SWizard™

updated on:
March 2013
Revision 5.0

This 32-bit program reads excitation energies and oscillator strengths of electronic transitions from output files generated by ***ADF 200x***, ***Gaussian 98, Gaussian 03***, ***Gaussian 09***, ***HyperChem 4.x-7.x***, ***CNDO/INDO***, ***ZINDO,*** and free-format ASCII text files and produces ASCII text tables containing electronic absorption spectra and the tables with transition assingments.

SWizard also can read vibrational frequencies and intensities from ***Gaussian 98/03/09*** output files (and free-format files) and produces ASCII text tables containing an IR or Raman absorption spectra.

System Requirements:

Supported operating systems:	MS Windows 2000 and Windows XP (32-bit) **ONLY**
Other requirements:	PC with *Pentium-II* processor or higher. The program is designed to use the minimum amount of computer memory.

SWizard processes output files from the following programs:

ADF 2000, ADF 2002, etc. (Scientific Computing & Modelling NV)

Gaussian 98, Gaussian 03, Gaussian 09 (Gaussian, Inc.)

HyperChem 4.x - 7.x (HyperCube, Inc.)

CNDO/INDO (by J. R. Reimers, U. of Sydney, Australia)

ZINDO (by M.C.Zerner, Quantum Theory Project, U. of Florida, USA; ZINDO is available in *Cerius*^{2} (Accelrys Inc.) and *CAChe* (Fujitsu Inc.))

In addition, *SWizard* can read **free-format ASCII text files** (please use **`log`** / **`out`** extensions to name the corresponding data files) containing energies and intensities of electronic transitions or molecular vibrations. The format of this file should be as follows:

Band energy 1	*Oscillator strength 1*	*Half-bandwidth 1*
Band energy 2	*Oscillator strength 2*	*Half-bandwidth 2*
Band energy 3	*Oscillator strength 3*	*Half-bandwidth 3*
...	*...*	*...*
Band energy N	*Oscillator strength N*	*Half-bandwidth N*

with a final blank line. Use only blank spaces (not **`Tab`**) to format your data in these ASCII text files.

You can use wavenumbers (cm^{-1}) or electron volts (eV) to specity energies and half-bandwidths.

Calculation of Absorption Profiles

Absorption profiles are calculated using the following models. Instead of evaluating the half-bandwidths, $\Delta_{1/2,I}$, for each transition, $\Delta_{1/2,I}$ can be taken as empirical parameters. For electronic transitions, $\Delta_{1/2,I}$ values depend on the nature of donor and acceptor orbitals . Then, an absorption profile is calculated as a sum of *Gaussian* or/and *Lorentzian* bands using the following equations:

Gaussian Model:

$$\varepsilon(\omega) = c_1 \sum_I \frac{f_I}{\Delta_{1/2,I}} \exp(-2.773 \frac{(\omega-\omega_I)^2}{\Delta^2_{1/2,I}}) \ , \qquad (1)$$

Lorentzian Model:

$$\varepsilon(\omega) = c_2 \sum_I \frac{f_I}{\Delta_{1/2,I}} \frac{0.25\Delta^2_{1/2,I}}{(\omega-\omega_I)^2 + 0.25\Delta^2_{1/2,I}} , \qquad (2)$$

Pseudo-Voigt Model (a convolution of both the *Gaussian* and *Lorentzian* functions with weights *W* and 1-*W* respectively)

$$\varepsilon(\omega) = W * c_1 \sum_I \frac{f_I}{\Delta_{1/2,I}} \exp(-2.773 \frac{(\omega-\omega_I)^2}{\Delta^2_{1/2,I}}) +$$

$$+ (1-W) c_2 \sum_I \frac{f_I}{\Delta_{1/2,I}} \frac{0.25\Delta^2_{1/2,I}}{(\omega-\omega_I)^2 + 0.25\Delta^2_{1/2,I}} , \qquad (3)$$

where molar absorptivity (molar extinction coefficient), ε, is given in units of mol^{-1} L cm^{-1}. The sums in Eqns. 1-3 include all allowed electronic transitions with energies, ω_I (expressed in cm^{-1}), half-bandwidths, $\Delta_{1/2,I}$ (expressed in cm^{-1}), and oscillator strengths, f_I. So, the total integrated intensity under an absorption profile obtained from Eqns. 1-3 is equal to a sum of the oscillator strengths:

$$4.32\times10^{-9}\int\varepsilon(\omega)d\omega=\sum_{I}f_{I}\ . \qquad (4)$$

A **Gaussian shape** can be chosen for spectroscopic bands with *inhomogeneous* line broadening (such as charge-transfer absorption bands of large polyatomic molecules in solution).

