
	File | Print Preview		Displays the active window on the screen as it appears in the printout.
	File | Print		Prints the active window.
	File | Printer Setup	N/A	Allows you to change the printer options
	File | Export	N/A	Exports the diagram in the active Diagram window to a graphics file.
	File | Exit	N/A	Closes the OOISpecLine application.
Edit	Edit | Undo		Undoes the last command. Up to 12 consecutive changes can be undone in one Diagram window.
	Edit | Redo		Cancels the last Undo command.
	Edit | Refresh	N/A	Refreshes the active Diagram window. This command deletes all false displays on the screen that may be lingering after a lot of editing.
	Edit | Display		Opens the **Display** dialog box, enabling you to change the display values of the axis. You can also access this command in the **Context** menu by clicking the right mouse button in the Diagram window.
	Edit | Scaling		Opens the Scaling dialog box, allowing you to shift and stretch the spectrum. Use this function to adjust different spectra's wavelength and signal. You can also access this command in the **Context** menu by clicking the right mouse button in the Diagram window.

Menu	Command	Icon	Description
Edit (Cont'd)	Edit | Adjust Wavelength	N/A	Changes the wavelength of the selected spectrum where the line cursor is located. This function makes it easy for you to adjust a spectrum, provided you know the exact wavelength of specific lines or band structures. You can also access this command in the **Context** menu by clicking the right mouse button in the Diagram window.
	Edit | Arithmetic of Spectra		Opens the **Combine Spectra** dialog box, which allows you to combine two overlaid spectra with arithmetic functions. Use this function to simplify the comparison of spectra.
	Edit | Wavelength of Spectra		Converts the wavelength unit of the selected spectrum to nanometers. This conversion is necessary to carry out a line identification process. A conversion from all customary formats is possible.
	Edit | Smooth Data		Enables you to smooth data using several filter functions. This smoothed data is then displayed as a new spectrum in the diagram.
	Edit | Integral		Launches the function for evaluating integrals of lines and band structures in the current Diagram window.
	Edit | Zoom in	N/A	Allows you to zoom in on the part of the spectrum selected by clicking the left mouse button and drawing a circle on the spectrum. This function is always available in the active Diagram window.
	Edit | XY-Autoscale		Displays the selected spectrum in its entirety. The display ranges of the wavelength and the signal correspond to minimum and maximum values of the selected spectrum.
Identification	Identification | Open Line Identification		Activates/deactivates all functions for the peak finding and line identification processes for the selected spectrum. The peak finding and line identification functions are applied to the currently selected spectrum.
	Identification | Identify Spectrum	N/A	Launches the peak finding and line identification functions according to the given parameters. This menu command is the same as clicking the **Start** button in the **Line Identification** dialog box with the **Identify spectrum** option selected.

Menu	Command	Icon	Description
Identification (Cont'd)	Identification | Display Line Positions From Database	N/A	Launches the database search and display of database lines according to the given parameters. This menu command is the same as clicking the **Start** button in the **Line Identification** dialog box with the **Display line positions from Database** option selected.
	Identification | Add Line		Adds a peak to the list for the identification process. After invoking this command, the cursor in the Diagram window changes to a cross. Move the cursor to the desired position and confirm by clicking on it. The exact position of the cursor in the diagram is displayed in the lower right button in the status bar. This command is also available in the **Context** menu by clicking the right mouse button in the Diagram window.
	Identification | Delete Line		Deletes the selected peak from the list for the identification process. Select a peak by clicking on the peak's mark. This command is also available in the **Context** menu by clicking the right mouse button in the Diagram window.
	Line Search | Delete All Lines	N/A	Deletes all peaks from the list for the identification process. This command is also available in the **Context** menu by clicking the right mouse button in the Diagram window.
	Identification | Wavelength of Peak	N/A	Adjusts the wavelength of the selected peak. This allows you to easily adjust the spectrum, if you know the exact wavelength value of the peak. This command is also available in the **Context** menu by clicking the right mouse button in the Diagram window.
	Identification | Line Info		Displays all the available information about the selected peak, including the wavelength and signal values, and a list of all lines and band structures found in the identification process with details for each line. Select a peak by clicking on the peak's mark. This command is also available in the **Context** menu by clicking the right mouse button in the Diagram window.

Menu	Command	Icon	Description
Identification (Cont'd)	Identification | Edit Line Entries	N/A	Lists all lines and band structures found with the identification process for the selected peak. You can then delete unwanted entries. Select a peak by clicking on the peak's mark. This command is also available in the **Context** menu by clicking the right mouse button in the Diagram window.
Database	Database | Open		Launches an OOISpecLine database search. An integrated database search enables you to search for specific lines and band structures of atoms, ions or molecules in the database.
	Database | Close	N/A	Closes the Database window.
	Database | Save result as	N/A	The list containing the line information is saved as an Excel (CSV), an RTF or an ASCII file.
View	View | Toolbar	N/A	Displays or hides the toolbar (toggle).
	View Status Bar	N/A	Displays or hides the status bar (toggle)
	View | Line Cursor	N/A	Displays or hides the line cursor in the diagram (toggle). The exact position of the line cursor in the diagram is displayed in the lower right corner in the status bar. Use either the mouse or the arrow keys to move the cursor. For larger operations, you can also use the Shift and Ctrl keys.
	View | Legend	N/A	Displays or hides the diagram's legend (toggle). Use **View | Text Options** to control the legend's position and display.
	View | Black/White Picture	N/A	Controls the display in the Diagram window to appear in black and white or color (toggle).
	View | Horizontal Lines	N/A	Displays or hides the horizontal lines in the diagram (toggle).
	View | Vertical Lines	N/A	Displays or hides the vertical lines in the diagram (toggle).
	View | Logarithmic x Axis	N/A	Displays the x-axis in a logarithmic or linear scale.
	View | Logarithmic y Axis	N/A	Displays the y-axis in a logarithmic or linear scale.

Menu	Command	Icon	Description
View (Cont'd)	View Line Color	N/A	Enables you to change the line color of the currently selected spectrum.
	View | Text Options	N/A	Opens the dialog **Text Options** dialog box, which allows you to change the following: • labels for title and axis • position and text for legend • font and size of text
Window	Window | Cascade	N/A	Cascades the open windows.
	Window | Tile	N/A	Tiles the open windows.
	Window | Tile Horizontally	N/A	Horizontally tiles the open windows.
	Window | Arrange Icons	N/A	Displays the windows as icons.
	Window | Close Windows	N/A	Closes all windows.
Help	Help | OOISpecLine Help		Opens the OOISpecLine online help file. This is a PDF document, requiring Adobe Acrobat. If you do not have Adobe Acrobat installed on your computer, you can download this program from the Adobe website for free.
	Help | About	N/A	Displays information about the OOISpecLine software.

Toolbar

The toolbar displays the most important and often used menu commands as icons. By clicking on the icon, you can invoke its corresponding menu command. Toolbar icons are listed in the following table.

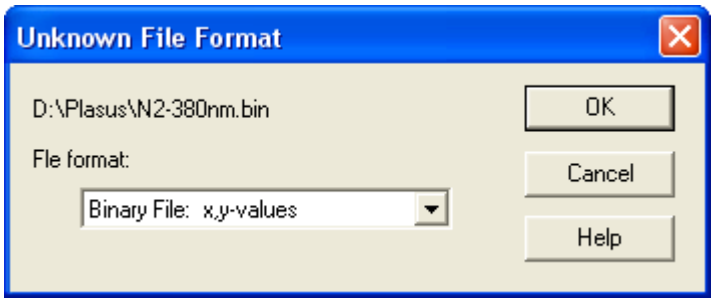
Icon	Action	Icon	Action
	Opens data file		Changes shift/dispersion of spectrum
	Closes window with all files		Smoothes data
	Saves the data file.		Arithmetic of spectra

Icon	Action	Icon	Action
	Independent database search		Convert wavelength format
	Overlay data file		Integral function
	Close overlaid data file		xy-Autoscale
	Information about the data files		x-Autoscale
	Print		y-Autoscale
	Print Preview		Activate/close line identification
	Copy diagram to clipboard		Add peak for the line identification process
	Undo last command		Delete the selected line marking
	Cancel last Undo command		Information about the selected line
	Change display values of axis		Help file

Dialog Boxes

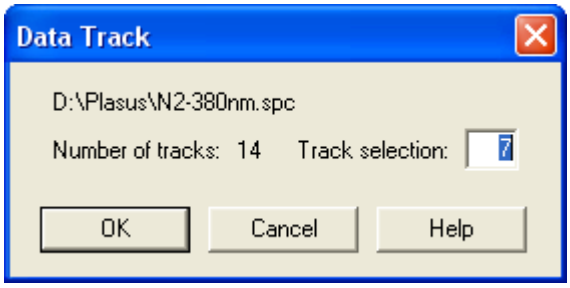
Unknown File Format

The data format of the opened file could not be identified. Select the correct format from the given list and click **OK**. See File Formats for a description of the supported file formats.



