

What is new in UNIFIT 2022?

Main focus of the advancement to the **version 2022** was in the improvement of the calculation procedure QPA (quantified peak areas) for the estimation of the spectrometer transmission function $T(E)$ (IERF). The functionality of the right mouse button was extended with design commands. A new input routine for the loading of SPECS Prodigy data was implemented. Two additional function of the Min/Max value definition of the fit parameters were implemented. The input dialogue for the fit parameters has now a call for the increasing and decreasing of the number of peak-fit components. The spectrum labelling and title functions were extended.

- i) The sub-programme for the generation of the spectrometer transmission function using reference peak pairs was improved. The following tasks were realized:
- Extending the $T(E)$ estimation from pure-element reference samples (Au, Ag, Cu, Ge) to well defined compounds (IL).
 - Plot of the input data and the $T(E)$ function in one sheet during the calculation and after loading the corresponding UNIFIT projects.
 - Changing of the fixed value $E_0 = 1000$ eV to a variable adjustable fit parameter E_0 .
 - Optimization of the fit procedure.
 - Optionally setting of the number of cycles (more than one) and sweeps per cycle.
 - Saving and reloading as UNIFIT project.
 - Improved saving and reloading of the estimated $T(E)$ functions.

The characterization of the new feature is:

- The calculation time is:
$$\text{Time} = \text{Number of cycles} \cdot \text{Number of sweeps} \cdot 11^{\text{number of free fit parameters}}$$
- The typical acquisition parameters of a measurement function are saved additionally with the estimated parameters of the $T(E)$ function (*.dat)(see Fig. 1). After a reloading the $T(E)$ function is displayed like after the calculation.
- The separation between:
 1. 'Calculation Transmission Function Al/Mg Excitation' and
 2. 'Calculation Transmission Function Synchrotron Excitation'is cancelled.
- The $T(E)$ approach can be saved and reloaded as UNIFIT project.
- After a reload the calculation can be continued and the input data can be displayed.
- $T(E) > 0$ at the displayed energy range.
- After pressing 'Calculate' (Fig. 1) the normalized intensities of the peak pairs and the curve of the $T(E)$ function are displayed in one plot.

- The dialogue for the definition of the fit parameters of the $T(E)$ function will be opened (see Fig. 2). Additionally, the fit conditions can be defined with:
 1. Number of sweeps per cycle.
 2. Number of cycles.
 3. Break condition (The iteration stops if the error (SSD) lower a defined value (e.g. 0.05).
 4. The function $T(E)$ can be normalized ($T(E_0) = 1$).

The following information are displayed (also after a iteration):

1. Error of the iteration.
2. Calculation time (zero before the iteration was started).

The fit parameters can be saved and reloaded.

