

# Spekwin32, Guidance for: *GaussFit*

*GaussFit* does:

assist in modelling/ deconvolution of the vibronic transitions of absorbance & fluorescence spectra, following Franck-Condon principles

## Sequence of steps:

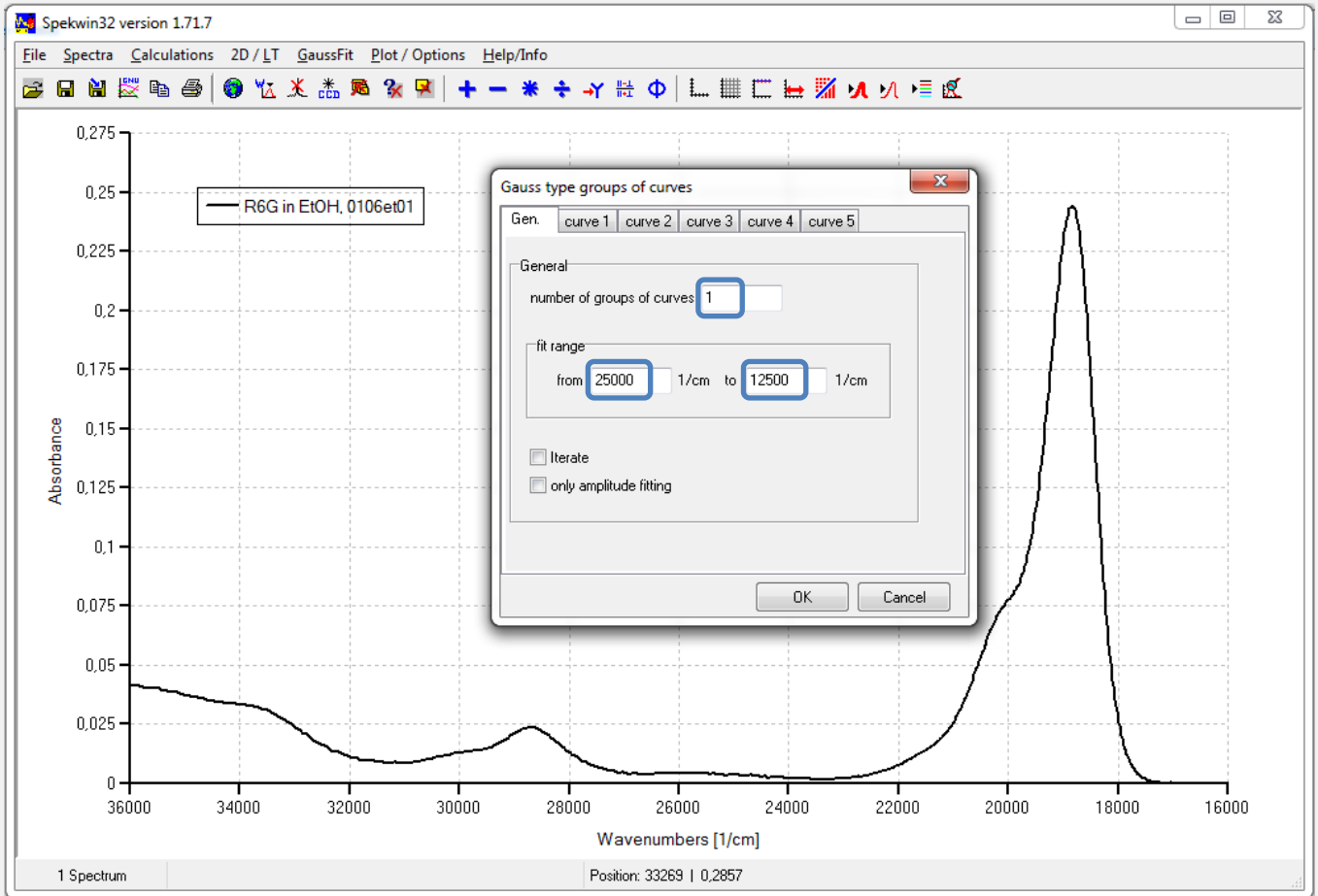
1. Load absorbance spectrum
2. Change to wavenumbers scale
3. Open GaussFit menu (Manually...)
4. Define fit range & number of groups of curves
5. Define initial values for vibration bands
6. Iterate
7. Play around with parameters & fit options
8. Repeat 6 & 7 until satisfied