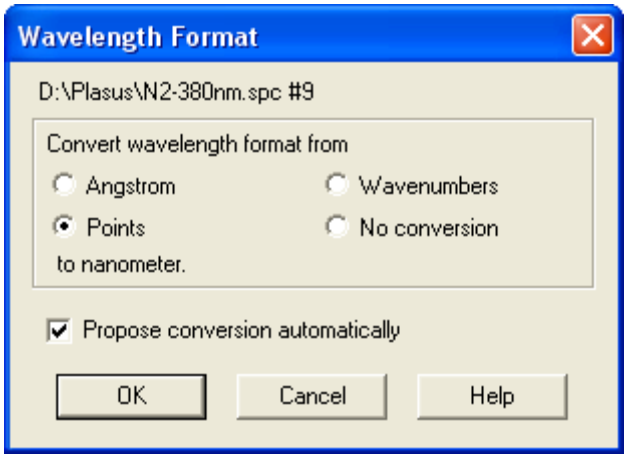
Data Track

The opened file contains more than one data track. Select the data track to be displayed and click **OK**. The data tracks are listed according to the specific file format. Refer to the documentation for the corresponding data acquisition program for more information about the nomenclature of data tracks. You can open several data tracks in one Graphics window by applying the **File | Overlay File** command for each of the different data tracks.



Wavelength Format

OOISpecLine has detected that the wavelength of the data file is given in the units checked in the list below. For the line identification process, a conversion of the wavelength format to nanometers is necessary. Click OK to confirm the conversion to nanometers. To skip the unit check while opening a new data file, uncheck **Propose conversion automatically**. You can convert the wavelength format later using the **Edit | Wavelength Format** menu command.



Wavelength Scaling

The wavelength units in the opened data file are either not given or given in pixel/points. The data is displayed as a function of the data points. For scaling the wavelength, two options are available:

- **2 Points** – Specify the wavelength of two data points in nanometers and click **OK**.
- **Point and dispersion** – Specify the wavelength of one data point in nanometers and the dispersion of the spectral data in nanometers/points and click **OK**.

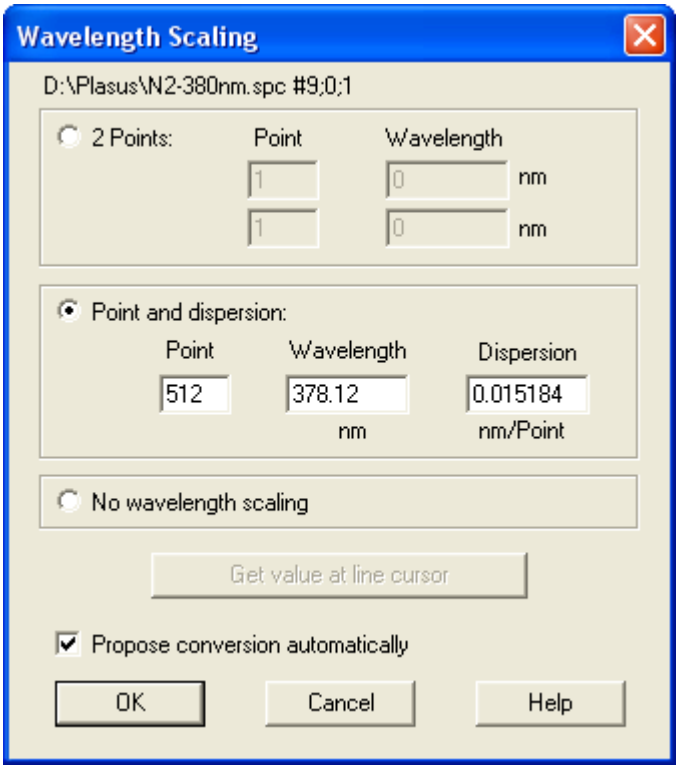
If the line cursor is activated in the opened data file, you can take the data points directly from the line cursor position. Use the following procedure.

► *Procedure*

To take data points directly from the line cursor position,

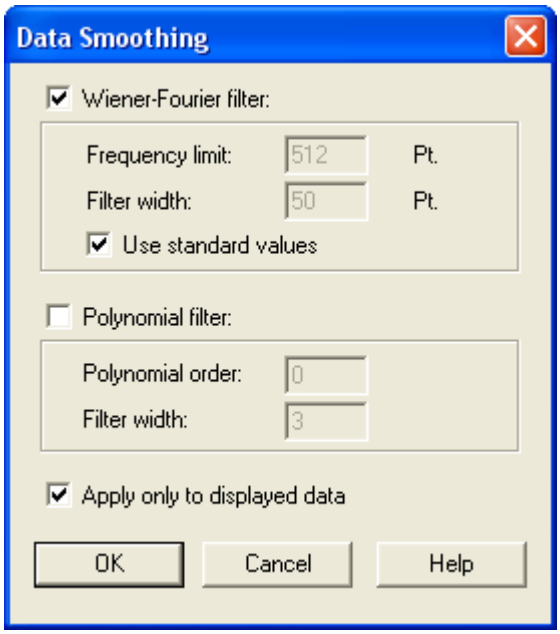
1. Move the line cursor to the desired position in the diagram,
2. Set the cursor to the edit box in the dialog box for the selected data point.
3. Click the **Get value at line cursor** button. The point or pixel number is copied to the edit box.

To skip the unit check while opening a new data file, uncheck the **Propose conversion automatically** box. You can convert the wavelength format later using the menu command **Edit | Wavelength Format** menu command.



Data Smoothing

For noisy data several filter functions are available for smoothing the spectral data. In this dialog you can set the parameters of the different filter functions.



Wiener-Fourier filter

If you choose this filter type the spectral data is smoothed according to the method of the Wiener-Fourier filter. The values for the frequency limit and the band width of the low-pass filter may be either set by the user or set to standard values, which are extracted from the data automatically by OOISpecLine. The later is recommended for a first run, where the extracted standard values will be displayed in the edit boxes and can be changed if necessary.

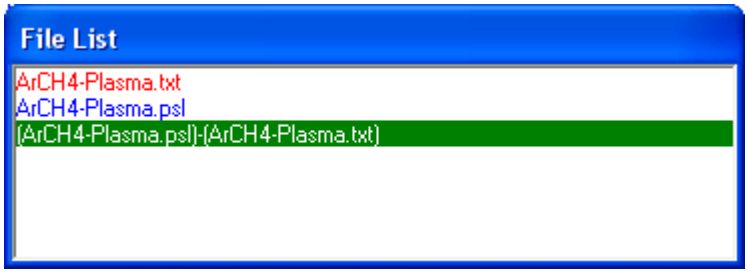
If both filter types are selected, the Wiener-Fourier filter is applied first to the spectral data followed by the polynomial filter.

Polynomial filter

According to the Savatzky-Golay technique, the polynomial order and the filter width must be specified for the polynomial filter.

File List

In this dialog box all displayed spectra opened in one diagram window are listed. The file name of the spectrum is displayed in the same color as the spectral curve.



A spectrum must first be selected before it is evaluated and processed. Select a spectrum by selecting its corresponding file in this dialog box. The selected spectrum is highlighted in the file list and the file name is displayed in the title bar of the Diagram window.

Display

Use this dialog box to change the range displayed in the diagram. The Display dialog box is available for Diagram windows and remains open until you close it.

