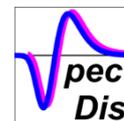# SpecDis Manual

Version 1.71

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T. Bruhn, A. Schaumlöffel, Y. Hemberger. G. Pescitelli, SpecDis, Version 1.70.1, Berlin, Germany, 2017, https://specdis-software.jimdo.com.

T. Bruhn, A. Schaumlöffel, Y. Hemberger, G. Bringmann, *Chirality* **2013**, *25*, 243-249.

T. Bruhn, G. Pescitelli, *Chirality* **2016**, *28*, 466-474.

System Requirements

Version 1.70.1 of SpecDis has been tested under Win 7 SP1 (32+64Bit), Windows 10, and Linux GTK2 64Bit (OpenSuse Leap 42.3). If you observe administrator-right problems install SpecDis on a partitioned drive other than C:\. Windows 8 has not been tested in detail but SpecDis should work under this OS, too.

Capabilities (selection)

- Automatic extraction of heats of formation and spectral data (excited states, IR/VCD, ORD) from output files
- Gaussian and Lorentzian curve generation
- Direct comparison of calculated spectra with experimental or calculated data
- Application of a shift (UV correction) or scaling factor
- Provide an enantiomeric ECD/VCD spectrum
- Arithmetic or Boltzmann weighted summation of spectra
- Plot results with Gnuplot in a "what you see is what you get" manner (up to 5 curves)
- Plot UV and CD traces of HPLC runs
- Generate spectral curves that can be processed in other software like Excel or Origin
- Read ORD values from Gaussian03/09/16 calculations and do a Boltzmann statistical weighting
- Read TD and/or MRCI results of Gaussian03/09/16, TURBOMOLE (escf,ricc2; tested up to version 6.7), ORCA (including 4.x), DALTON 2013, ADF (2013), and NWChem (2014)
- Calculate similarity factors for matching of ECD/UV or VCD/IR curves
- Determination of a suited band width and/or shift/scaling factor using the similarity factor or a cross section algorithm
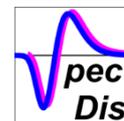
Installation

Copy SpecDis to a directory of your choice, on first start the software will generate the *SpecDis.ini* in the same directory (your settings will be saved in this file).

To use the plotting routine within SpecDis you have to install Gnuplot on your system. Gnuplot is freely available under the following link: www.gnuplot.info/

To get plots from gnuplot, SpecDis needs the directory of the file wgnuplot.exe (for Windows systems): Go to File → Settings and use the search button, normally the executable can be found in the \bin or the \binary directory of your gnuplot installation path:
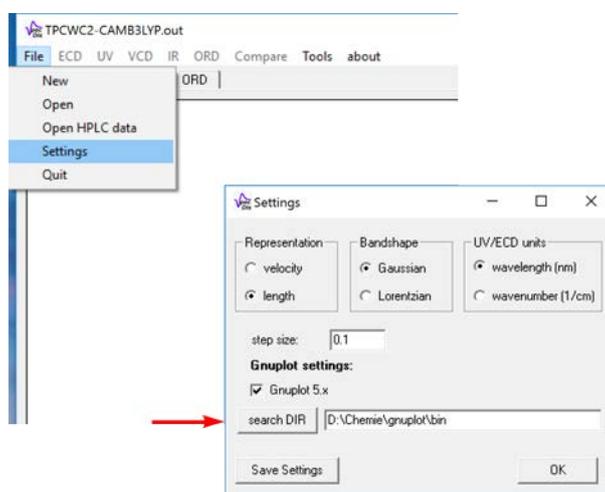
For the linux version SpecDis needs the path to the file 'gnuplot', usually this is /usr/bin. As Linux does not have default fonts you have to make sure that the Arial and symbol fonts are available on your system or you have to change the fonts in the new plotting settings in the ECD/UV or VCD/IR tab.

