Visual EPR

Everyday programs for magnetic resonance users

2015

JANUARY

S	M	T	W	T	F	S
				1	2	3
4	5	6	7	8	9	10
11	12	13	14	15	16	17
18	19	20	21	22	23	24
25	26	27	28	29	30	31

FEBRUARY

S	M	T	W	T	F	S
1	2	3	4	5	6	7
8	9	10	11	12	13	14
15	16	17	18	19	20	21
22	23	24	25	26	27	28

MARCH

S	M	T	W	T	F	S
1	2	3	4	5	6	7
8	9	10	11	12	13	14
15	16	17	18	19	20	21
22	23	24	25	26	27	28
29	30	31				

APRIL

S	M	T	W	T	F	S
			1	2	3	4
5	6	7	8	9	10	11
12	13	14	15	16	17	18
19	20	21	22	23	24	25
26	27	28	29	30		

MAY

S	M	T	W	T	F	S
					1	2
3	4	5	6	7	8	9
10	11	12	13	14	15	16
17	18	19	20	21	22	23
24	25	26	27	28	29	30
31						

JUNE

S	M	T	W	T	F	S
	1	2	3	4	5	6
7	8	9	10	11	12	13
14	15	16	17	18	19	20
21	22	23	24	25	26	27
28	29	30				

JULY

S	M	T	W	T	F	S
			1	2	3	4
5	6	7	8	9	10	11
12	13	14	15	16	17	18
19	20	21	22	23	24	25
26	27	28	29	30	31	

AUGUST

S	M	T	W	T	F	S
						1
2	3	4	5	6	7	8
9	10	11	12	13	14	15
16	17	18	19	20	21	22
23	24	25	26	27	28	29
30	31					

SEPTEMBER

S	M	T	W	T	F	S
		1	2	3	4	5
6	7	8	9	10	11	12
13	14	15	16	17	18	19
20	21	22	23	24	25	26
27	28	29	30			

OCTOBER

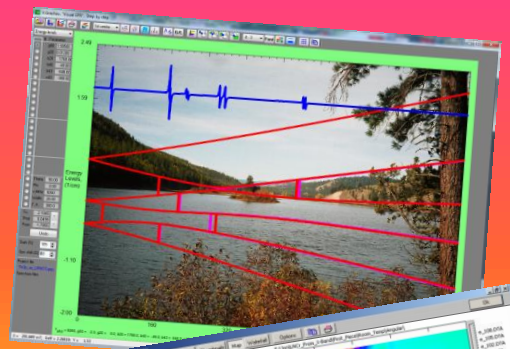
S	M	T	W	T	F	S
				1	2	3
4	5	6	7	8	9	10
11	12	13	14	15	16	17
18	19	20	21	22	23	24
25	26	27	28	29	30	31

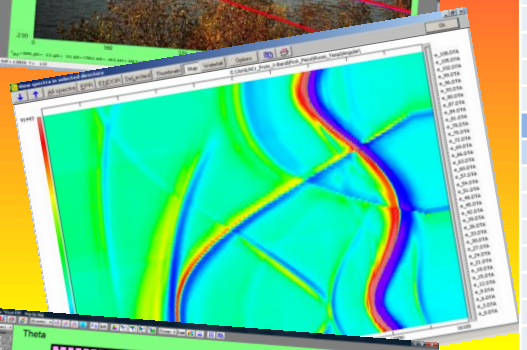
NOVEMBER

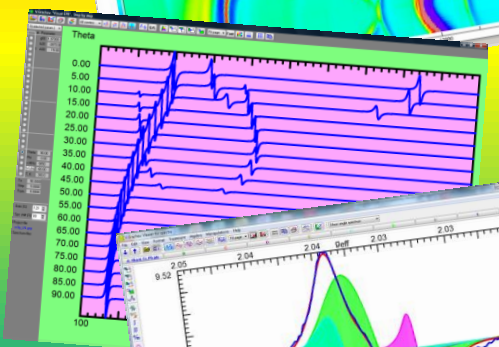
S	M	T	W	T	F	S
1	2	3	4	5	6	7
8	9	10	11	12	13	14
15	16	17	18	19	20	21
22	23	24	25	26	27	28
29	30					