Wavelength

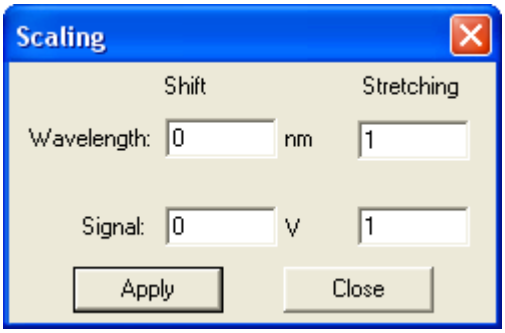
Only the data of the given wavelength range is displayed in the diagram.

Signal

Only the data of the given signal range is displayed in the diagram.

Scaling

Use this dialog box to shift a spectrum or change the dispersion, which may be necessary if the wavelength or the dispersion could not be specified exactly during the data acquisition process. The Scaling dialog box is available for Diagram windows and remains open until you close it.



Wavelength

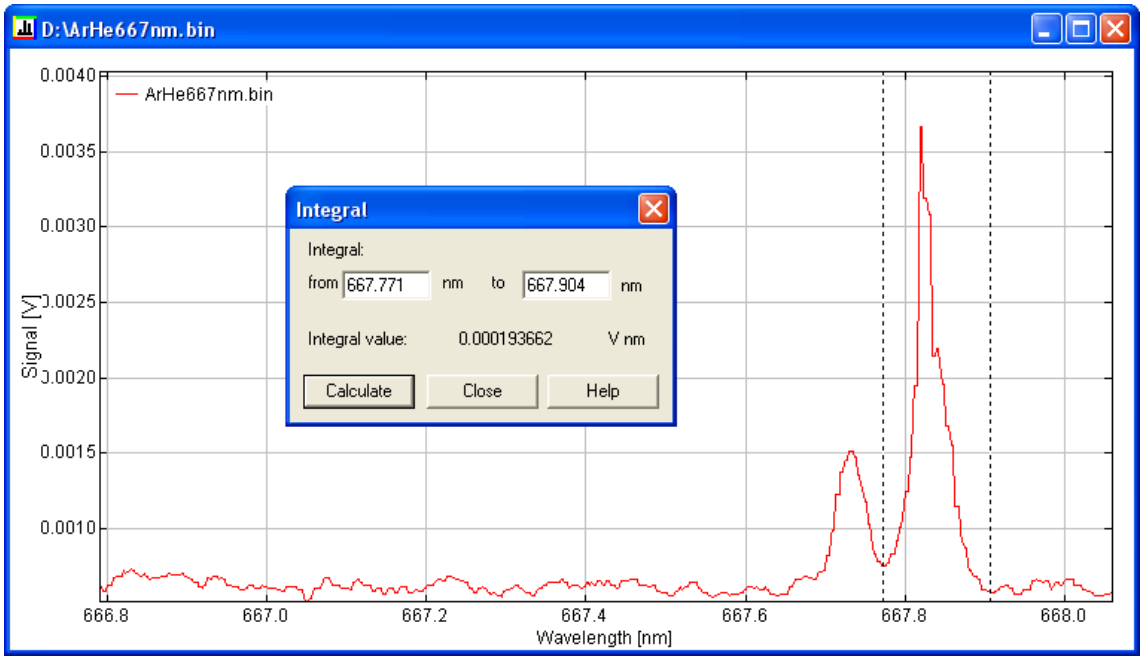
The spectrum shifts by the specified wavelength and compresses (<1) or stretches (>1) according to the specified dispersion value. The reference point for compressing and stretching the data is set to the smallest wavelength value of the spectrum. For an easy and precise comparison of overlaid spectra, it is recommended that you adjust the wavelength scale as well as the underground and peak values of the signal.

Signal

The spectrum shifts by the specified signal and compresses (<1) or stretches (>1) according to the specified dispersion value.

Integral

Use the Integral dialog box to easily calculate integrals of lines and band structures. Two vertical, dashed lines are displayed in the graph to represent the limits of the integral. These lines can be moved using the mouse or the keyboard (L and R keys along with the arrow keys). The Integral dialog box is available for Diagram windows and remains open until you close it.



Integral

Displays the current wavelength limits of the integral. If you want to specify exact values, enter the limits here. The integral is calculated after you click **Calculate**.

Integral value

Displays the current integral value calculated from the data.

Adjust Wavelength at Line Cursor

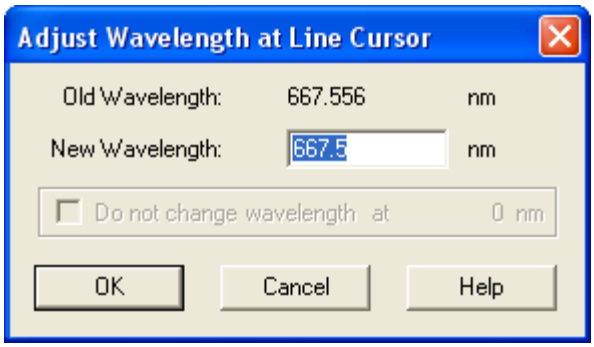
If you know the exact wavelength of a line or structure, you can easily adjust the spectrum using this dialog box.

► *Procedure*

1. Move the line cursor to the desired wavelength position.
2. Open the **Adjust Wavelength at Line Cursor** dialog box with the **Edit | Adjust Wavelength** command.
3. Enter the correct wavelength in the **New Wavelength** field.

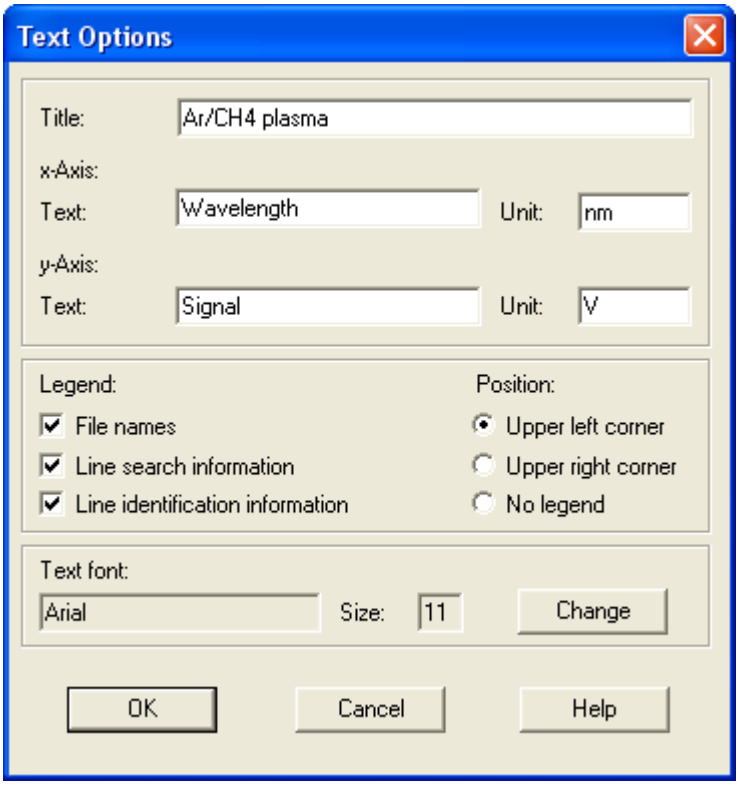
   If two lines or structures can be assigned with exact wavelength values, the spectrum can be adjusted by applying this command twice: For the first position, proceed as described above, then move the line cursor to the second position in the spectrum and open this dialog box again. Enter the correct New Wavelength for the second data point and select the check box **Do not modify wavelength at ... nm**. The specified wavelength here is the value of the changed position.

4. Click **OK**. The spectrum is shifted, stretched and/or compressed according to the given parameters.



Text Options

Use this dialog box to change the labels, legend and text font.



Labels

Enter the title, as well as the labels and units of the axes as they should appear in the Diagram window.

Legend

Specify the information to be displayed in the legend and where the legend appears in the diagram.

Text font

Select the text font of the labels. You can change it by clicking **Change** and selecting another font from the given list.

