

Introduction

Welcome to the reference documentation for LT10. Here you can find details about features and utilities of this software. If you're new to LT10 start with <u>Getting started with LT10</u>.

Feel free in using left contents panel and links at the top of each page to navigate to desired subjects.

LT10

Modern operating systems besides of their many advantages raise compatibility issues for programs compiled in former languages. It is one of the reasons why the new program for numerical analysis of positron annihilation lifetime spectra was built. As it is the continuation of well known LT series it inherits most of the features available and solutions used in LT (numerical routines and analysis logic). Like in previous versions, operating on series of spectra makes possible to correlate selected parameters belonging to different spectra of a series. Despite of features already implemented earlier, designing new version was perfect opportunity to include features yet unavailable in other versions of the program. Moreover, the completely new user interface was designed to make those features easy to use. New structure of the program supported with checked logic makes the computer analysis flexible and versatile.

Requirements

Since LT10, requires Microsoft .NET Framework 3.5 to work, requirements for this framework applies to LT10 also. (Below are presented requirements for framework available on Microsoft website:

http://download.microsoft.com/download/9/a/e/9ae0f6cc-7032-408e-9ca7-989f9e4af4ec/dotNetReadMe.htm)

Supported Architectures

- x86
- x64
- ia64 (Windows Server 2008)

Supported Operating Systems

- Microsoft Windows XP
- Microsoft Windows Server 2003
- Windows Vista
- Windows Server 2008
- Windows 7

Hardware Requirements

Minimum

400 MHz CPU, 96 MB RAM, 800x600 256-color display

Recommended

1.0 GHz or higher CPU, 256 MB or more RAM, 1024x768 high-color 32bit display

Up to 500 MB of hard disk space may be required

Framework

Required framework is available to download at this address: http://msdn.microsoft.com/en-us/netframework/aa569263.aspx

See			<u>Theoretical</u>	<u>Parameter</u>	Parameters	<u>Fit</u>
also	<u>Project</u>	<u>Document</u>	<u>model</u>	<u>Status</u>	Grid	Window

Getting started with LT10

Introduction

Once you've downloaded and installed LT10 you have are able to run program. Below you can see the main window which appears after program execution.



This window is the desktop of the LT10 program which holds opened projects. You are allowed to open multiple projects as if they were a documents in MDI application. To switch between them use either *Windows* menu or keyboard shortcut Ctrl+Tab.

New Project

In order to work with spectra series you have to either open existing project or

create the new one. This section presents wizard which creates new project.

To create a new project choose *File* -> *New*. All you have to do is to choose <u>theoretical model</u> and spectra of interest. It is done by clicking proper button in <u>documents</u> tree in *New Project* dialog (see figure below).

New Project	
Documents	
Add Remove	
Document	
Document Name	Document01
Theoretical Model	(Define)
Spectra	(Define)
	Ok Cancel

Although, project will contain one document by default, with chosen theoretical model and spectra, document count may be changed with *Add/Remove* buttons in *New Project* dialog. When working with multiple documents with different theoretical models and spectra it is adviced to name each document by clicking default document name.

note

Both theoretical model and spectra of each document, although

chosen while creating new project, may be modified after project is created in project's *Propeties*. New documents may be added as well.

Once project is created, theoretical function paramter must be set to its initial value, as close to the real one as possible. The more exact values is provided the more reliable analysis result can be expected.

Parameters are logically grouped in four groups:

- sample parameters (dependent on theoretical model)
- source parameters (intensities and lifetimes of number of components)
- prompt parameters (resolution curve parameters)
- range parameters (analysis range, zero channel and background)

Some of them (like range and prompt parameters) already have default initial value, other (like sample and source parameters) should be provided manually. Also component count (if possible) should be manually adjusted like in sample or source case with special spin edit below proper <u>parameters grid</u>.

ectrum1		Commo 💌	Commo 🔻	Commo T		8
ectrum1		Concerns a succession of the s		Gommo	Local Free M	
	1	100	0.202	0	0	0.202
ectrum2	2		-	-	0	0.202
ectrum3	3	-	-	-	0	0.202
ectrum4	4	-	-		0	0.202
ectrum5	5	-	-	-	0	0.202
ectrum6	6	-	-	-	0	0.202
ectrum7	7	-	-	-	0	0.202
ectrum8	8	-	-	-	0	0.202
ectrum9	9		-	-	0	0.202
ectrum10	10		-	-	0	0.202

note

Some of theoretical models like Trapping Models have fixed component count to 1. In those cases component count cannot be changed and there is no spin edit below parameters grid.