Since Version 1.60, gnuplot 4.6 is supported, plotting of png will only work with versions 4.6 and higher, as the new terminal pngcairo is used. If you use version 5.x check the corresponding checkbox in the settings, otherwise line thickness and color for eps do not fit.

File Formats

SpecDis is a software either to analyze excited-states calculations from Gaussian 03/09/16, Turbomole, ORCA, Dalton, NWChem, ADF, and the sTDA software from Grimme, VCD calculations from Gaussian09/16, or to analyze and plot HPLC-UV and CD chromatograms with Gnuplot. For these purposes SpecDis can read several file formats but needs certain file extensions to recognize the different formats:

Calculated Data:
Gaussian03/09/16, Turbomole, ORCA, DALTON, ADF, NWChem: *.out* or *.log*
DFT/MRCI: *.cd* and *.uv*
sTDA: *.dat
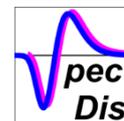
SpecDis can use these files directly without any editing but it only reads excited states in the range of 100 to 4000 nm. VCD and IR data will be read from Gaussain09/16 files only (use the VCD keyword even if you only need IR, otherwise SpecDis cannot read the data) in the range from 0 to 4000 cm^{-1}, thus negative frequencies are ignored.

SpecDis has an own file format called *.bil. The first line is a comment line, followed by two columns with tab separated values. Which values are given is written in the comment line. This file format is needed for the Boltzmann statistical and the arithmetical summation of single ECD/UV, VCD/IR, or ORD spectra. Furthermore, it can be used to import spectra from other QM software by writing your own scripts that create the bil files from this unsupported software. To differentiate the bil files every method has its own file extension so that the extension is build up by a method token and the .bil extension (*.'token'.bil). The tokens are *cd* for ECD (e.g. *.cd.bil*), *uv* for UV, *vc* for VCD, *ir* for IR, and *or* for ORD. The same tokens are used for experimental spectra (see below).

<u>Experimental Data:</u>

SpecDis will read UV/ECD data from 100 nm to 4000 nm, only!

UV and ECD spectra:
Spectra from JASCO Spectrometers:
SpecDis can directly read the Jasco ASCII file format, but you have to change the file-extension for UV or CD spectra to *.uv.exp.xy* or *.cd.exp.xy*, respectively.

IR/VCD spectra:
Again spectra from JASCO spectrometers can be read directly when they are in the Jasco ASCII file format (change extension to *.ir.exp.xy* or *.vc.exp.xy*).

ASCII Files:
These files should have the same extension as mentioned above (*uv.exp.xy* and *cd.exp.xy* or *.ir.exp.xy* or *.vc.exp.xy*)! SpecDis can read xy-files with tab spaced numbers (first nanometers/inverse cm, second R/f values) and no empty line at the end of the file. In the case of UV spectra it can read *.csv* files (semicolon separated files), too.

HPLC-UV or HPLC-CD:
SpecDis reads these files as pure xy-files, that means two numbers (first x, second y) which are tab separated (or semicolon separated). Use *.ccd* or *.cuv* as file-extensions, so that SpecDis recognizes them as CD or UV spectra, respectively. The range of the displayed chromatogram will be automatically selected from the file by SpecDis but you can also choose the retention time range (zoom) of interest in the corresponding edit box.
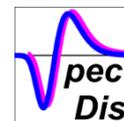
Table 1. File extensions for experimental data.