Line Identification

To activate line identification, by select the **Identification | Open Line Identification** menu command. The **Line Identification** dialog box appears, allowing you to control the peak finding and line identification processes.

Identify spectrum

Depending on your selection, a peak finding and/or a line identification process is carried out. After finding all line peaks in the spectrum, the Find peaks process can be switched off.

Display line positions from database

The line positions from the database will be displayed in the spectrum.

Information Window

The information window keeps track of the current status of the peak finding and line identification processes and records all previous actions.

Start

The **Start** button launches peak finding, line identification, and/or the database search according to the specified parameters.

Options

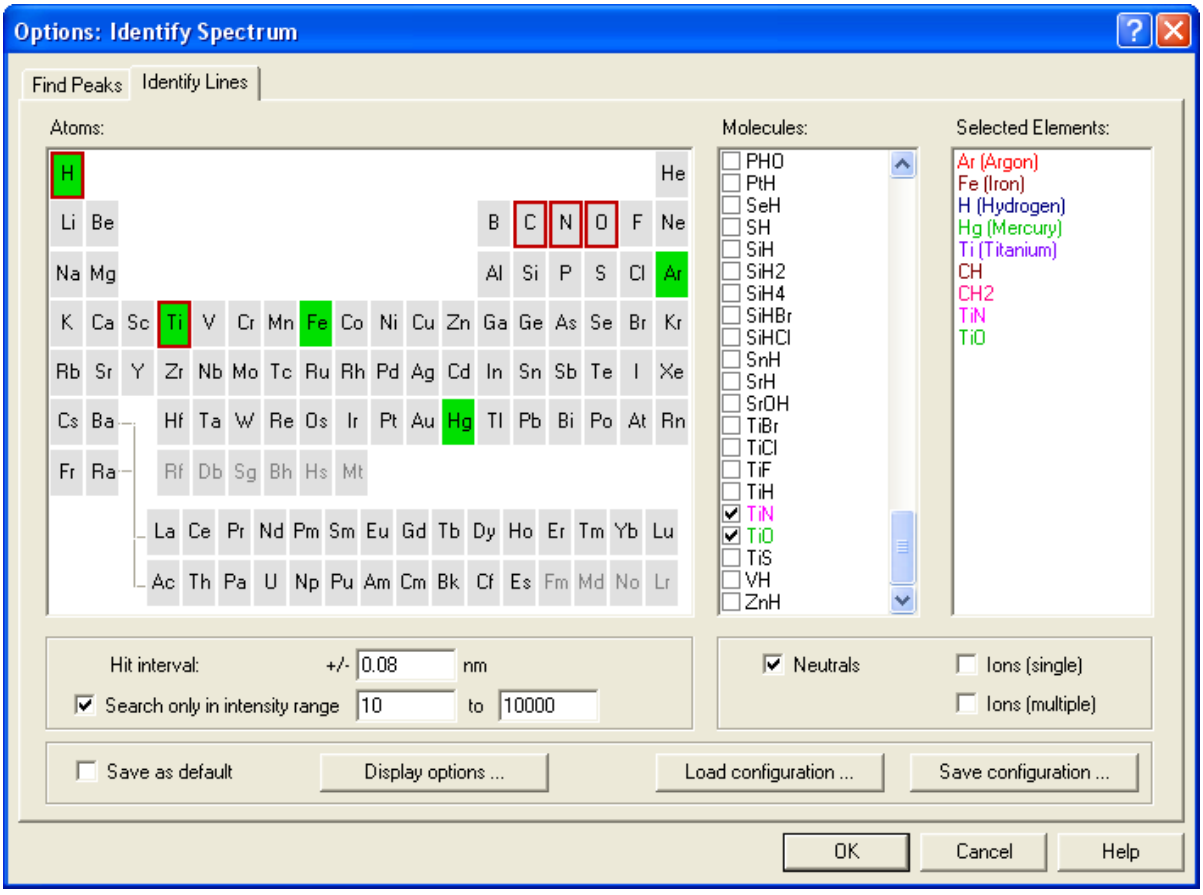
The button **Options** button opens either the **Options: Identify Spectrum** or the **Options: Display Line Positions From Database** dialog box for you to select the line identification or the database search, respectively.

Close

Click **Close** to deactivate the line identification mode.

Options: Identify Spectrum: Identify Lines Tab

All parameters for the line identification process are set in this screen. Select the atoms, molecules and ions to be included in the identification process in this register.



Atoms

Click on the atom(s) in the periodic table to be considered in the line identification of the spectrum. Selected atoms have green background color. A red border indicates that molecules containing this atom are also selected. Use the **Context** menu by clicking the right mouse button to select and deselect all atoms and molecules.

Molecules

This field lists all molecules containing at least one of the atoms selected in the periodic table. Check the box in front of the molecule for the line identification process. Use the **Context** menu by clicking the right mouse button to select and deselect all listed molecules.

Selected Elements

This list contains all atoms and molecules selected for the line identification process. You can use this list as a summary and check.

Hit interval

Use this field to specify how precisely the peak wavelength must fit the wavelength from the database. If the value from the database lies within the limits of the hit interval, the line or band is selected for identification. If no lines are identified, either the hit interval is too small or the element selection is incorrect.

Intensity range

If you want to identify lines only in a given intensity range, please check the box and specify a lower and upper limit of the intensity range. Lines are set to be identified, if the value of the relative intensity given in the database lies in the specified intensity range. The unit of the specified values must correspond to the selection in the dialog *Display Options*.

Neutrals and Ions (single and multiple ionized)

Specify which types of selected elements should be scanned in the line identification process.

Save as default

Select this option when closing the dialog box to save the current values as the default values.

Display options...

Click this button to open the **Display Options** dialog box, in which you can change the display of the results in the spectrum and in the results tables.

Load configuration...

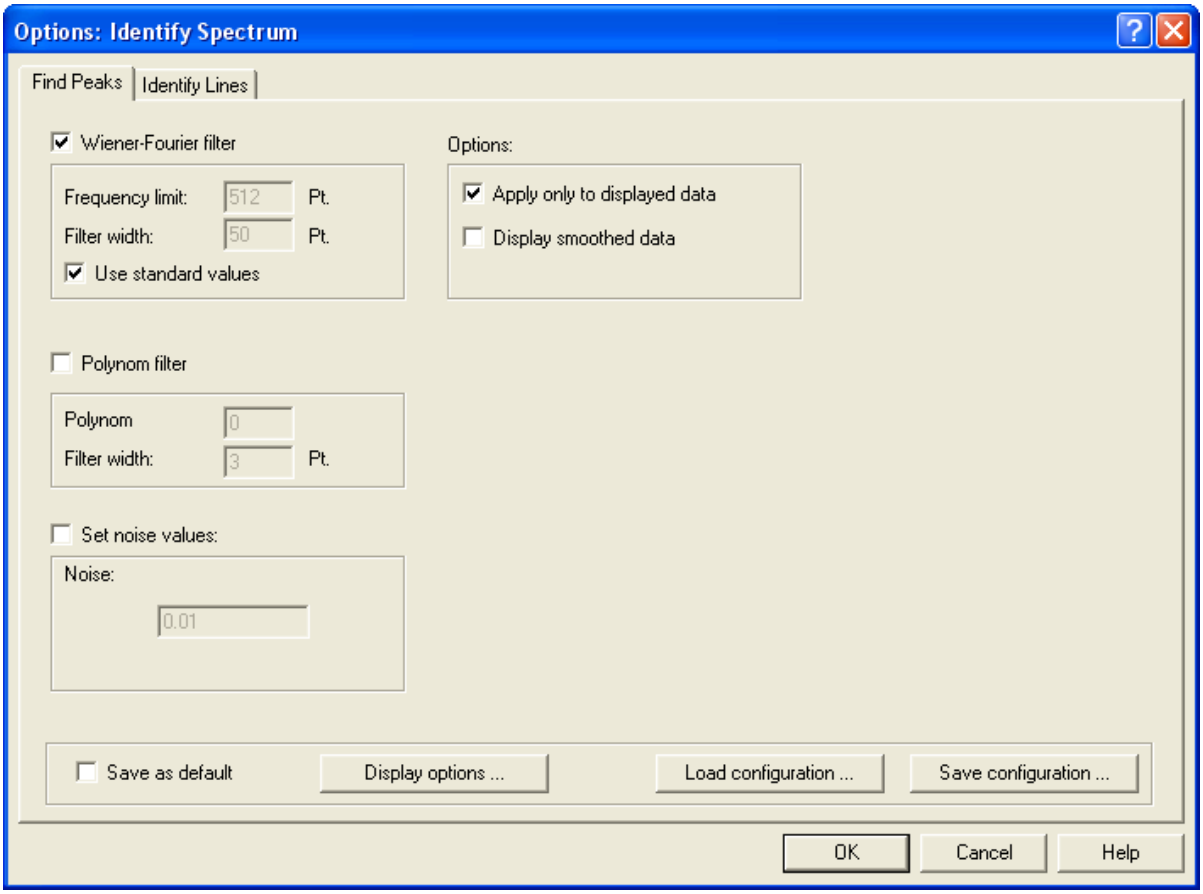
Click this button to load a stored configuration (atom and molecule selection, filter, hit interval,...) for the spectrum's line identification process.