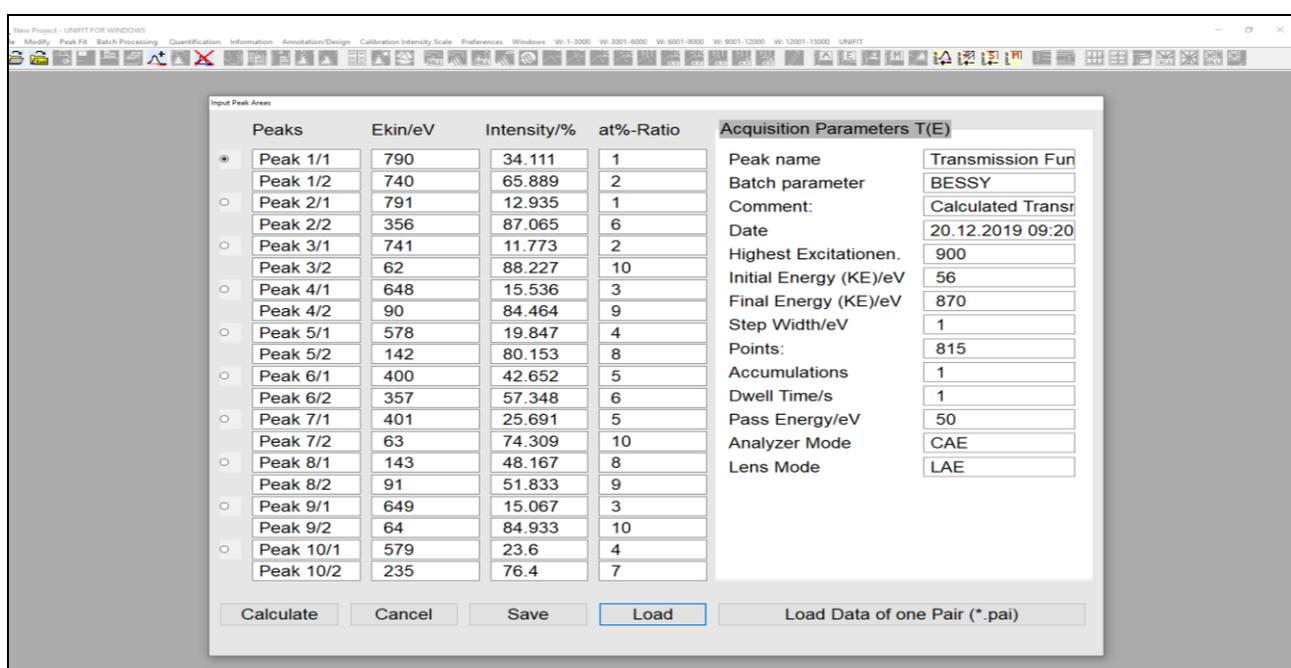


Fig. 1. Input dialogue for the estimation of the transmission function $T(E)$ using ten reference-peak pairs and appropriate acquisition parameters, example: IL

ii) A new input routine for the SPECS Prodigy data format was implemented. The input of XPS, REXPS and XAS data are supported:

Four loading options are offered (see Fig 3):

1. Spectrum
2. Ring Current
3. Mirror Current
4. TYR-Data
5. Free data block name, edit field

- One normalization option: normalizing to Ring Current.

- Option: Create sum curve of scans (slices).
- Incorrect input data are identified and changed to readable data.

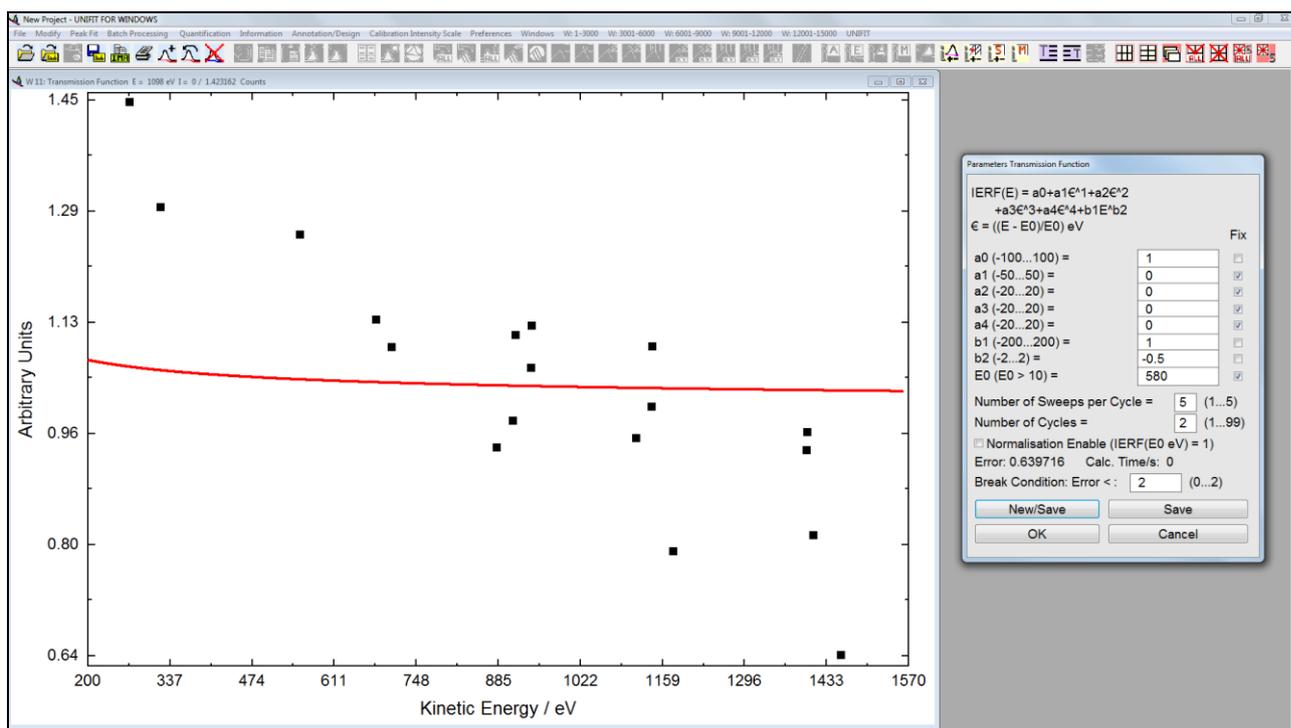


Fig. 2. Left: plot of the normalized reference pairs and the $T(E)$ function using the start parameters in one frame, right: input dialogue for the parameters of the $T(E)$ function and parameters for the controlling the estimation as well as the information for validation of the calculation