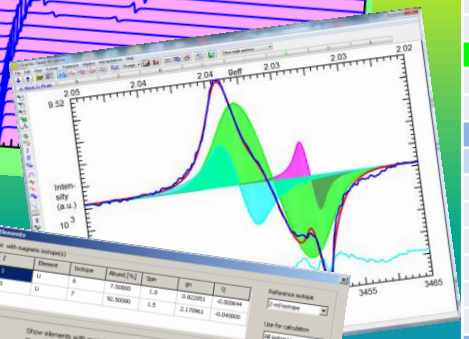
DECEMBER

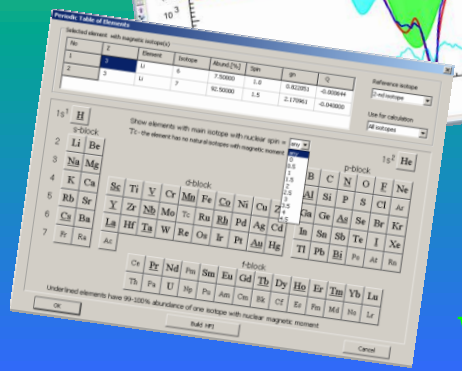
S	M	T	W	T	F	S
		1	2	3	4	5
6	7	8	9	10	11	12
13	14	15	16	17	18	19
20	21	22	23	24	25	26
27	28	29	30	31		

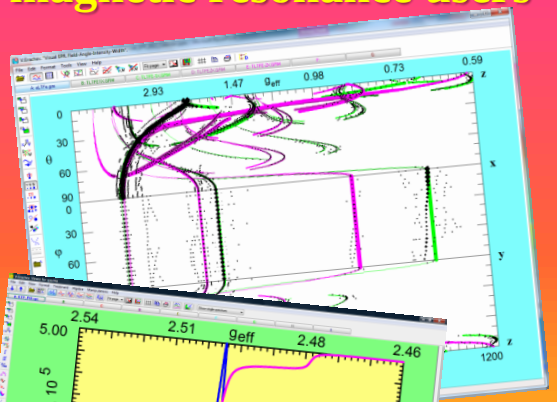


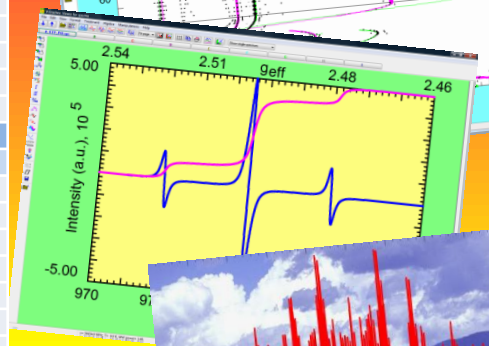


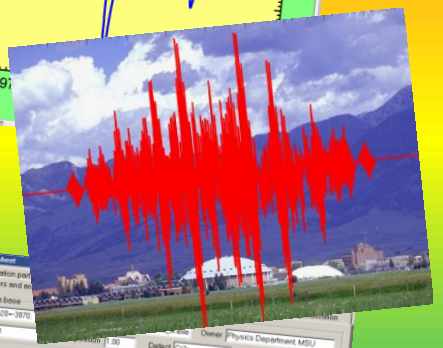


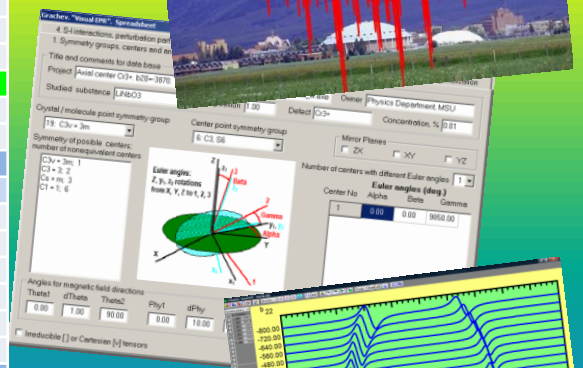


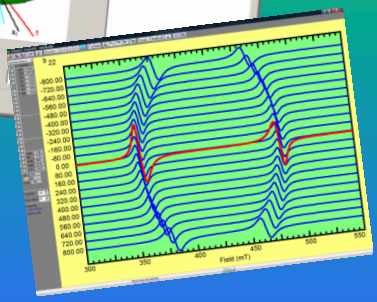












Valentyn Grachov

http://www.visual-epr.com

Why do you need "Visual EPR" programs?

There are several reasons, why you should prefer **Visual EPR**, but not other programs.