Save configuration...

Click this button to save the current configuration for the spectrum's line identification process.

Options Identify Spectrum: Find Peaks Tab

Set the parameters for the peak finding process using this screen.



Wiener-Fourier filter

Choose this filter type to smooth the spectral data according to the Wiener-Fourier filter method. The values for frequency limit and bandwidth of the low-pass filter can be set by you, or are set to standard values extracted from the data automatically by OOISpecLine. Standard values are recommended for a first run. The extracted standard values are displayed in the edit boxes and can be changed if necessary.

If both filter functions are selected, the Wiener-Fourier filter is applied first to the spectral data followed by the polynomial filter.

Polynomial filter

According to the Savatzky-Golay technique, the polynomial order and the filter width must be specified for the polynomial filter.

Set noise values

For finding peaks of lines and band structures, a noise value is necessary to distinguish between signal and noise. OOISpecLine calculates this value automatically from the data. To change this value, check the box and enter the value. For a first run, it is recommended that you calculate the noise value automatically. The extracted standard values are displayed in the edit box and can then be changed, if necessary.

Options

This field enables you to set the following optional parameters:

- Check **Apply only to displayed data** to search for peaks and identify lines and band structures only in the displayed part of the spectrum. This can save time, especially if the spectral data consists of a large number of data points.
- Check **Display smoothed data** to display the smoothed spectrum in the diagram.

Save as default

Select this option to save the current values as default values when this dialog box is closed.

Display options...

Click this button to open the **Display Options** dialog box, in which you can change the display of the results in the spectrum and in the results tables.

Load configuration...

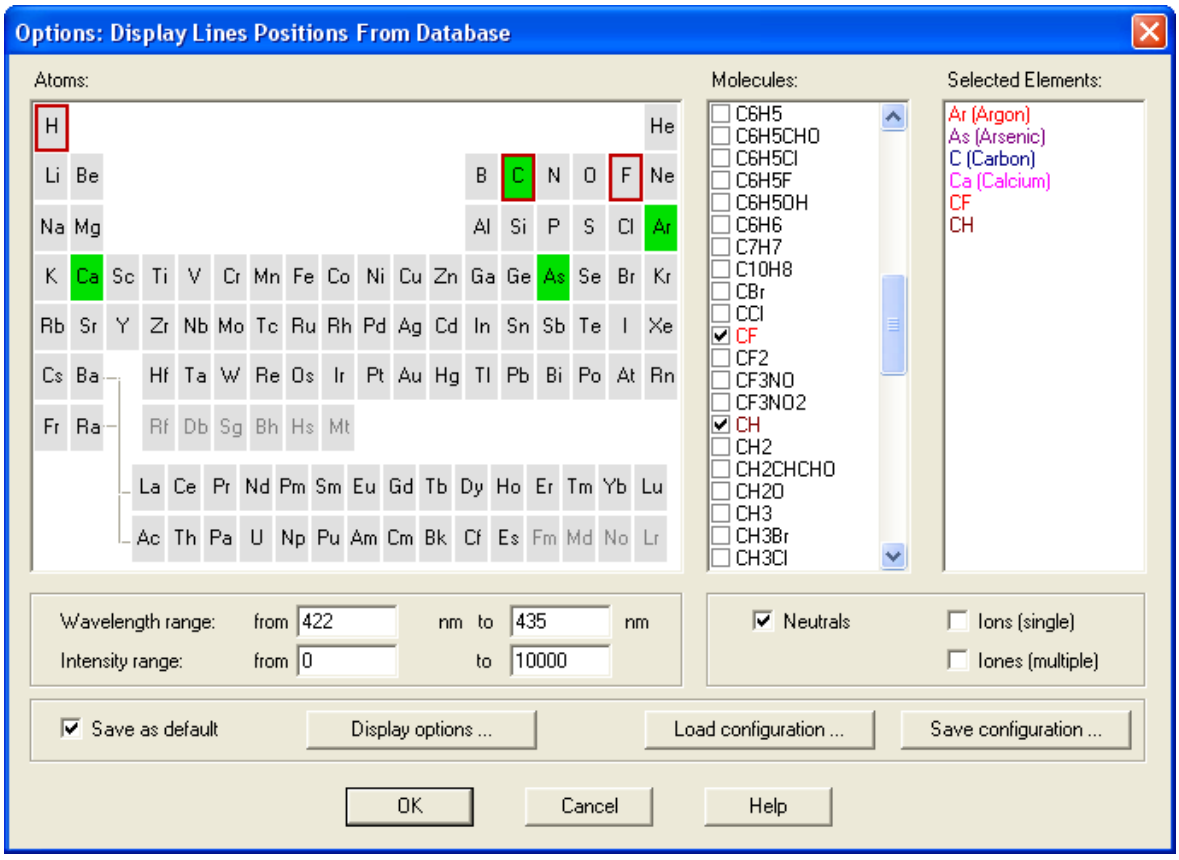
Click this button to load a stored configuration (atom and molecule selection, filter, hit interval,...) for the spectrum's line identification process.

Save configuration...

Click this button to save the current configuration for the spectrum's line identification process.

Options: Display Line Positions From Database

According to selection in this dialog the database will be searched for lines of atoms, ions and molecules and they will be displayed in the spectrum.



Atoms

Click on the atom(s) in the periodic table to be considered in the database search. Selected atoms have green background color. A red border indicates that molecules containing this atom are also selected. Use the **Context** menu by clicking the right mouse button to select and deselect all atoms and molecules.

Molecules

This field lists all molecules containing at least one of the atoms selected in the periodic table. Check the box in front of the molecule for the database search. Use the **Context** menu by clicking the right mouse button to select and deselect all listed molecules.

Selected Elements

This list contains all atoms and molecules selected for the database search. You can use this list as a summary and checklist.

Wavelength range

Use this field to specify the wavelength range in which the database should be searched for lines and band structures of the selected atoms, molecules and ions.

Intensity range

Use this field to specify the intensity range in which the database should be searched for lines and band structures of the selected atoms, molecules and ions. The units of the specified values must correspond to the selection in the dialog **Display Options** dialog box.

Neutrals and Ions (single and multiple ionized)

Use this field to specify which types of the selected elements should be scanned in the line identification process.

Save as default

Select this option to save the current values as default values when this dialog box is closed.

Display options...

Click this button to open the **Display Options** dialog box, in which you can change the display of the results in the spectrum and in the results tables.

Load configuration...

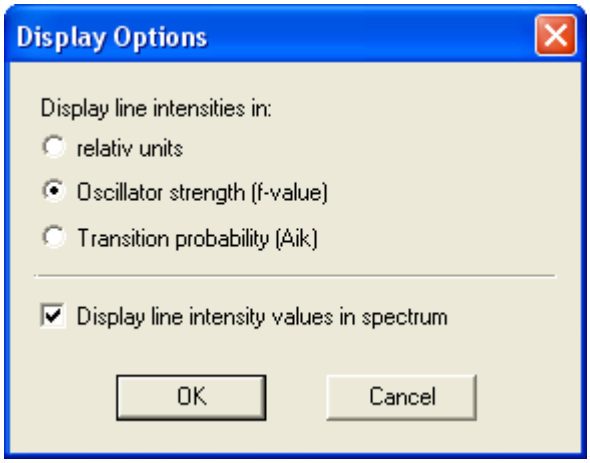
Click this button to load a stored configuration (atom and molecule selection, filter, hit interval,...) for the database search.