Experimental Data	SpecDis file extension
ECD spectrum: JASCO ASCII-File (*.txt)	*cd.exp.xy
UV spectrum: JASCO ASCII-File (*.txt)	*uv.exp.xy
ECD spectrum, tab or semicolon separated (nm;$\Delta\varepsilon$)	*cd.exp.xy
UV spectrum, tab or semicolon separated (nm;abs)	*uv.exp.xy
UV spectrum, *.csv (nm;abs)	*uv.exp.xy
VCD spectrum, tab or semicolon separated (cm^{-1};$\Delta\varepsilon$)	*vc.exp.xy
IR spectrum, tab or semicolon separated (cm^{-1}; ε)	*ir.exp.xy
ORD spectrum, (nm;specific rotation)	*or.exp.xy
HPLC-UV chromatogram	*.cuv
HPLC-CD chromatogram	*.ccd

Settings

The most important settings are the choice of the bandshape (Lorentz or Gauss) and the representation of the calculated results (dipole-velocity or dipole-length gauge) that should be used in SpecDis. Keep in mind that ORCA provides ECD values only from the length formalism (except for sTD calculation). SpecDis only reads data from ONE formalism, thus, if you change the representation you have to reload your calculated data!
Since version 1.70 you also have the choice between wavelength and wavenumbers for ECD/UV plots.
The 'save settings' button saves 'plot settings' and the 'checkbox settings' (search in subfolders or in the same folder) for extract heat/spectra, too.

General Usage of SpecDis

The easiest way to use SpecDis is to drag a *.log* or *.out* file of Gaussian03/09/16 or ORCA and drop it to SpecDis. If this does not work use the menu File → Open. The Spectra will then be drawn automatically. You can switch between the different pages to see the ECD/UV or VCD/IR spectra. It is possible to choose different wavelength ranges by editing the numbers on the upper right side, the range of the y-axis is automatically chosen. To compare with other spectra you have to use the *Compare* menu, via Drag&Drop always a new session is started and old data will get lost. A short description of the main features is given in the following:
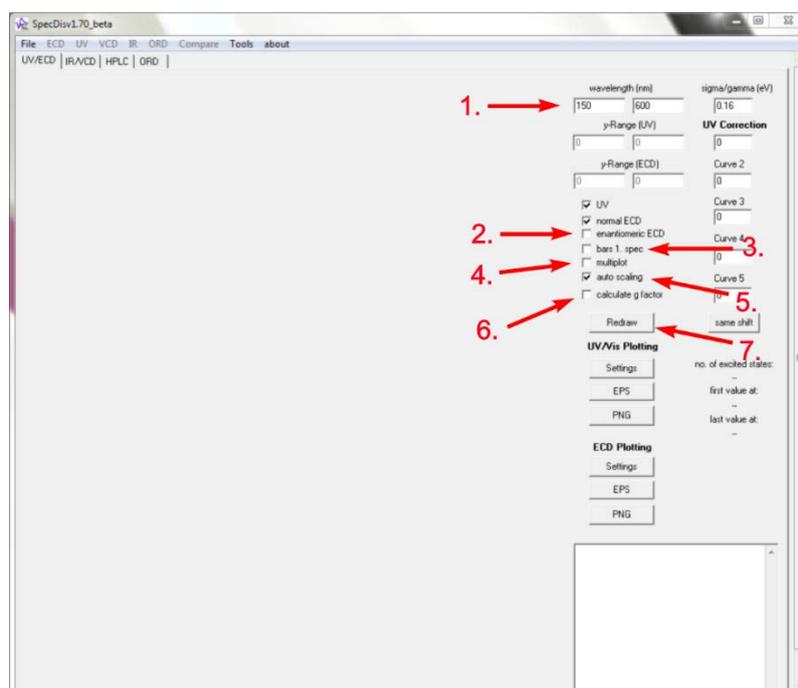
1. Wavelength region, sigma/gamma value, and UV correction

Here the region is selected in which the spectra are drawn, if units are set to wavenumber two new edit fields will appear in which wavenumber will be given (the values for the wavelength fields will be calculated automatically in this case). Depending on the choice of the bandshape in the settings one can give a sigma (Gaussian band shape) or gamma (Lorentzian) value. In case of wavelength units the UV correction is given as a shift in nm, while for wavenumbers a scaling factor has to be chosen, SpecDis will automatically adapt this to the selected units. The UV shift is a pure empirical approach and safes much computational time. However, the shape of experimental and calculated UV spectra should be quite identical (same number of peaks, comparable relative intensities of the peaks), otherwise one should check if there are problems in the calculation or the measurements (e.g. choose better functionals/basis sets/methods).[4,3,1]
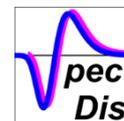
2. Enantiomeric ECD/VCD spectrum