Fitting theoretical curves to the experimental data

To run calculations, there must be one of the parameters grid displayed, since the parameters grid defines which spectra will be fitted.

note

Displayed parameters grid doesn't determine fitting parameter set but spectra which will be fitted. For example, if displayed parameters grid is *sample*, other parameters will be fitted as well, as long as spectrum included in *sample* group is also included in other parameter groups.

note

Attempting to run calculations when displaying other page than that holding parameters grid (eg. *Search*) results in showing message box instructing to choose one of the parameters grid.

Calculations may be run in following ways:

- 1. calculations for first spectrum in currently displayed parameters grid *Fit first spectrum*
- 2. calculations for all spectra in currently displayed parameters grid *Fit series of spectra*
- 3. calculations for custom spectrum in currently displayed parameters grid *Fit [spectrum_name]* in parameters grid's context menu

note	
While runni	ing calculations for either first spectrum or for all
spectra in cu	urrently displayed series can be achived by using
calculations	5 toolbar \blacktriangleright Fit first spectra \clubsuit Fit series of spectra $times$ Cancel calculations
(or <i>Project</i>)	menu), fitting custom spectrum can be done only
through par	ameters grid's context menu.

Every time calculations is about to run, *Search* tab of project is activated to allow user to follow calculations progress.

note

User may disable automatic switching to *Search* tab of project by deselecting *Switch to Search tab after calculations run* check box in *General* tab of *Tools* -> *Options* dialog.

Finished calculations, as well as each calculations progress, are prompted by proper entry in *Events* box in *Search* tab. Moreover, if calculations were run for single spectrum, special <u>fit window</u> appears with displayed fit for chosen spectrum, when calculations are over. If those fits are dissatisfactory, calculations may be repeated by clicking button *Fit again* in this window.

Bindings

There are two kind of bindings available in LT10:

- Interodument parameter (*Create interdocument value* button)
- Shared group (*Join document groups* button)

Both binding can be created in *Project properties -> Bindings* view.

FeAlMe_4states.ltpp	
prompt [nk] ranges [nk]	
Project properties Search Nikiel_gru2010 Kapton_maj2011 sample [all] source [Ni src]	
Indict projectes Search Nikiel_gru2010 Kapton_maj2011 sample [aii] source [Ni src] Initial Values Documents Join document groups Bindings 3. nk Document Groups	

note

To distinguish type of binding in bindings view, both binding types are marked with different colors.

Document

Document in LT10 is a spectra holder with binded <u>theoretical model</u>.

Each document has its own tab page in owning <u>project's</u> form. User interface of document is also tab page control, which contain as many tab pages holding <u>parameter grids</u> as many parameter groups are defined in theoretical model.

Spectrum	Key value	zero	start	stop	background	
					Commo 💌	
pectrum1	1	220	176	1797	15	adjust
pectrum2	2	220	176	1797	-	adjust
pectrum3	3	220	176	1797	-	adjust
pectrum4	4	220	176	1797	-	adjust
spectrum5	5	220	176	1797	-	adjust
spectrum6	6	220	176	1797		adjust
spectrum7	7	220	176	1797	-	adjust
spectrum8	8	220	176	1797		adjust
spectrum9	9	220	176	1797	- /	adjust
	10	220	17/	1707		odiust

See also Parameters Grid

Fit window

Tool which shows fit quality. Every time calculations for first spectra in each document ends with showing this window. Moreover, after series calculations you may see fit quality of any spectrum in series by choosing <u>parameters grid's</u> *context menu -> Show spectrum fit*. The top chart contains such series as

- Experimental spectrum
- Theoretical curve
- Curves representing each component in each group



The bottom chart in fit window shows fit quality. The more even graph the better fit. If fit is not satisfying try clicking "Fit again".