Save configuration...

Click this button to save the current configuration for the database search.

Line Identification: Display Options

Use this dialog box to control the display of the results in the spectrum and in the results tables.



Display line intensities in:

Select the units for the line strength:

- **relative units** – The line strength in relative units is related to the f-value of the atomic line. A relative line strength of 1000 corresponds to an f-value of 1. If no data is available for an element, the relative line strengths will be normalized to the strongest line or band set to 1000.
- **Oscillator strength (f-value)**
- **Transition probability (A_{ik})**

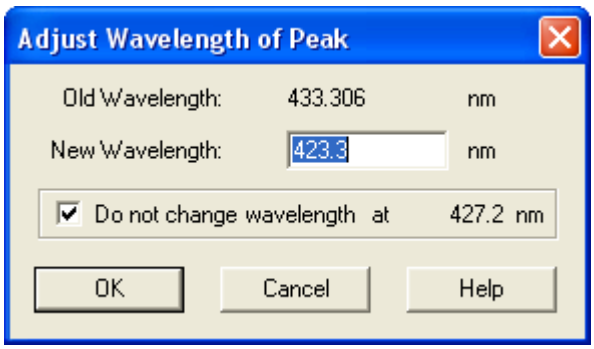
If no oscillator strength or transition probability is given in the database, no value is displayed.

Display line intensity values in spectrum

The values of the line intensities are displayed in the spectrum as well as the element name and the wavelength.

Adjust Wavelength of Peak

Use this dialog box to adjust the spectrum if a peak is identified in the spectrum but the wavelength does not match exactly the value from the database.



► *Procedure*

To adjust the spectrum,

1. Select the specific line.
2. Select the **Identification | Wavelength of Peak** menu command to open the **Adjust Wavelength of Peak** dialog box.
3. Enter the correct wavelength from the database as the **New Wavelength**.
4. Click **OK**. The spectrum is adjusted according to the given parameters.

If two identified lines or structures have been assigned exactly the same wavelength values, you can adjust the spectrum by applying this command twice. See the following procedure.

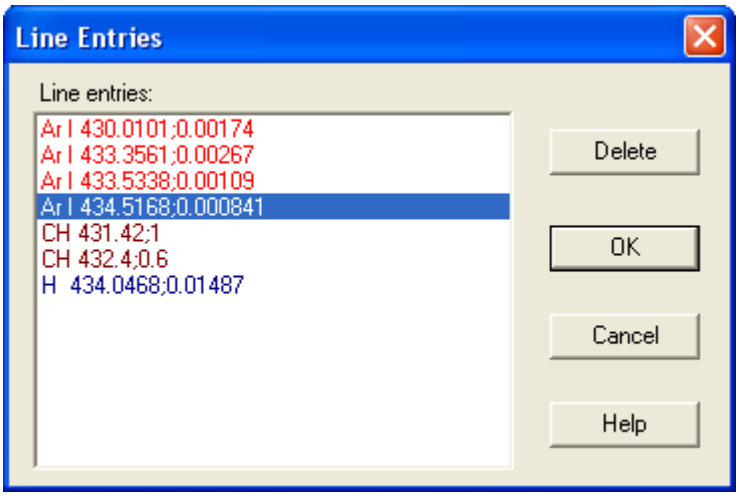
► *Procedure*

To adjust a spectrum when two identified lines or structures have been assigned the same wavelength values,

1. For the first line, follow the previous procedure (on page 37) for adjusting the spectrum.
2. Select the second line in the spectrum.
3. Select the **Identification | Wavelength of Peak** menu command to open the **Adjust Wavelength of Peak** dialog box.
3. Enter the correct wavelength for the second line as the **New Wavelength**.
4. Check the **Do not modify wavelength at ... nm** box. The specified wavelength here is the value of the line changed before.
5. Click **OK**. The spectrum is shifted and stretched or compressed according to the specified wavelength values. Now the spectrum is adjusted correctly and all other peaks should be identified as well.

Line Entries

Use this dialog box to delete any unneeded lines and band structures identified in the line identification process.

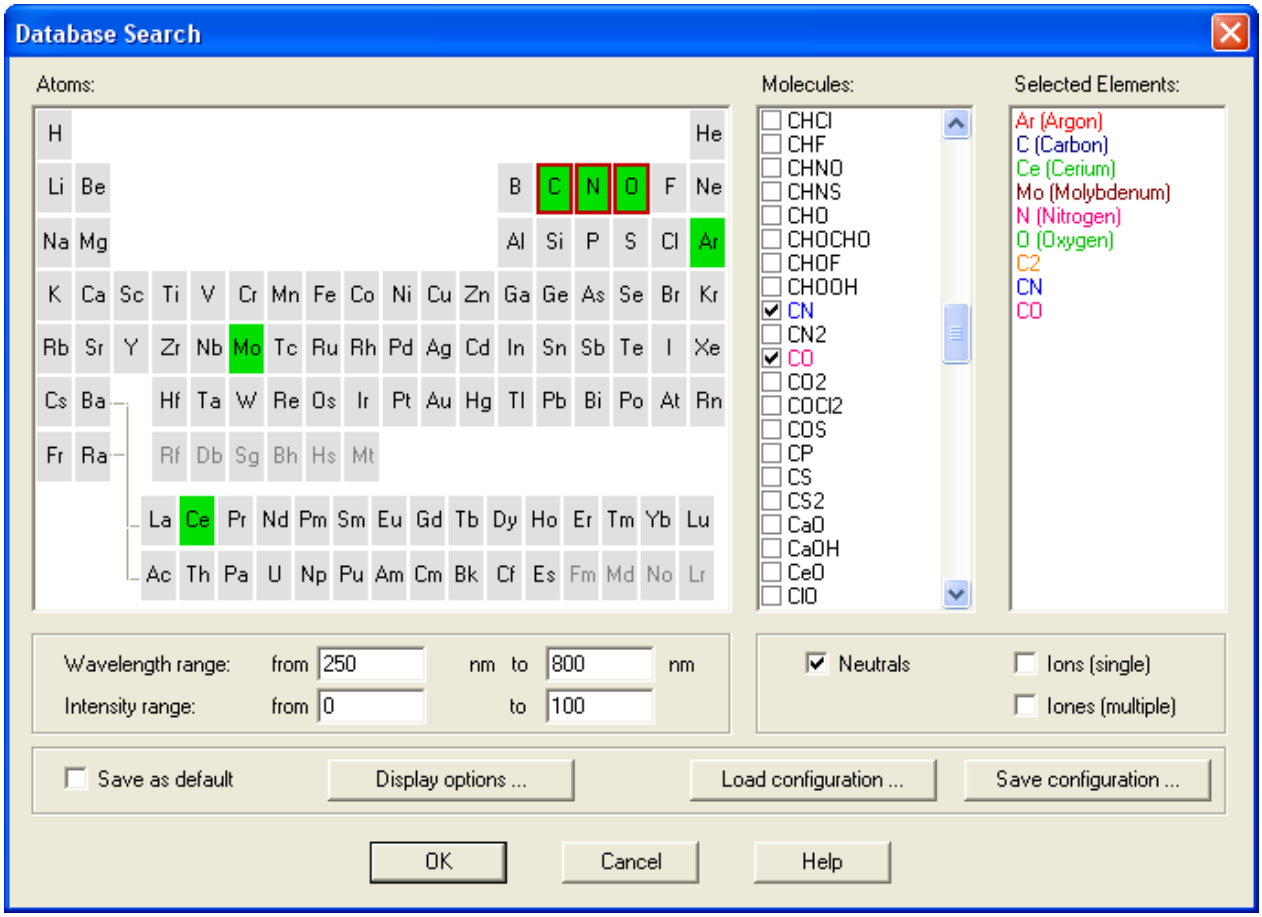


Line entries

This list contains all identified lines of the selected peak. Select the entries you wish to delete. To add deleted entries again, you must launch a new line identification process.