Just check 'enantiomeric ECD' (or VCD) on the right side, the enantiomeric spectrum will be drawn now (the enantiomeric spectrum is simply calculated by multiplication of the Δε values with (-1)). To save this spectrum be sure that 'normal ECD' (or VCD) is unchecked and open 'ECD-spectra' (or VCD) → 'Save cd.bil' (Save vc.bil) or 'Save xy'.

3. Bar Spectra

If this checkbox is checked a bar spectrum of the first curve is shown (either in UV and in the ECD, if enantiomeric ECD is checked a bar spectrum of it is displayed, too).

4. Multiplot

Normally SpecDis will display only two curves at once, thus the second one will get replaced automatically each time you add a spectrum. By checking the multiplot checkbox, SpecDis displays up to five spectra. Furthermore, you can choose at which position (curve2, 3, 4, or 5) the newly loaded spectrum will be placed.

5. Autoscaling

As default SpecDis uses relative intensity values to draw the spectra, the highest peak is set to 90% of the height of the diagram and all other values are scaled to fit this value. To get an impression of how the values of two spectra 'behave' in absolute units, you can switch off the 'auto scaling' checkbox. Keep in mind that this checkbox has no influence on the absolute values of the spectra, it just changes the presentation of the spectra in the images/plots. Saved curves still have the absolute values from the calculation or the measurement.

6. Peak Picking

The Peak picking tool is quite simple, you have to select a range in which a peak has to be find by left clicking in the spectrum, keep the mouse button pressed and move the yellow rectangle to the position you need and release the button. SpecDis will now search the highest value in the region and checks if the neighbored values are both smaller. If so, SpecDis determines it as a peak and will give the wavelength/wavenumber above the peak in the spectrum and in the small memo field on the right side. To determine minima (i.e. troughs in the ECD/VCD) use the right mouse button to select a range. SpecDis also checks if you selected the range in the ECD/VCD spectrum or in the UV/IR spectrum and will accordingly pick the peak. If both – UV/IR and ECD/VCD – are loaded and if the g-factor checkbock is selected a g value is calculated at the selected ECD/VCD peak. Make sure that the value makes sense, id est both spectra have to be in absolute values.
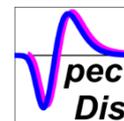
7. Redraw

Sometimes it is useful to completely redraw the spectra, especially when using the peak picking tool. By pressing *Redraw* the results of the peak picking in the spectra are removed.

Plot spectra with gnuplot

To get Gnuplot plots, SpecDis needs to know where the wgnuplot.exe is (have a look at the installation instructions above).

To get an eps file of the spectra shown in SpecDis, you have to use the 'Plot EPS' button (to get a png file use the 'Plot PNG' button). Choose a name for the plt-file in which all relevant input for gnuplot is saved. This routine will also save all visible curves as an xy file. Then SpecDis automatically plots the spectra which are currently shown in the open tab. This works in a "What You See Is What You Get" manner for most of the spectra, only for HPLC-UV traces (here additionally a 3D plot is possible) and for VCD/IR spectra the gnuplot spectra look different. All settings like the range and y-axis are taken as used before in SpecDis.

One important point here: while using "auto scaling", the y-range of the first ECD/UV spectrum is fitted to the range of the second one if it is an experimental curve and multiplot is deactivated. Otherwise all curves are adjusted to the one with the highest peaks (This is always done for VCD/IR). For ECD/UV it is recommend to read in the calculated spectrum first and the experimental one as second (if multiplot is not used). Just fool around with the ranges and the order of the spectra to get a feeling how to plot your spectra in the way you like it most.