Following:

execution of an example (absorbance of Rhodamine 6G, spectral data from „Test Spectra“ collection, subfolder: *csv files\Varian Cary50\0106et01.csv*)

after

- loading spectrum
- changing to wavenumbers scale
- opening Gaussfit window, you are here:

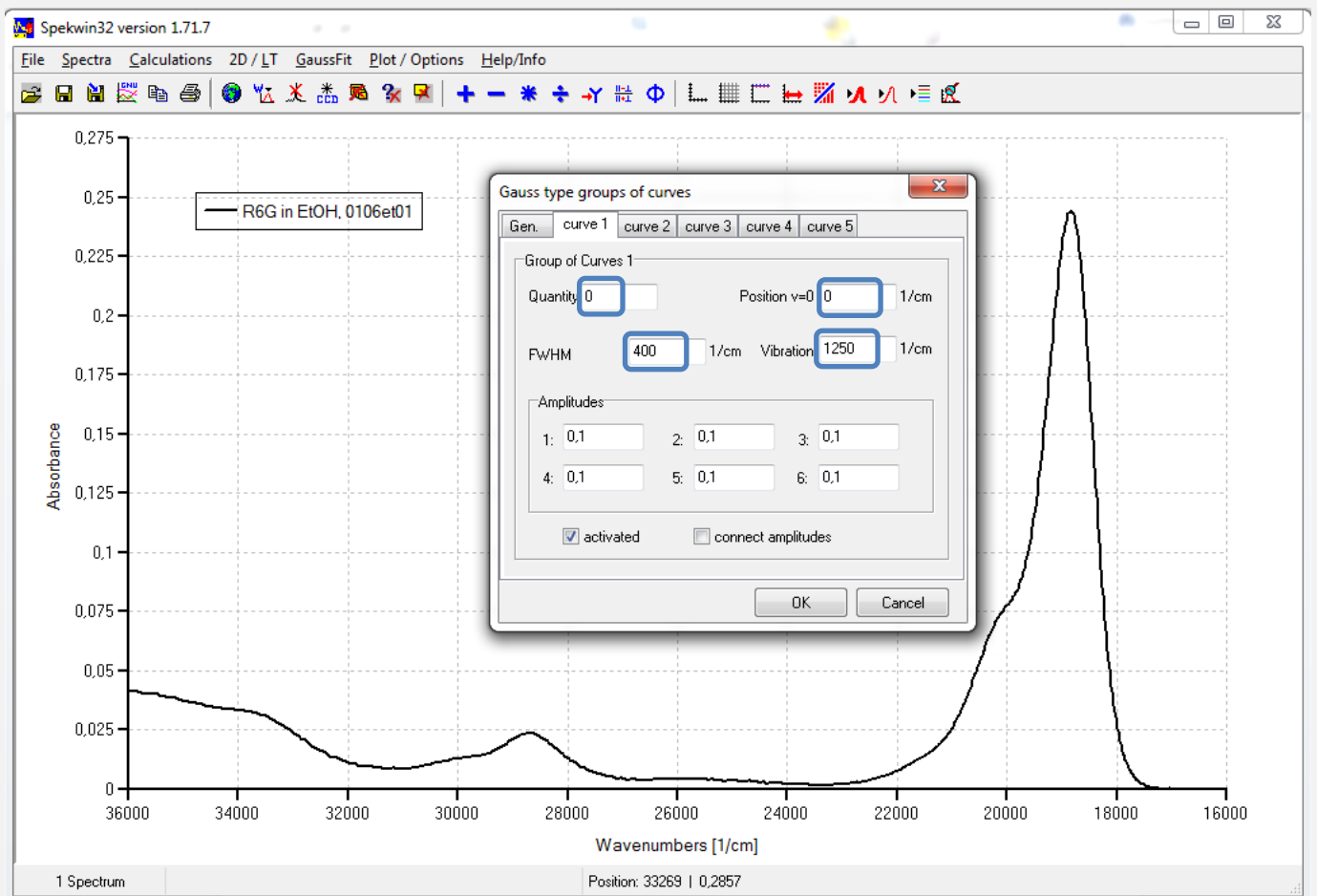


- For „number of groups of curves“ choose 1 initially, you might go up to two or three later, if necessary