Database Search

Us e this dialog box to set the parameters for a database search. The database can be searched for atomic and ion lines, as well as molecular bands. All entries found are listed in the Database window:



Atoms

Click on the atom(s) in the periodic table to be considered in the database search. Selected atoms have green background color. A red border indicates that molecules containing this atom are also selected. Use the **Context** menu by clicking the right mouse button to select and deselect all atoms and molecules.

Molecules

This field lists all molecules containing at least one of the atoms selected in the periodic table. Check the box in front of the molecule for the database search. Use the **Context** menu by clicking the right mouse button to select and deselect all listed molecules.

Selected Elements

This list contains all atoms and molecules selected for the database search. You can use this list as a summary and checklist.

Wavelength range

Use this field to specify the wavelength range in which the database should be searched for lines and band structures of the selected atoms, molecules and ions.

Intensity range

Use this field to specify the intensity range in which the database should be searched for lines and band structures of the selected atoms, molecules and ions. The units of the specified values must correspond to the selection in the dialog **Display Options** dialog box.

Neutrals and Ions (single and multiple ionized)

Use this field to specify which types of the selected elements should be scanned in the line identification process.

Save as default

Select this option to save the current values as default values when this dialog box is closed.

Display options...

Click this button to open the **Display Options** dialog box, in which you can change the display of the results in the spectrum and in the results tables.

Load configuration...

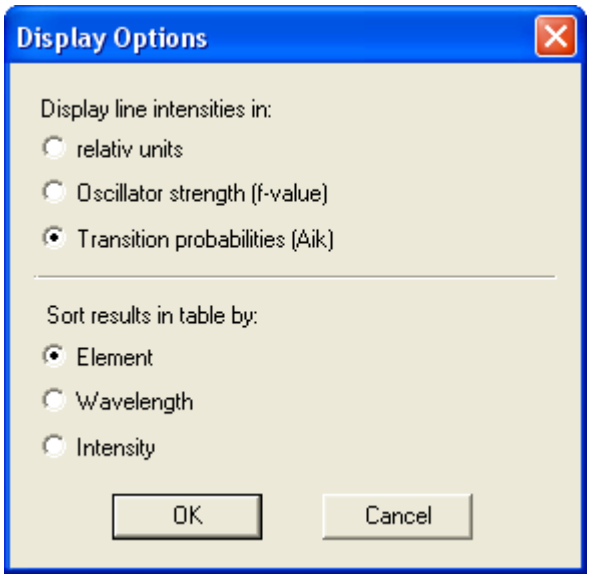
Click this button to load a stored configuration (atom and molecule selection, filter, hit interval,...) for the database search.

Save configuration...

Click this button to save the current configuration for the database search.

Database search: Display Options

Use this dialog box to control the display of the results in the spectrum and in the results tables. Also see *Line Identification: Display Options*).



Display line intensities in:

Select the units for the line strength:

- **relative units** – The line strength in relative units is related to the f-value of the atomic line. A relative line strength of 1000 corresponds to an f-value of 1. If no data is available for an element, the relative line strengths will be normalized to the strongest line or band set to 1000.
- **Oscillator strength (f-value)**
- **Transition probabilities (A_{ik})**

If no oscillator strength or transition probability is given in the database, no value is displayed.

Display line intensity values in spectrum

The values of the line intensities are displayed in the spectrum as well as the element name and the wavelength.

If no oscillator strength or transition probability is given in the database, no value is displayed.

Sort results in table by

Select to sort the results by element, wavelength, or intensity.

File Formats

Data Formats

OOISpecLine supports the following data formats:

OOISpecLine format (.psl)

ASCII-data including spectrum, line identification and database search.

ASCII format (.txt, .asc)

- one data set each line (end of line character: \n = 0A)
- data set: only y-value or x- and several y-values
- delimiter: semicolon, tabulator, white space, comma)

Hamamatsu ASCII format (.txt)

Hamamatsu-MPM format

Binary format (.bin)

- only y-values or x- and y-values alternately
- 32-bit wide floating point number

4SPEC format (.crv)

4SPEC format (Stanford Computer Optics, Inc.)

MAPS format (.mps)

MAPS format (Photometrics GmbH)

DaVis format (.prf)

DaVis format (LaVision GmbH)

OOIBase format (.sample,.scope,.reference, .dark,.sampledark)

OOIBase32 format (Ocean Optics, Inc.)

GRAMS format (.spc)

Old and new GRAMS format (Galactic, Inc.)

WinSpec format (.spe)

WinSpec format (Roper Scientific, Inc.)

Export Formats

Data Formats

OOISpecLine format (.psl)

ASCII-data including spectrum, line identification and database search.

Excel format (.csv)

Comma Separated Values for spreadsheet programs.

Binary format (.bin)

- only y-values or x- and y-values alternately
- 32-bit wide floating point number

ASCII format (.txt,.asc)

- one data set each line (end of line character: \n = 0A)
- data set: only y-value or x- und y-value (delimitate character: ; , space)

Graphic Formats

Windows Bitmap format (.bmp)

Windows Bitmap

Windows Metafile format (.wmf)

Windows Metafile

Corel Presentations (.wpg)

Corel Presentations graphics

Sources of Database

The database of **OOISpecLine** for atoms, ions and molecules is compiled from public sources only. The most important sources are listed below.

Atoms and atomic ions

R. Kurucz, CD-ROM No.23, Harvard-Smithsonian Center for Astrophysics, 1995

NIST Atomic Spectra Database, National Institute of Standards and Technology, Ver. 2.0, 1999, http://physics.nist.gov/cgi-bin/AtData/main_asd

A.R. Striganov, N.S. Sventitskii, *Tables of Spectral Lines of Neutral and Ionized Atoms*, IFI/Plenum, 1968

W.L. Wiese et al., *Atomic Transition Probabilities*, Vol I & II, NBSDS 1966 & 1969

Molecules and molecular ions

Pearse & Gaydon, *The Identification of Molecular Spectra*, Chapman and Hall Ltd, 1976

H.M. Crosswhite (Ed.), *The Hydrogen Molecule Wavelength Tables of H.G. Dieke*, Wiley-Interscience, 1972

Appendix B

Ionization States

Table 1 provides a list of elements with their ionization states. The ionization states are given in spectroscopic notation as follows:

- I = Neutrals
- II = Single ionized elements
- III = Double ionized elements, etc.

Table 2 lists the element compounds in OOISpecLine.

Note

These tables are subject to change without notice.

Table 1: Elements with their Ionization States

Z	Element	Symbol	Ionization State	Z	Element	Symbol	Ionization State
1	Hydrogen	H, D, T	I	51	Antimon	Sb	I-V
2	Helium	He	I-II	52	Tellurium	Te	I-II
3	Lithium	Li	I-III	53	Iodine	I	I-V
4	Beryllium	Be	I-IV	54	Xenon	Xe	I-VIII
5	Boron	B	I-V	55	Cesium	Cs	I-IV
6	Carbon	C	I-V	56	Barium	Ba	I-V
7	Nitrogen	N	I-VII	57	Lanthanum	La	I-V
8	Oxygen	O	I-VII	58	Cerium	Ce	I-V
9	Fluorine	F	I-VIII	59	Praseodymium	Pr	I-V
10	Neon	Ne	I-IX	60	Neodymium	Nd	I-II