Important: Keep in mind, that SpecDis normally does not know whether your values are in molar or relative units (in some cases it will detect this from the cd.exp.xy file). As a default it assumes that you use relative CD ($\Delta\varepsilon$) values in mdeg and labels the y-axis according to this.

Note: Do not use blanks or the underline character within your file name, the generation of the *.eps* from the *.plt* file with gnuplot might fail otherwise. SpecDis removes blanks and underlines automatically!

Since version 1.60, it is possible to choose several gnuplot settings directly within SpecDis. Have a look at the settings buttons in the CD or UV tabs. The settings are more or less self-explaining, however, in the following a few details are given.

UV/ECD Plot settings
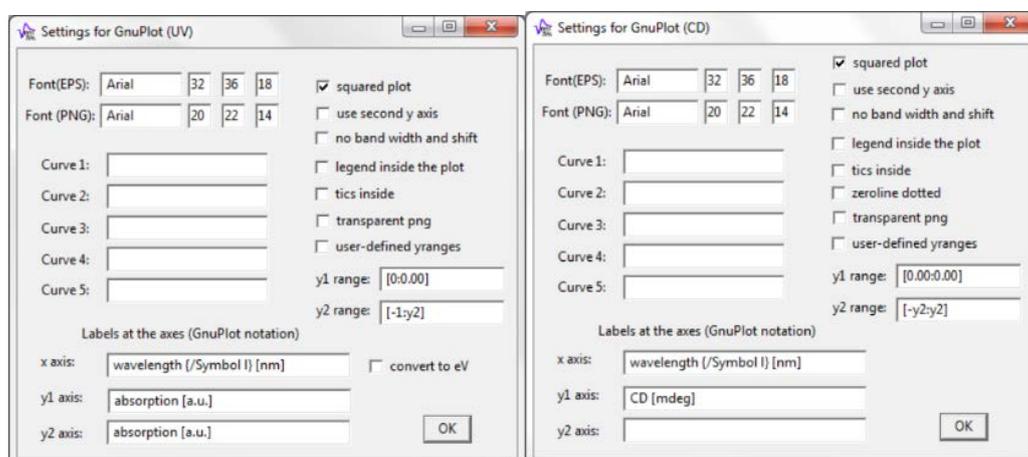
In the first line a font can be selected (for eps and png separately) and three different sizes, with the first one giving the general size in the plot (e.g. numbers at the axes), the second number defining the size of the labels at the axes, and the third one selects the size of the legend.
The checkboxes on the right side should be self-explaining, however, one should note that the use of a second y axis will divide the spectra in experimental and calculated spectra and both will have their own axis (autoscaling is automatically deactivated). A squared plot is an option of gnuplot by which the diagram has a square shape while it is a rectangle without this option.
In the plot settings one can change the names (which be used for the legend in the plot) of the curves, this is especially important if curves with identical names have been loaded. In this case the names have to be changed, otherwise it is not possible to plot the spectra.
The labels at the axis have to be given in gnuplot notation, it is thus also possible to use symbols and so on. For details have a look in the gnuplot manual.

IR/VCD Plot settings

The settings are quite similar to UV/ECD, but here only two font sizes are selectable, the general size (e.g. labels and numbers at the axes) and the size of the legend. IR and VCD curves will be plotted in different diagrams by default, only if the overlay checkbox is checked all curves will be in one diagram.
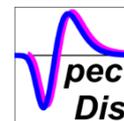
Comparisons and Tools

Comparison

Once you have loaded a calculated spectrum you can compare it with other calculated or experimental spectra. Open Compare → … with CD/UV spectra if you want to compare a CD spectrum with a UV or CD spectrum or open Compare → …with UV spectrum if you want to compare a UV spectrum with another one (and so on for IR/VCD, ORD, or chromatograms). **Note:** For a full comparison of calculated and experimental data, always read a calculated spectrum first, otherwise the shift and σ-value options will be disabled.