A **Lorentzian shape** can be chosen for spectroscopic bands with *homogeneous* line broadening [for more details, please refer to: J. I. Steinfeld "*Molecules and Radiation: An Introduction to Modern Molecular Spectroscopy*" The MIT Press: Cambridge, MA, 1981; pages 22-24].

In the current version of the program, you can use:

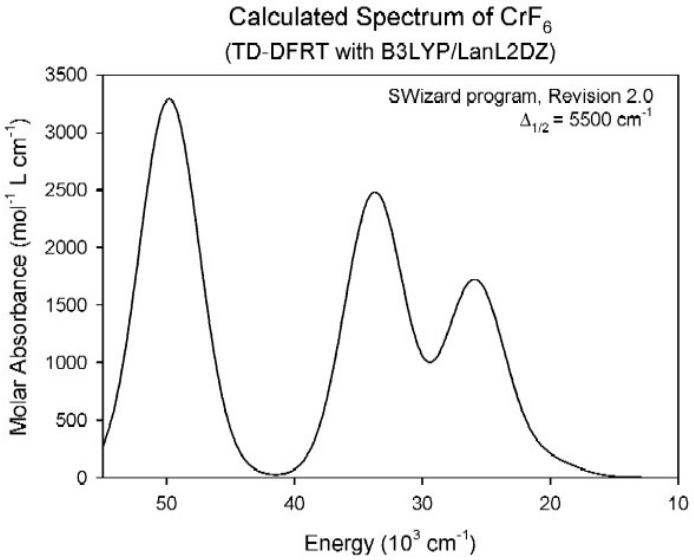
1. **the average half-bandwidth for all bands** (post-processing of *HyperChem*, *Gaussian 98*, CNDO/INDO output files). This is a good approximation if the electronic transitions in the spectrum are of similar nature;
2. **different half-bandwidths for different bands**. You have to specify half-bandwidths in a separate ASCII file. If you use free-format input files, you should specify $\Delta_{1/2,I}$. for each band in the third column of the input file (see page 2 of this manual).

Working with SWizard:

To start to the program execute ***SWizard.exe***. The program parameters are specified in the *parametr.txt* file. You can modify default SWizard parameters to fit your needs.

SWizard will read calculated excitation energies and oscillator strengths of electronic transitions from an output file and will produce an ASCII text table containing the absorption spectrum curve in the following format:

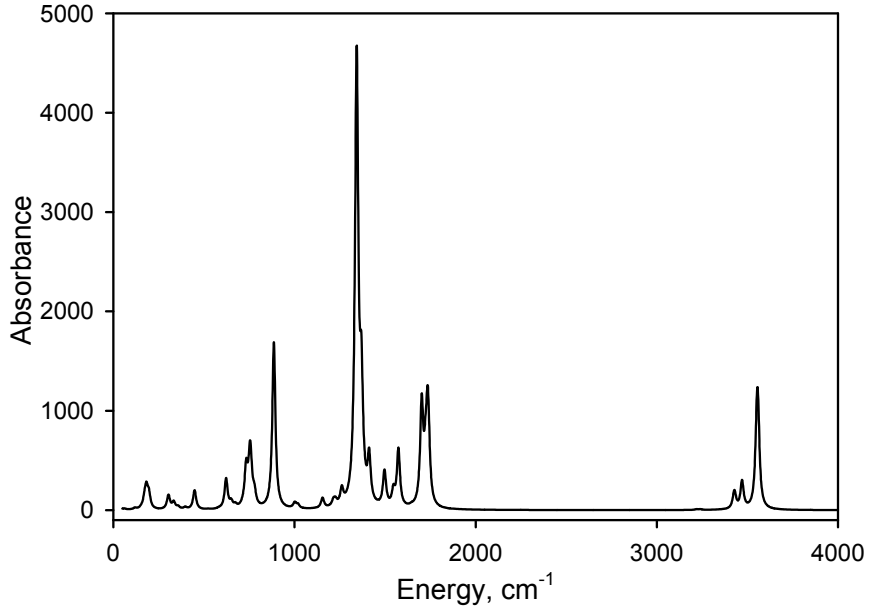
1st column:	**Energy**	**(10^3 cm^{-1})**
2nd column**:**	**Wavelength**	**(nm)**
3rd column:	**Molar absorptivity, ε**	**(cm^{-1} L mol^{-1})**
4th column:	**log(ε)**	
5th column:	**Simulation data for future reference**	