Z	Element	Symbol	Ionization State	Z	Element	Symbol	Ionization State
11	Sodium	Na	I-IX	61	Promethium	Pm	I-II
12	Magnesium	Mg	I-XII	62	Samarium	Sm	I-II
13	Aluminum	Al	I-XIII	63	Europium	Eu	I-III
14	Silicon	Si	I-XII	64	Gadolinium	Gd	I-IV
15	Phosphorus	P	I-XIII	65	Terbium	Tb	I-IV
16	Sulfur	S	I-XVI	66	Dysprosium	Dy	I-II
17	Chlorine	Cl	I-X	67	Holmium	Ho	I-II
18	Argon	Ar	I-XIV	68	Erbium	Er	I-III
19	Potassium	K	I-XIV	69	Thulium	Tm	I-III
20	Calcium	Ca	I-XV	70	Ytterbium	Yb	I-IV
21	Scandium	Sc	I-XXI	71	Lutetium	Lu	I-V
22	Titanium	Ti	I-XXI	72	Hafnium	Hf	I-V
23	Vanadium	V	I-XXII	73	Tantalum	Ta	I-V
24	Chromium	Cr	I-XXIII	74	Tungsten	W	I-II
25	Manganese	Mn	I-XXIV	75	Rhenium	Re	I-II
26	Iron	Fe	I-XXV	76	Osmium	Os	I-II
27	Cobalt	Co	I-XXVI	77	Iridium	Ir	I-II
28	Nickel	Ni	I-XXVII	78	Platinum	Pt	I-II
29	Copper	Cu	I-V	79	Gold	Au	I-III
30	Zinc	Zn	I-IV	80	Mercury	Hg	I-III
31	Gallium	Ga	I-V	81	Thallium	Tl	I-IV
32	Germanium	Ge	I-V	82	Lead	Pb	I-V
33	Arsenic	As	I-V	83	Bismuth	Bi	I-V
34	Selenium	Se	I-V	84	Polonium	Po	I

Z	Element	Symbol	Ionization State	Z	Element	Symbol	Ionization State
35	Bromine	Br	I-V	85	Astatine	At	I
36	Krypton	Kr	I-VIII	86	Radon	Rn	I
37	Rubidium	Rb	I-IV	87	Francium	Fr	I
38	Strontium	Sr	I-V	88	Radium	Ra	I-II
39	Yttrium	Y	I-V	89	Actinium	Ac	I-IV
40	Zirconium	Zr	I-V	90	Thorium	Th	I-IV
41	Niob	Nb	I-V	91	Protactinium	Pa	I-II
42	Molybdenum	Mo	I-IV	92	Uranium	U	I-II
43	Technetium	Tc	I-II	93	Neptunium	Np	I
44	Ruthenium	Ru	I-III	94	Plutonium	Pu	I-II
45	Rhodium	Rh	I-III	95	Americium	Am	I-II
46	Palladium	Pd	I-III	96	Curium	Cm	I-II
47	Silver	Ag	I-III	97	Berkelium	Bk	I-II
48	Cadmium	Cd	I-IV	98	Californium	Cf	I-II
49	Indium	In	I-V	99	Einsteinium	Es	I-II
50	Tin	Sn	I-V				

Table 2: Element Compounds in OOISpecLine

Element	Compunds
Aluminum molecules	Al_2, AlCl, AlF, AlH, AlH_+, AlN, AlO, AlS, AlBr
Arsenic molecules	As_2, AsCl, AsF, AsH, AsN, AsO, AsO_+, AsP, AsS, AsS_+, AsH_2
Barium molecules	BaCl, BaF, BaH, BaO, BaS
Beryllium molecules	BeCl, BeF, BeH, BeH_+, BeO, BeS
Boron molecules	B_2, BCl, BF, BH, BH_+, BN, BO, BO_+, BS, BBr, BO_2, BOF_2
Bromine molecules	Br_2, Br_{2+}, BrCl, BrF, BrO
Cadmium molecules	CdBr, CdCl, CdF, CdH, CdH_+
Calcium molecules	CaBr, CaOH, CaCl, CaF, CaH, CaO, CaS
Carbon molecules	Br, CHCl, CHF, CHNO, CHNS, CHO, CHOCHO, CHOF, CHOOH, CH_2O, CH_2CHCHO, CH_3Br, CH_3Cl, CH_3NO_2, CH_3O, C_2H_2, C_2H_4, C_2H_4O, C_2H_5, C_2H_5CHO, $C_2H_5NO_2$, C_3H_3, C_3H_5, C_3H_6O, C_4H_2, C_4H_{2+}, C_5H_5, C_6H_5, C_6H_5Cl, C_6H_5F, C_6H_5CHO, C_6H_5OH, C_6H_6, C_7H_7, $C_{10}H_8$, CF_3NO, $C_3F_7NO_2$, C_3F_7NO, CF_3NO_2, $COCl_2$, C_2O, C_3O_2, COS, COS_+, C_3S_2, C_2, C_{2+}, C_{2-}, C_3, CCl, CF, CF_2, CH, CH_+, CH_2, CH_3, CN, CN_+, CN_2, C_2N, C_2N_2, CO, CO_+, CO_2, CO_{2+}, CP, CS, CS_2, CS_{2+}
Cerium molecules	CeO
Chlorine molecules	Cl_2, Cl_{2+}, ClF, ClO, ClF_3, ClO_2
Chromium molecules	CrBr, CrCl, CrF, CrH, CrO, CrS
Copper molecules	Cu_2, CuCl, CuF, CuH, CuO, CuS, CuBr, CuOH
Fluorine molecules	F_2, F_{2+}, FCO, F_2CO
Gallium molecules	Ga_2, GaCl, GaF, GaH, GaO, GaBr
Germanium molecules	GeBr, GeCl, GeF, GeH, GeO, GeS
Gold molecules	Au_2, AuCl, AuH
Helium molecules	He_2, HeNe
Hydrogen molecules	H_2, HBr, HBr_+, HCP, HNF, HNO, HNO_2, HS_2, H_2S, H_2S_+, HCN, HCl, HCl_+, HF, HF_+, H_2O, H_2O_+
Indium molecules	In_2,InCl,InF,InH,InO,InO_+,InBr,$InBr_2$,$InCl_2$

Element	Compunds
Iron molecules	FeBr, FeCl, FeF, FeO
Lithium molecules	Li_2, LiCl, LiH, LiBr
Magnesium molecules	Mg_2, MgCl, MgF, MgH, MgH_+, MgO, MgS, MgBr, MgOH
Mercury molecules	Hg_2, Hg_{2+}, HgCl, HgF, HgH, HgH_+, HgBr, $HgBr_2$, $HgCl_2$
Neon molecules	Ne_2
Nickel molecules	NiBr, NiCl, NiF, NiH, NiO
Nitrogen molecules	N_2, N_{2+}, NCl, NF, NH, NH_+, NH_2, NO, NO_2, N_2O, N_2O_+, NS, NS_+, N_3, NCO, NCS, NCl_2, NF_2, NH_3, N_2H_2, N_2H_4, NO_3, N_2O_3, N_2O_4, N_2O_5, NSF
Oxygen molecules	O_2, O_{2+}, O_3, OH, OH_+
Phosphorus molecules	P_2, P_{2+}, PCl, PF, PF_+, PH, PH_+, PN, PO, PO_+, PS, PS_+, PH_2 PH_3, PHO, POBr, $POBr_2$, POCl, $POCl_2$
Platinum molecules	PtC, PtH, PtO
Potassium molecules	K_2
Selenic molecules	Se_2, SeCl, SeH, SeO, SeS, SeBr, $SeBr_2$, $SeCl_2$, SeO_2
Silicon molecules	Si_2, SiC_2, SiCl, SiF, SiH, SiH_+, SiH_2, SiN, SiO, SiO_+, SiO_2, SiS, SiBr, $SiBr_+$, SiHBr, $SiCl_2$, SiHCl, SiF_2, SiF_3, SiH_4
Silver molecules	Ag_2, AgCl, AgF, AgH, AgO, AgBr
Sodium molecules	Na_2, NaF, NaH, NaK
Strontium molecules	SrBr, SrOH, SrCl, SrF, SrH, SrO
Sulfur molecules	S_2, SF, SH, SH_+, SO, SO_2, S_2O, S_3, S_4, SO_3
Tantalum molecules	TaO, TaO_+
Tin molecules	SnBr, SnCl, SnF, SnH, SnO, SnS
Titanium molecules	TiBr, TiCl, TiF, TiH, TiN, TiO, TiS
Tungsten molecules	WO
Vanadium molecules	VCl, VH, VO
Zinc molecules	Zn_2, ZnCl, ZnF, ZnH, ZnH_+, ZnO, ZnBr

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