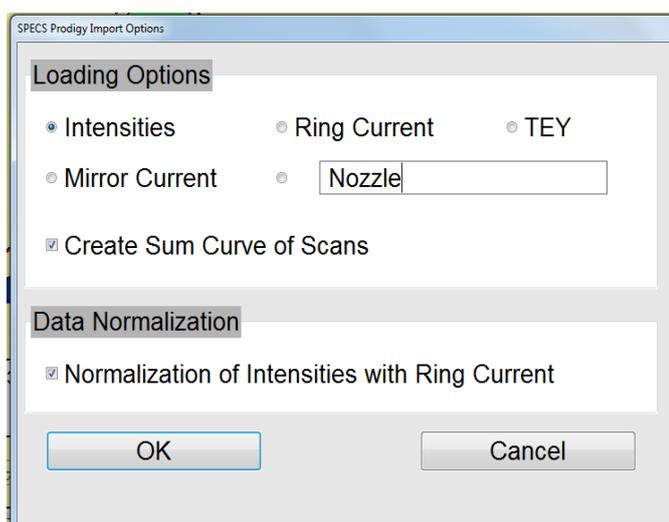


Fig. 3. Dialogue for the definition of the loading condition of the SPECS Prodigy data

- **XAS:**

1. Energy scale is calibrated to the external true excitation energy values.

2. Energy scale is converted to equidistant steps using linear interpolation of the intensities.
3. Minimum of the step width: 0.02 eV

- **XPS:**

Data of a RESXPS measurement are identified automatically.

- iii) Two new options for the definition of the Min/Max values of the fit parameters were implemented (Fig. 4). The Min/Max values of the positions of all defined peak-fit components may be defined using the position of the peak-fit component.

The Min/Max values can be defined:

1. All maxima and minima: position of peak-fit component +0.2 eV and -0.2 eV
2. All maxima and minima: position of peak-fit component +0.4 eV and -0.4 eV