Values in bottom chart are calculated with equation:

$$D[i] = \frac{T[i] - E[i]}{\sqrt{E[i]}}$$

where

i - channel number

E[i] - value of experimental spectrum at channel i

T[i] - value of theoretical curve at channel i

D[i] - difference between theory and experiment at channel i



Good fit



It is possible to change the color of visible components in the top chart or even hide some of the components. To do that expand series list by clicking *Series* button on the top toolbar



Charts may be saved to either bitmap 🗏 (*.bmp file with top and bottom charts

with selected series) or tab-separated files 🗒 (data which was used to draw charts)

If there are more documents in project and fit window appeared after fitting first spectra or fit window was called manually from parameters grid, you may switch displaying spectrum fit with combo box at toolbar.



Parameter Status

Most of parameters in LT10 besides of value has a status used to control parameter value's freedom degree in calculations process and range of binding in series of spectra. Therefore available statuses are combinations of freedom degree specificators and range of binding specificators.

Range of binding specificators

Common

All spectra within a document have one common value.

Local

Each spectrum has a private value.

Freedom degree specificators

Free

Parameter value is free to change in calculations process.

Fixed

Parameter value can not be changed by minimalization procedure.

There are four standard combinations of specyficators mentioned above which defines statuses available to choose:

- Local Free
- Local Fixed
- Common Free
- Common Fixed

Parameter statuses may be set with status controllers placed at the top of <u>parameters grid</u> as shown in picture below.

e int ₁ fwhm ₁		shift ₁	int ₂		fwhm ₂	shift ₂	
Commo 💌	Commo 💌	Local Free 🔽	Commo	•	Commo 💌	Local Fix 💌	
85.979	0.24498	Local Free			0.18405	-6.8941	
-	-	Local Fixed Common Free			-	-6.8941	
-	-	Common Fixed			-	-6.8941	
		mixed			-	-6.8941	
-	-	0.0025282	-		-	-6.89	
	int 1 Commo 85.979 - - - - - - - - -	int 1 fwhm 1 Commo Commo C 85.979 0.24498 	int 1 fwhm 1 shift 1 Commo Commo Local Free 85.979 0.24498 Local Free - - Local Free - - Common Free - - Common Free - - Common Free - - 0.0025282	int 1 fwhm 1 shift 1 int 2 Commo Commo Local Free Commo 85.979 0.24498 Local Free Commo - - Local Free Commo - - Common Free Common Free - - Common Free Common Free - - Common Free Common Free - - 0.0025282 -	int 1 fwhm 1 shift 1 int 2 Commo Commo Local Free Commo 85.979 0.24498 Local Free Commo - - Common Free - - Common Free - - Common Free - - Common Free - - 0.0025282	int 1 fwhm 1 shift 1 int 2 fwhm 2 Commo Commo Local Free Commo Commo Commo 85.979 0.24498 Local Free Commo 0.18405 - - Local Fixed Common Free - 0.18405 - - Common Fixed nixed - - - 0.0025282 - -	

note

It is possible to set statuses of few parameters within one grid at the same time. To do that follow this steps:

- select controllers which statuses you want to change (controller is selected when its text is marked white; to select controllers use ctrl key or simply drag cursor through controller cells)
- 2. press spacebar to activate lastly selected controller
- 3. with mouse left button expand active controller
- 4. select desired status

All selected controllers will gain status chosen for the last controller in selection range.

Beside four standard statuses there are two additional parameter statuses for binded parameters (<u>interdocument parameter</u>).

- Binded Free
- Binded Fixed

To distinguish parameter status on parameters grid, each status has binded different color.

note

Statuses colors may be adjusted in *Options* dialog (*Paramters grid* tab) available in menu *Tools* -> *Options*.