Compare more than two spectra: You have to check the 'multiplot' checkbox to compare more than two spectra, as long as 'multiplot' is unchecked SpecDis will only replace the second spectrum. With selected multiplot, you have to choose at which position (2-5) the new spectrum has to be loaded. If you want to delete a curve you also have to use the Compare …with menu, instead of loading you can select a curve and subsequently remove it. Every curve may be corrected by an individual shift/factor (see right side of SpecDis).

Export Data

It is possible to export calculated curves as xy files (ASCII). These files can be easily imported into Excel, Origin, or any other software of your choice to be further processed there. To save a curve as an xy file open the corresponding menu (ECD, UV, VCD, or IR) and choose 'Save xy'. SpecDis saves the curve in the range that is visible in the tabs (without any corrections!) and the step size for ECD/UV can be changed in the settings (default is 0.1 nm, which is also the smallest possible value). For VCD/IR spectra the step size is hardcoded to 1 cm^{-1}.

If you interested in the results of the excited states/frequency calculations you can export so-called bil files. These are tab separated files giving the excitation energy (in nm) and the corresponding R/f value or the vibrational energy and the R/VA values.

Extract Energies/Generate Heat-files for Boltzmann Weighting

Heat files contain one line with the energy in kcal/mol, these files are needed for the Boltzmann statistical weighting of spectra. The *.heat* files can be generated from Gaussian or ORCA *.log* or *.out* files with the heat extraction tool (Tools → extract heat). Just choose the directory in which the files (or the subdirectories, if you checked this box) can be found.

SpecDis will look (if chosen only in every subdirectory) for *.log* and *.out* files. Mind that SpecDis reads only energies of selected methods for Gaussian03, but with Gaussian09/16 it should work with all semiempirical, HF, all DFT methods and with MP2 calculations. ORCA and MOPAC2007/2009/2012 energies can be extracted for every method. All *.heat* files will be written to a new 'heat' directory in the chosen directory.

Of course these heat-files can be created manually, if the energies were from other software packages or from other methods. Create a txt-file for example with the windows editor which contains one line: HEAT OF FORMATION = 0.0 kcal/mol where the number should contain the energy in kcal/mol. Save the file and edit the name so that it has the same name as the corresponding *.bil* file with the file extension *.heat*.
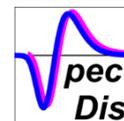
Since Version 1.63 SpecDis searches either in subfolders only or in the chosen directory only, check or uncheck the corresponding checkbox within the extract-heat tool. To simplify the workflow you can save your selection, go to Settings in the File menu and press the 'Save Settings' button.

Since 1.70 it is possible to extract Gibbs free energies from Gaussian09/16 calculations, a checkbox has been added to the tool and since version 1.71 Gibbs free energies of ORCA 4.x freq calculations are supported, too (keep in mind that only the standard value of ORCA is used (rotational symmetry = 3), make sure that it fits to your symmetry).

Extract Spectra

Like in the case of the heat extraction SpecDis will search for excited state calculation in subdirectories or in the selected folder only, depending whether the subdirectory checkbox is checked or not. Open Tools → extract spectra and choose the directory in which all the files can be found. SpecDis looks for *.*log* or *.*out* files and writes the corresponding *.*bil* files in a new 'spectra' directory in the initially chosen main directory.

Sum Spectra

For the Boltzmann-weighted summation of spectra, you need *.*bil* files and a *.*heat* files with the same name as the *.*bil* file. Select the bil files with the 'Select Files' button (select the first file and then press shift and click the last file to select). If not chosen otherwise, SpecDis will look for the heat files in the same directory as the bil files. Alternatively, you can select another folder, where SpecDis searches the heat files by clicking on 'Select Dir'. Once selected, SpecDis will not remove the dir, if nothing has been selected before, SpecDis proposes the upper directory of that of the bil files.