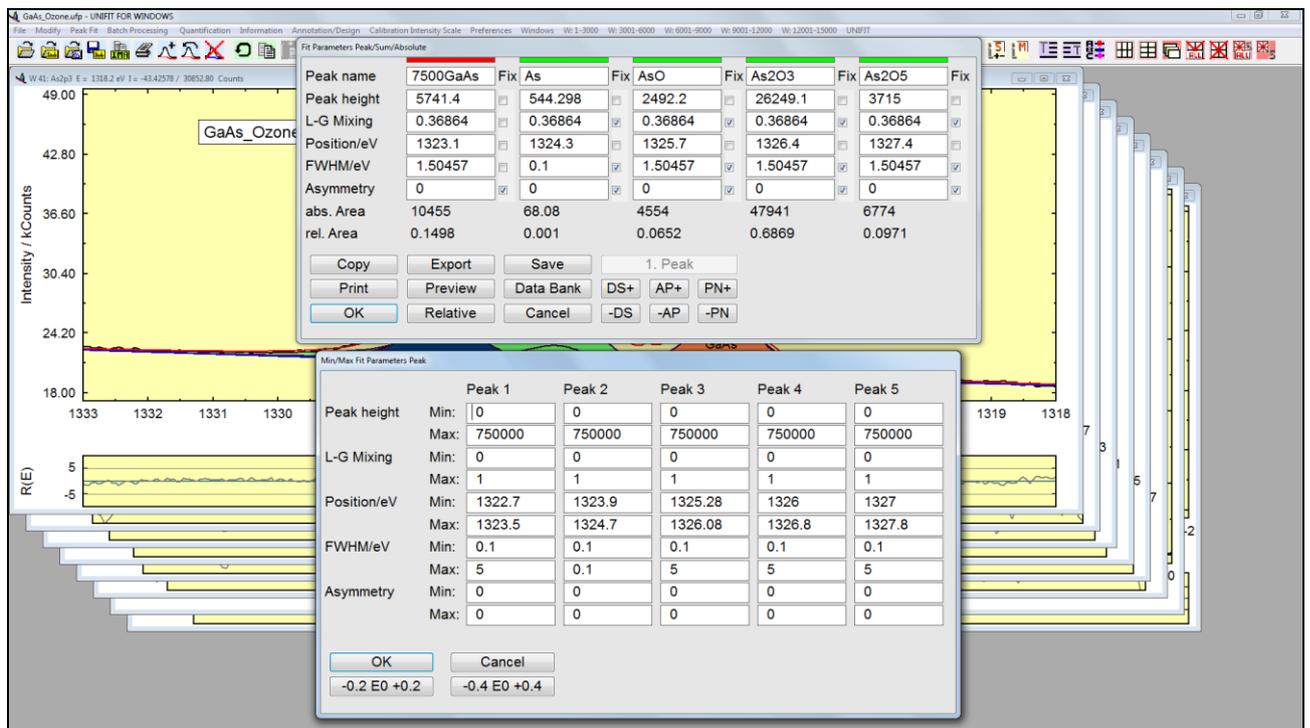


Fig. 4. Top: Dialogue for the definition fit parameters, bottom: dialogue of the Min/Max values of the fit parameters with the two new controls

- iv) The number of the peak-fit components can be increased or decreased using a separate control implemented into the dialogue for the definition of the start parameters of the peak fit (see Fig. 4). The controls are titled with 'PN+' and '-PN'.
- v) New functions were implemented into the dialogue 'Spectrum Labelling 1' (see Fig 5) and 'Spectrum Title 1' (see Fig 6).
1. The x- and y position of the labelling of the spectra can be defined.
 2. The mouse operation for the positioning after a definition of a spectrum label was removed.
 3. An additional label is placed with a short shift of the x and y position.
 4. The new command 'OK Plus New Labelling' or 'OK Plus New Title' allows the definition

of more than one label or title with a short closing and reopening of the dialogue
'Spectrum Labelling 1' or 'Spectrum Title 1'.

5. The commands '-DS' and 'DS+' permits the simultaneous decreasing and increasing of the text size without closing the dialogue.

The changed text size is saved automatically and is used for a new activation of a dialogue.

vi) The New functions were implemented into the dialogue 'Spectrum Labelling 2' (see Fig 7) and 'Spectrum Title 2' (see Fig 8). These programme features allow an integration of a formatted text, figures or pictures into the spectra windows.

vii) The functionality of the popup menu of standard-spectra windows using the right mouse button was extended by:

1. Spectrum Labelling 2
2. Spectrum Title 2
3. Activate Resizing 'Spectrum labelling 2'
4. Activate Resizing 'Spectrum Title 2'

viii) The order to increase the secure use of the program UNIFIT, open dialogues are closed in two cases:

- a) Automatic without an information message on changing the active window:
- b) With an information message in case of saving a Unifit project, export of data, export of images and printing out operations.