Parameters	Grid
------------	------

t ci_sim2								
Project proper	ties Search	Document	01					
sample sourc	sample source prompt ranges							
Spectrum	Key value	int 1	τ ₁	int ₂	τ 2	int ₃	τ ₃	T avg
		Commo 💌	Commo 💌	Commo 💌	Local Free 🔽	Commo 💌	Commo 💌	
ci20	1	59.8043	0.126125	30.198	0.200057	9.99768	1.30145	0.265956
ci22	2	-	-	-	0.220013	-	-	0.271983
ci23	3	-	-	-	0.229905	-	-	0.27497
ci24	4	-	-	-	0.240345	-	-	0.278122
ci26	5	-	-	-	0.26002	-	-	0.284064
ci28	6	-	-	-	0.279836	-	-	0.290048
Component co	Component count							

Parameters grid is a tool designed to edit parameter values and statuses for series of spectra in single parameters group. Most of parameters grids have similar set of columns: name of spectrum, key value and columns holding parameters specific for actual parameters group.

Hiding columns

Columns in parameters grid may be hidden to obtain greater clarity of situation if some of parameters always have the same value and status or these values are not interesting at the moment.

To hide/show column in parameters grid deselect/select items in *grid's context menu -> Visible columns*

note

Hiding column with free parameters will NOT exclude those parameters from calculations! To exclude parameter from calculations set its status to Fixed (any of following are possible: Common Fixed, Local Fixed and Binded Fixed. See <u>Parameter</u> <u>Status</u>)

sim2X Diject properties Search Document01X mple source prompt ranges								
Spectrum	Key value	int 1	τ1	int ₂	τ2	int 3	r 3	τ _{avg}
Visible	columns	•	Spectrum	1			Sommo 💌	
:i20 Copy		Ctrl + C	 Key value 	e			.30145	0.265956
:i22 Paste		Ctrl + V	✓ int 1				-	0.271983
:i23 3		-	✓ τ ₁				-	0.27497
:i24 4		-	✓ int 2				-	0.278122
:i26 5		-	✓ τ₂				-	0.284064
:i28 6		-	✓ int 3				-	0.290048
20 6 - 0.290048								

Sorting spectra

Spectrum, Key value and *Model* columns are sortable. (*Model* column is displayed when parameters grid displays spectra from more than one document - see <u>Bindings</u>) To sort spectra by one of these columns simply click header of the

column you want to sort by.

note

Sorting one parameters grid automatically affects other parameter grids, holding the same spectra.

S	ee			<u>Theoretical</u>	<u>Parameter</u>	Parameters
al	SO	<u>Bindings</u>	<u>Document</u>	<u>model</u>	<u>Status</u>	Grid

Project

Project in LT10 is collection of <u>documents</u>. LT10 allows to work with multiple projects as if they were documents in MDI application. Moreover projects may run their calculations simultaneously without necessarity of running another instances of whole LT10 application.

note

User has to be cautious in running big number of calculations since each project runs its calculations in new thread. Multiple threads on single-CPU computers may affect on speed of the calculations.

Project window

Every project window in LT10 program acts like document in MDI Application and is simply collection of tab pages. Beside of tab pages which contain tracking and modifing controls there are additional tab pages responsible for managing parameters of each document in project.

Project properties tab

Set of properties specific for particular project.

Initial values

Defines how initial parameter values for spectra in series are obtained: either by automatically copying values from previous spectrum in series or using those, determined in previous calculations.

Documents

Documents present in project. Both spectra series and theoretical model of each document may be modified.

Bindings

Overview of all <u>bindings</u> defined in project. Both interdocument parameters and shared groups are displayed.

LtProject.ltpp	
Project properties Search Docu	Iment01
Initial Values Documents Define I	how values are obtained while processing series of spectra
Bindings	O Calculate
	Get specified by user
LtProject.ltpp	
Project properties Search	Document01
Initial Values Documents A	dd Remove
Bindings	Theoretical model Document Spectra
	Multiexponential Document01 spectrum1 (9 more)
FeAlMe_4states.ltpp	
prompt [nk] ranges [nk	
Project properties Sear	rch Nikiel_gru2010 Kapton_maj2011 sample [all] source [Ni src]
Initial Values	
Bindings	
	1. all
	Document Groups
	Nikiel_gru2010
	Nikiel_kwi2011 sample
	Kapton_maj2011
	remove rename modify
	remove rename modify

Search tab

Search tab presents actual state of running calculations. The tab is divided into three parts

Events

Text area which displays information about such events in calculation process as changes in fit variance, time when calculations finished and so on.