1. The programs were developed during many years. Could you spend so much time to write your own program?
2. They have very simple and convenient interface (they were developed for undergraduate students) and are flexible enough to solve most of your tasks. For instance, a change of point group symmetry, values of electron and nuclear spins, any parameters of spin-Hamiltonian or number of equivalent centers takes few seconds.
3. They are very fast. Using conventional desktop or laptop you can calculate spectra of the Gd^{3+} or Mn^{2+} in few minutes.
4. They have been tested in several spectroscopic groups from different countries. They work under **Windows** operational system.

You can treat measured spectra and build angular dependence using **View_spw.exe**, simulate spectra and compare experimental and calculated angular dependencies using **Fields_w.exe**, then view and treat angular dependencies using **FAIW.exe** preparing them for publication .

These everyday programs will facilitate and accelerate experimental data treatment, enhance trustworthiness of obtained results, improve accuracy of determined characteristics, and increase efficiency of conducted research in laboratories, which need in characterization of magnetic properties.

View_spw.exe is the program for preliminary treatment of EPR, ENDOR and other spectra. The program allows:

1. To browse all spectra in directory (or, selectively, EPR or ENDOR only) - it helps you in a few seconds to find the spectrum needed;
2. To convert a spectrum from one format to another - the program recognizes several different formats: two binary formats - byte (BRUKER) and single (WIN-EPR), two ASCII formats - one column (Y) format with signal intensities only and two column (X and Y) format with sweeping parameter values and intensities (the last are usually used for graphical programs, like “ORIGIN”, “GRAPHER”,...), *.sta, *.fls and *.jdx -formats;
3. To estimate line positions (g-factor, resonance magnetic field or frequency) and distance (splitting) between any points in a spectrum;
4. To carry out filtering of the spectrum using one of 9 filters with variable width: movement, Gaussian, Lorentzian, polynomial, Fourier filters etc;
5. To carry out peak-peaking of a spectrum;
6. To decompose complicated spectrum with overlapped lines to separate Gaussian and Lorentzian derivatives, to compare several spectra on one screen; to carry out algebraic transformations of 9 spectra: R = A + k*B+…;
7. To prepare the file with angular dependencies of the spectra collecting the positions and intensities of resonance lines (from all peak-files) and the values of polar and azimuthal angles.

No one known program does grant you these possibilities.

FIELDS_w.exe calculates angular dependencies of resonance magnetic fields and intensities of EPR lines for the rotation of magnetic field in any plane. The program imitates a sweep of the static magnetic field from B_{min} to B_{max}. Near resonance it uses cubic interpolation of energy level dependencies on magnetic field; far from resonance it increases this step. The program has a spreadsheet for the input of all necessary parameters for simulation of EPR spectra and their dependencies: the parameters of Zeeman interactions, the parameters of zero-field splitting (crystalline field) and hyperfine interactions in the Spin-Hamiltonian, microwave frequency, Euler angles for equivalent centers (if present), spins of particles, initial and final orientations of the external magnetic field ,which are characterized by polar and azimuthal angles, steps on angles etc. The parameters can be saved in <*.gep> file for further use.

Using **“*Simulation form*”** it is possible to simulate interactively resonance fields for given spin-Hamiltonian parameters and to compare simulated and experimental spectra and their angular dependence.

Using **“*Step by step form*”** it is possible to obtain the following dependencies:

1. Positions of energy levels on magnetic field;
2. Differences of energy levels on magnetic field;
3. Transition intensities on magnetic field;
4. EPR spectrum shape on line width and line shape (Gaussian, Lorentzian and their derivatives), azimuthal or polar angles, any parameter of Spin-Hamiltonian, microwave frequency, and temperature.

FAIW.exe is powerful tool for viewing, comparing and transformation of 2-3-4 dimensional arrays of EPR, ENDOR or other data.

It visualizes experimental or calculated angular dependencies of resonance magnetic fields (EPR) or resonance frequencies (ENDOR) and convert into special symbols the information about other resonance line characteristics - intensity and width. It allows also to extract the points, what you need, from array of experimental data and to prepare the data for fitting, to shift all points on definite angle and save the result, to exclude from experimental data those points, which are close to calculated angular dependencies. It has many other useful visual procedures, which transform data in the table of the file treated.

It works with special ASCII files. These files are output files of **View_spw.exe** (experimental angular dependencies, <*.grt> or <*.gem>) or **Fields_w.exe** (calculated angular dependencies, <*.grt> or <*.grm>). The program has large sets of symbols for the representation of experimental data and sets of color lines for the representation of calculated angular dependencies. This allows convenient comparison of calculated and experimental data and preparation of the graph for publication.