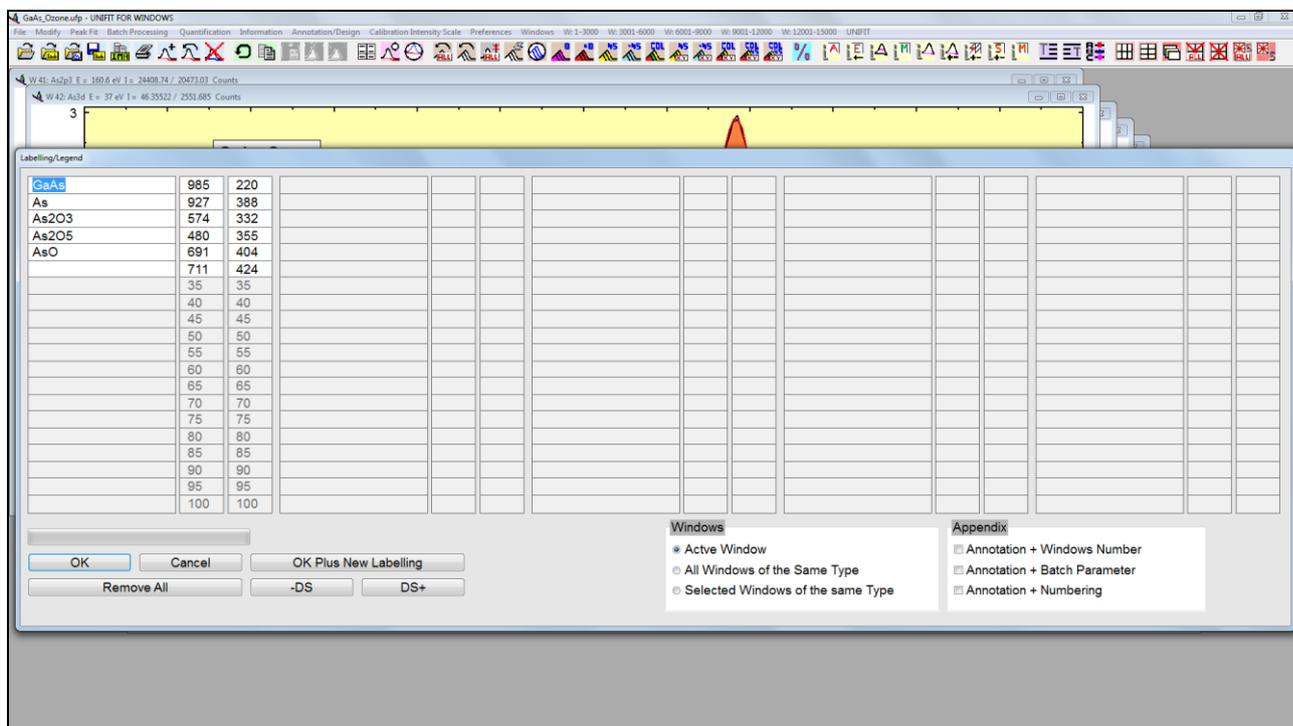


Fig. 5. Dialogue 'Annotation/Design – Spectrum Labelling 1'

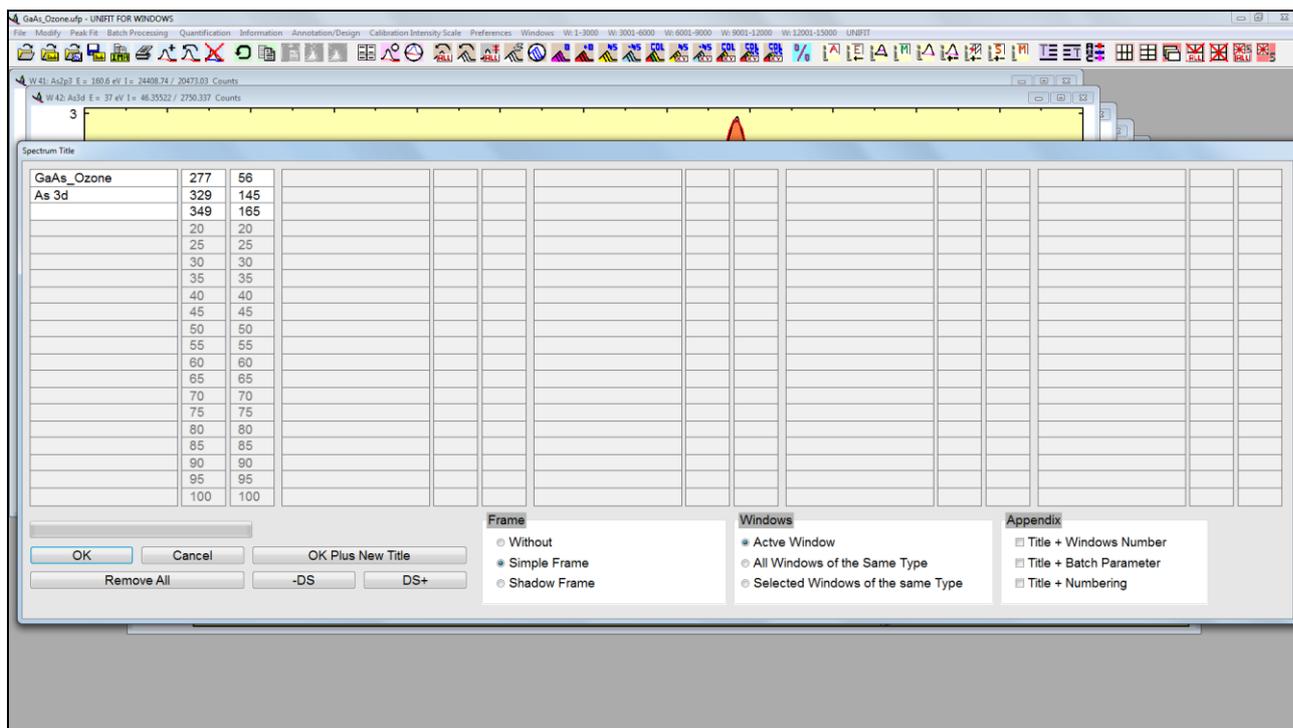


Fig. 6. Dialogue 'Annotation/Design – Spectrum Title 1'