To sum up spectra start the tool, choose the method and the files you want to sum up and click the ok button. After that a spectrum is generated, which can be saved via the corresponding menus. The used weighting factors are displayed in the text field (you can use copy&paste here). Default temperature for the weighting is 298 K, you can change the temperature by changing the number in the edit field.

Similarity Factors

This tool helps you to find optimal shifts/scaling factors in combination with an optimal σ/γ value, minimizing the personal bias that might occur if you find these values 'by hand'. SpecDis compares to curves by two different algorithms (cross section or similarity, see below) and determines the best values in the given range. In case of UV/IR spectra SpecDis uses the cross section algorithm, in case of ECD/VCD it uses the similarity algorithm. By contrast to the previous version, SpecDis now searches for the best Δ_{ESI} value (before it searched for the best similarity). For details have a look in the next section and the cited literature.

Note: Load a calculated spectrum first, then add an experimental one. SpecDis will perform a scaling of the intensities, the scaling factor is given and is in best case close to one.

Theoretical Background

SpecDis uses a number of equations that will be shortly introduced here for details on the equations have a look at the cited literature.

Calculation of Gauss Curves for ECD/UV

To get spectra from calculations that can be compared with the experiment you have to lay gauss curves over the single oscillator or rotational strength values (calculations for ECD and UV **are done in eV**! and will only subsequently **converted** to nm or cm^{-1}). The line-shape ECD curves $\Delta\varepsilon(\lambda)$ were obtained from the 'bar-type' spectra by utilizing a Gauss distribution[2,6] according to:

$$\Delta\varepsilon(\lambda) = \frac{1}{22.96\times10^{-40}} \cdot \frac{1}{\sigma\sqrt{\pi}} \sum_k E_{0k} R_{0k} \exp\left[-\left\{\frac{(E-E_{0k})}{\sigma}\right\}^2\right],$$

where λ_k and R_{0k} are the wavelength and the rotatory strength of the kth electronic transition, respectively, and σ is the exponential half-width, i.e., half the bandwidth of the CD band at $1/e$ peak height. The default σ-value in SpecDis is 0.16 eV which is in many cases a good alignment but other values in the range of 0.05 eV to 0.4 eV are usual, too. For the UV spectra a similar formula is used with the oscillator strength instead of the rotational strength and a constant factor of 2.870 x 10^4 instead of 1/22.96 x 10^{-40}. In the end SpecDis produces molar values by these equation, i.e. the ECD and the UV is given in Mol^{-1}cm^{-1} ($\Delta\varepsilon$ and ε).

Lorentz Curves for UV/ECD or IR/VCD

The formula used to get Lorentz curves for ECD is the following:

$$\Delta\varepsilon(\lambda) = \frac{1}{22.96\times10^{-40}} \cdot \frac{1}{\sqrt{\pi}} \sum_k E_{0k} R_{0k} \frac{\gamma}{(E-E_{0k})^2 + \gamma^2}$$

where γ is half the bandwith at half peak height, λ_k and R_{0k} are the wavelength and the rotatory strength of the kth electronic transition.

For UV spectra the constant is replaced by 2.870 x 10^4 and of course oscillator strength is used instead of rotational strength values.