Common values

List of all parameters with common values in each document and each group (Common Free and Common Fixed statuses, see also: parameter status)

Local values

This group box contains chart which presents relationships between chosen parameters and spectrum index in series currently fitted. If there are any parameters with local values (Local Free and Local Fixed statuses) those parameters are available to choose in *Parameter* combo box.

note

Although chart is good view of changes made by calculations process, user is allowed to switch this option off which may slightly increase calculations speed.

korzysci.ltpp	
Project properties Search Document01	
Events	Common values
[14:18:59]	τ ₁ sample Document01 0.202
Lalculations started for series of spectra	τ ₁ source Document01 0.125
[14:19:02] $y^2 = 1.016074316$	int 2 source Document01 4
Iteration 1 (Function call count: 1)	τ _{2 source Document01} 0.386
	int 3 source Document01 1
[14:19:03] Calculations time: 00:00:04.056	τ _{3 source Document01} 2
Calculations finished. Global $\chi^2 = 1.0198$	Contrib. source Document01 50
Local values	
Show local values	Ţ
chart diamoter the random chart	
0.77	ectri ectri be ctri
0.66	
0.44	
0.33	
0.11	
Ľ.	

Document tab

This tab page contains another tab pages control which holds as many parameter grids as many parameter groups exist in chosen theoretical model. Moreover, parameter names, their amount and properties depends on model binded to this document. Screenshot of such document is presented below (binded theoretical model is multiexponential model used to positron anihilation spectroscopy analysis).

Spectrum	Key value	zero	start	stop	background	
					Commo 💌	
pectrum1	1	220	176	1797	15	adjust
spectrum2	2	220	176	1797		adjust
spectrum3	3	220	176	1797	-	adjust
spectrum4	4	220	176	1797	-	adjust
spectrum5	5	220	176	1797		adjust
spectrum6	6	220	176	1797	-	adjust
spectrum7	7	220	176	1797	-	adjust
spectrum8	8	220	176	1797	-	adjust
spectrum9	9	220	176	1797	- /- /- /- /- /- /- /- /-	adjust
	10	220	17/	1707		odiuat

As shown in picture document tab caption is equal to the one provided while creating owning project.

The layout of each page in document is similar. The top part of page is occupied by grid containing parameters for each spectrum. Since some of the parameters may have statuses (a combinations of range specificatos: common, local with freedom degree specificators: fixed, free; for more about statuses see also: <u>parameter status</u>) one of the top rows in grid holds controls which allows to

change those statuses for chosen parameters. Each spectrum in document has corresponding row with parameters which belongs to the just-displaying group tab page.

note

Whereas most of the parameter values are editable in parameters grid - some of them aren't. For example in groups where component count is variable - value of first intensity (if such parameter exist in the group) is not editable and is changing while providing values of intensities for other components. Value of this intensity adapts to other intensities to make sum of all in group equal to 100%.

Below grid, there are often additional group-specific tools. For example there may be component count setter, default values provider or other handy tools.

Theoretical Model

Theoretical model is a definition of curve which is fitted to the experimental data. In this connection it have an influence on parameters used to build the curve (their amount, how they are grouped, and whether parameters may construct components).

While choosing theoretical model in *Theoretical Model* dialog, parameters defined in the model are listed in bottom group box. There are also may be found such additional informations as its name, description and path to the assembly, where model is implemented.

Heoretical Model	<u>_0×</u>
Anihilation models	
Multiexponential Wided multiexponential Two states trapping model Three states trapping model	
 Model description Multiexponential Simple theoretical model which uses sample components built from lifel intensity parameters Prameters in groups unpacked components: int, π. source: int, π. prompt: int, fwhm, shift, πleft, πight. ranges: zero, start, stop, background. Assembly 	ime and
E:\NĒED\lib\anh.dll	
UK	Lancei