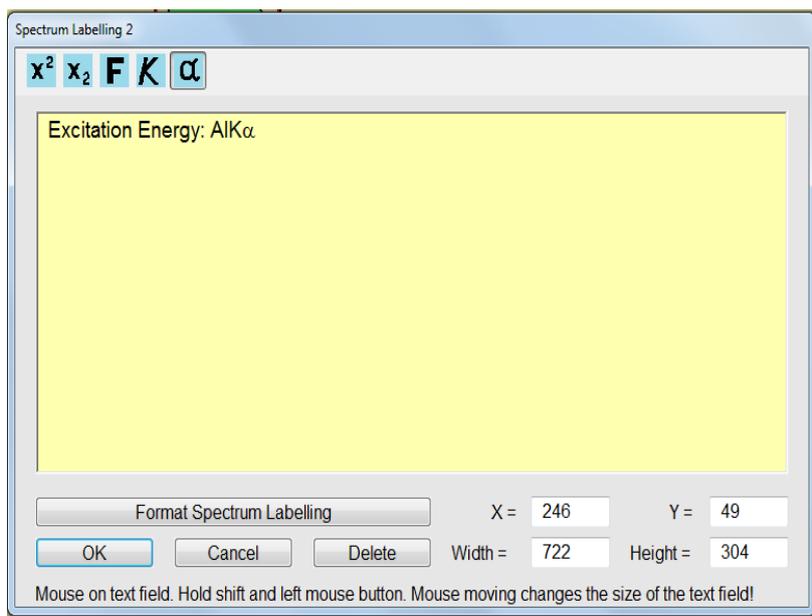


Fig. 7. Dialogue 'Annotation/Design – Spectrum Labelling 2'

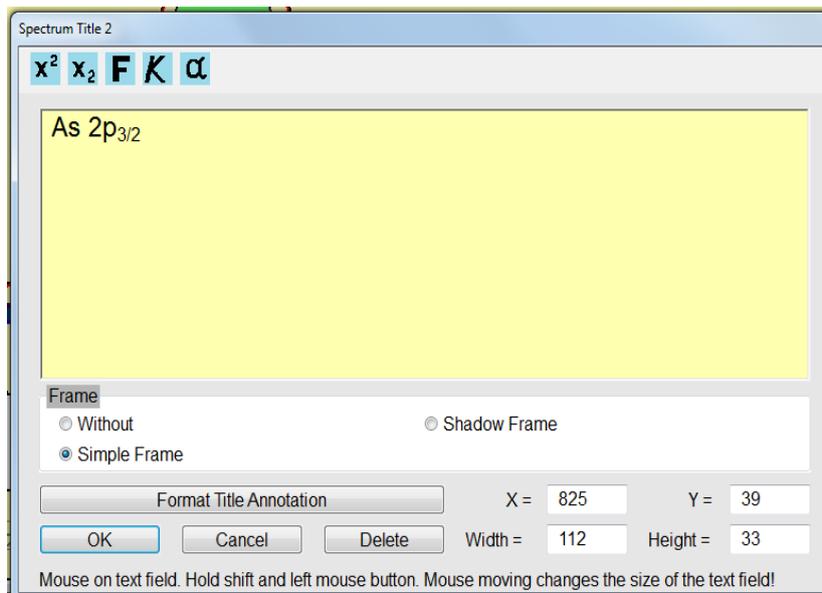


Fig.8. Dialogue 'Annotation/Design – Spectrum Title 2'

- ix) The programme-internal spectra names can be modified manually. Five options are offered:
- Spectrum name without extension (multi region measurement),
 - Spectrum name plus batch parameter (SDP, ARXPS),
 - Spectrum name plus x-Axis (line scan),
 - Spectrum name plus y-Axis (line scan),
 - Spectrum name plus x-axis and plus y-axis (multipoint measurement, mapping),
 - Spectrum name plus batch parameter plus x-axis and plus y-axis (SDP mapping).