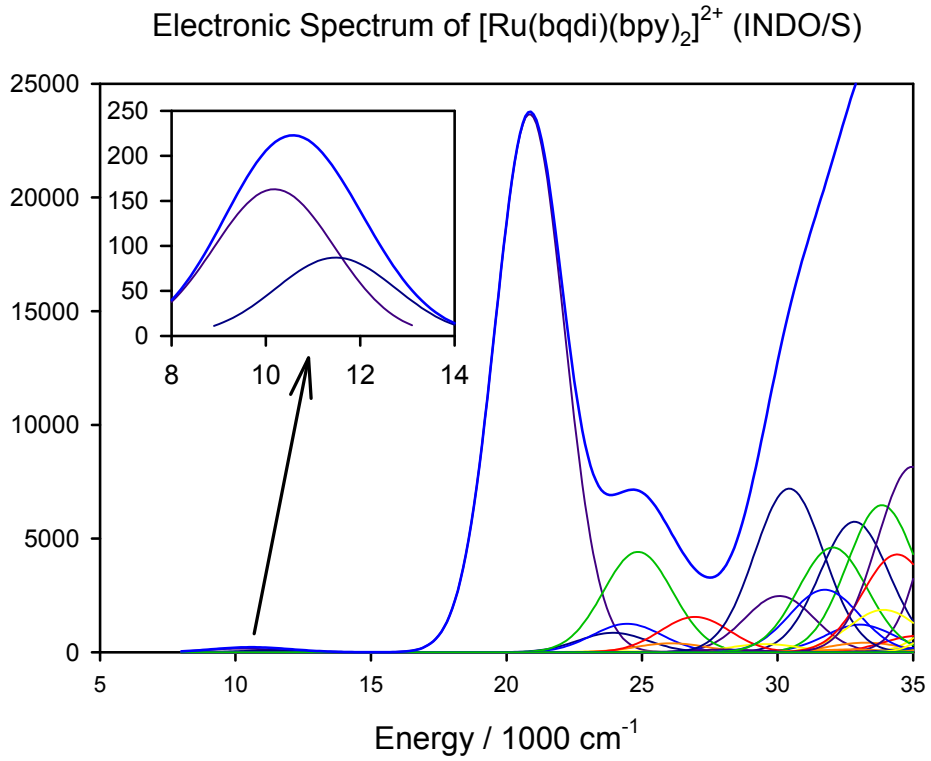
In addition to an absorption spectrum file, a table with transition assignments is created by *SWizard* (for *HyperChem* and *Gaussian 98/03/09* output files only).

In the case of IR/ Raman data, SWizard will produce an ASCII text table containing the absorption spectrum curve in the following format:

1st column:	**Energy**	**(cm^{-1})**
2rd column:	**Molar absorptivity, ε**	**(cm^{-1} L mol^{-1})**
3th column:	**log(ε)**	
4th column:	**Simulation data for future reference**	



As an additional option (the **PRINT = ALL** keyword in the *SWizard* parameter file), contributions of individual bands to an absorption spectrum can be calculated and written to an ASCII file (*SWIZARD2.DAT*). Here is an example:



The format of the *SWIZARD2.DAT* file:

1st column:	**Energy**	**(10^3 cm^{-1})**
2nd column:	**Molar absorptivity**	**(cm^{-1} L mol^{-1})**
3-nth columns:	**Contributions from individual absorption bands**	**(cm^{-1} L mol^{-1})**

Please note that individual contributions are printed only if they exceed the 1/10000th of the maximum molar absorptivity in the selected frequency range.

You can import SWizard output files to your favorite software for graphs (*MS Excel*, *Quattro Pro*, *Origin*, *SigmaPlot*, *KaleidaGraph*, etc.) to plot simulated spectra. One example is shown below:

5. SWizard limitations:

Maximum number of bands in calculations **3000***

this limit is **500 transitions for electronic spectrum calculations for Gaussian 98/03/09 and **2000** for HyperChem.*

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UV-Vis absorption (or IR/Raman) spectra were calculated using the SWizard program [1,2].

1. S. I. Gorelsky, SWizard program, revision X.X, http://www.sg-chem.net/

2. S. I. Gorelsky, A. B. P. Lever, *J. Organomet. Chem.* **2001**, *635*, 187-196

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