- *Fit range*: defines the data range to be used for fitting. Type in left and right border in wavenumbers into the left and right edit box. This example: 22000, 18000  
The fit range will not change during iteration
- Switch to „curve 1“ tab.

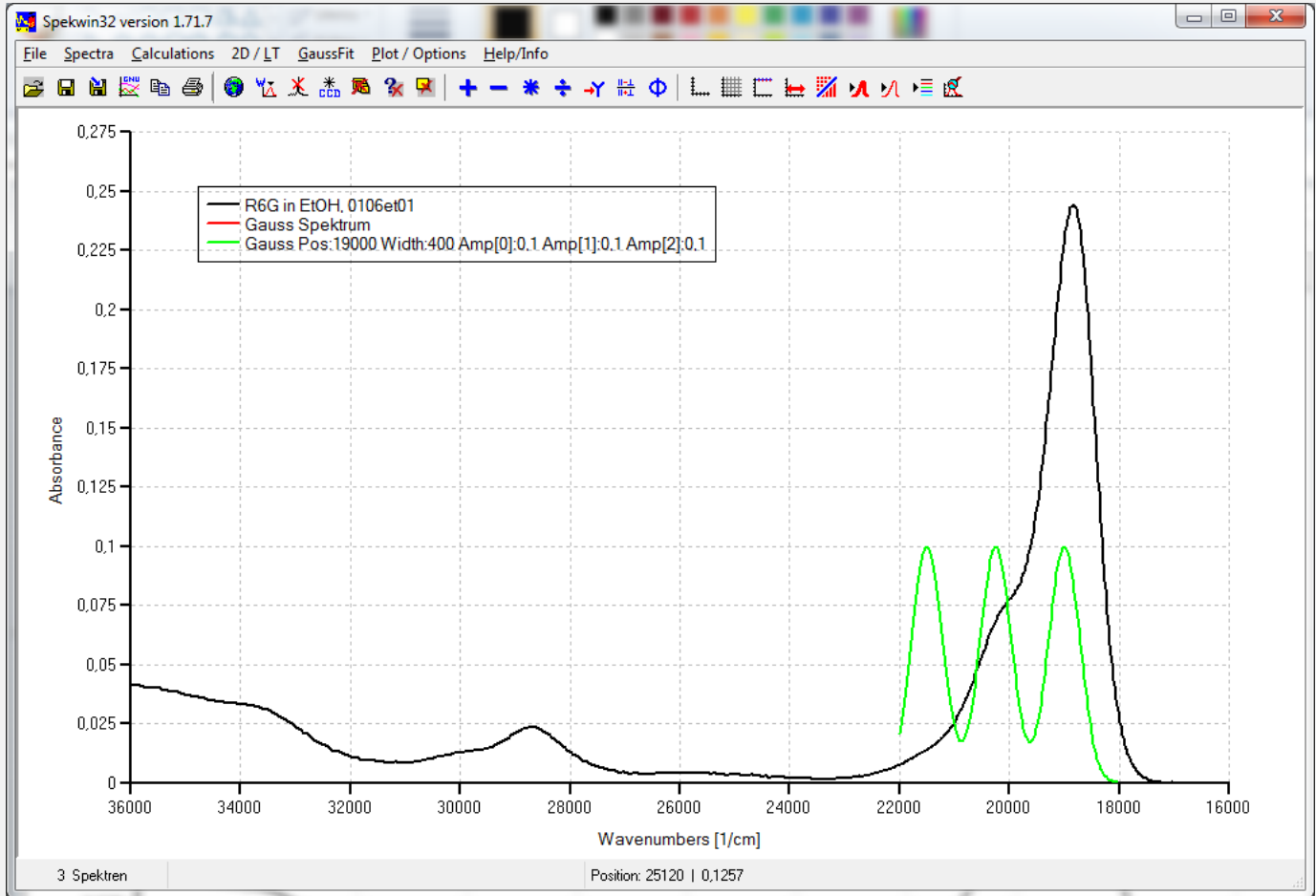
Now define for first group of curves:

- „Quantity“: is the expected number of vibronic bands that make up the transition to be fitted. **This example: 3** (you can see the maximum at 19000, a shoulder at 20000 and a faint shoulder at 22000)
- „Position“: type in a rough estimate of the center of the first gauss curve (the 0-0 transition). **This example: 19000?**
- „FWHM“: defines the width of the Gauss curves, 400 is a good start.
- „Vibration“: defines the distance of the vibronic progression, 1250 is a good start
- Ignore „amplitudes“ for this time.

Position, FWHM, Vibration, amplitudes will change during iteration, Quantity stays fixed.



Now press [OK] and the initial Gauss spectrum (red) is generated, consisting of the individual Gauss curves (green) summed up.

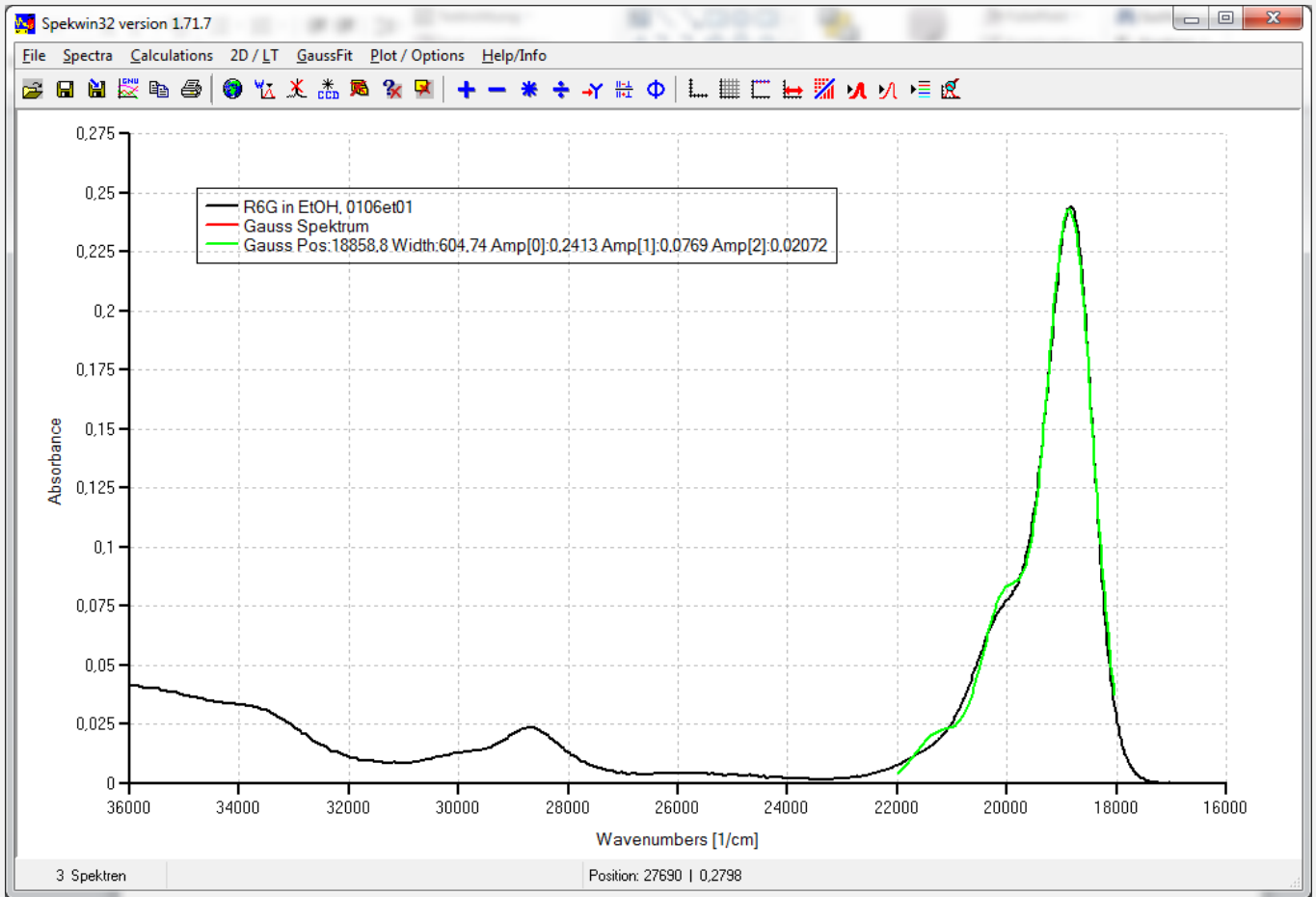


Not very impressive... but it is just what you typed in: three identical Gauss curves, with intensity values set to 0.1

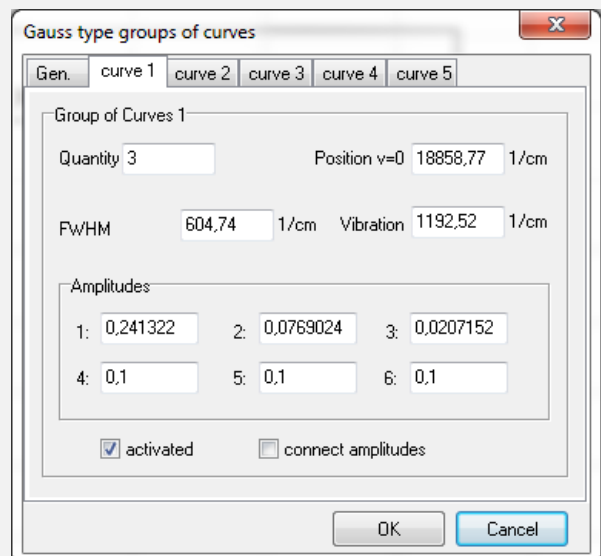
Now

- open again the GaussFit window
- go to first tab *Gen.*
- activate „*Iterate*“
- press [OK]
- Lean back and...

...enjoy your first iterated Gauss spectrum, fairly resembling the original data.



From the GaussFit window, you will see the parameters that have been found during iteration.



Now play around, using all the options:

- From the *Gen* tab
  - „*Iterate*“ will try to optimize Position, FWHM, Vibration, and amplitudes of all activated curves at the same time (which is too much sometimes).
  - With „*only amplitude fitting*“ activated, it won't shift around the bands in x direction but only optimize the amplitudes.
  - Increase the number of sets of Gauss curves.
- From the curve 1 tab (and the other curve tabs)
  - With „*connect amplitudes*“ activated, the given amplitude ratio will remain unchanged during iteration.
  - On deselecting „*activated*“, the current curves tab will be completely ignored during iteration.
  - Change the quantity of connected Gauss curves and vary the other parameters-

### **Final remark:**

The GaussFit function is not suited for fitting of NIR, FTIR or Raman spectra. It produces spectra from groups of curves separated by constant distances which is appropriate for absorbance/ fluorescence spectra described by the Franck-Condon-scheme.