For VCD and IR always the Lorentz curves are used with the following equations (calculations are done in wavenumbers):[3]

VCD: $\quad \Delta\varepsilon(\upsilon) = \frac{1}{229600\times10^{-44}} \cdot \frac{1}{\pi} \sum_k \upsilon_{0k} R_{0k} \frac{\gamma}{(\upsilon-\upsilon_{0k})^2 + \gamma^2}$

IR: $\quad\;\; \varepsilon(\upsilon) = \frac{1}{91.48\times10^{-40}} \cdot \frac{1}{\pi} \sum_k \upsilon_{0k} D_{0k} \frac{\gamma}{(\upsilon-\upsilon_{0k})^2 + \gamma^2}$
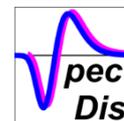
The constants are fitted to the units given from Gaussion09 (for VCD in 10^{-44} and for IR in 10^{-40} cgs units). Keep in mind that the absolute values from GaussView (version 5.09) are by a factor of 10^4 higher as in SpecDis (most probably due to a missing conversion to the 10^{-44} units in Gaussview).

Boltzmann weighting:[4]
Experimental CD spectra are a summation of the CD spectra of every conformer of the structure measured. To get a better accordance of experiment and calculation you have to consider this behaviour. Therefore a PES scan has to be done, to find all conformers in a certain range around the "global" minimum structure. From the thus obtained energies one can get weighting factors for every conformer using the following formula:

$$\frac{N_i}{N} = \frac{g_i e^{-E_i / k_B T}}{Z(T)}$$

with $N = \sum_i N_i$ and $Z(T) = \sum_i g_i e^{-E_i / k_B T}$

In this formula i is the number of conformers found by the PES scan, T is in SpecDis defined as 298 K and g_i is assumed to be 1, as every conformer should be unique. Energies of the single conformers will be used as relative energies to the lowest lying structure found during the PES scan and k_B is the Boltzmann constant. The intensities of the single spectra will be multiplied with this factor and after that added up to the overall spectrum, which can be compared with the experiment (energies for SpecDis have to be in kcal/mol!).

Similarity factors

This feature is in the tools menu and can be used to determine similarity factors as they are described by Bultinck *et al.* for IR and VCD spectra.[5,6] One can use this similarity factor or a cross section algorithm to automatically determine a suited bandwidth value and UV shift. For this you have to read in the calculated UV and CD spectra first and then add the experimental spectrum. SpecDis will check if parameters like wavelength region and intensities fit to each other (e.g. if the experimental UV is given in relative units, the calculated spectrum will be normalized to 1 or calculated intensities will be scaled if there is a large discrepancy) and will then run the algorithms for the given set of wavelength range, bandwidth values, and shifts. Users insight on the quality of measurements and calculations is indispensable here, otherwise, this algorithm might produce nonsense![6]

Formula used for the cross section algorithm:

$$\left| \int_{\lambda_1}^{\lambda_2} f(x)dx - \int_{\lambda_1}^{\lambda_2} g(x)dx \right|$$

With f(x) as the calculated curve and g(x) as the experimental curve. The cross sections of the curves are calculated for all possible combinations of the given parameters and the smallest ones are chosen as the best values.

Formulas used for the similarity factor:

UV/IR similarity:
$$S = \frac{\int_{\lambda_1}^{\lambda_2} f(x)g(x)dx}{\sqrt{\int_{\lambda_1}^{\lambda_2} f^2(x)dx \int_{\lambda_1}^{\lambda_2} g^2(x)dx}}$$

ECD/VCD similarity:
$$\Sigma_{fg} = \frac{\phi^{++}S^{++} + \phi^{--}S^{--}}{\phi^{++} + \phi^{-}}$$

Weighting factor for positive values (negative parts are calculated analogously):

$$\phi^{++} = \int_{f(x)>0} f(x)dx + \int_{g(x)>0} g(x)dx$$

Enantiomeric Similarity Index Δ:
$$\Delta = \left| \Sigma_{fg} - \Sigma_{fg_{Enantiomer}} \right|$$

For details see reference [6].

The similarity tool can also be used for VCD/IR using the cross section algorithm for IR or the similarity algorithm for IR and VCD as described by Bultinck et al.[5] SpecDis uses the results of the cross section algorithm (if IR is compared) to find the best γ value and scaling factor. Like in the case for UV the similarity algorithm tends to too high γ values.

References

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