ECISVIEW: An interactive toolbox for optical model development

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Abstract

The software package ECISVIEW is a graphical interface built around the multi-disciplinary nuclear reaction code ECIS-95 [1]. The basic purpose of ECISVIEW is the possibility to change optical potential parameters interactively, with the keyboard or the mouse, and to display the calculated result immediately on the screen. The key feature of the working method is that the user can specify the value of optical potential parameters as *any* mathematical function of the energy, A, Z or user defined parameters. This enables us to obtain conveniently the optimal optical potential parameters for a given nucleus over the whole energy region of interest. ECISVIEW makes it possible to simultaneously study the dependence of all calculated angular distributions, polarizations and total cross sections on optical model parameters. This method is perhaps more than 100 times faster than the conventional method of preparing an input file, running the code, editing the output file and finally viewing the data with a graphical program. ECISVIEW has been developed (JvW and AK) at ECN Petten, and has been extensively used (AK and JPD) at CEA, Bruyères-le-Châtel. As an example, we present a spherical 0-200 MeV nucleon optical model for ^{90}Zr. A demonstration of ECISVIEW has been given at this Specialists' Meeting.

1 Introduction

The search for the best set of optical model parameters for a certain nucleus, or for a range of nuclei, is a well-known and tedious problem. Some optical model codes have built-in search routines, usually on a χ^2-basis, that attempt to adjust the parameters to the experimental data according to search criteria given by the user. Although this problem could, in principle, be solved numerically, the final set of parameters often gives a result that does not come up to the expectations if judged by eye. Even though quite adequate results for global nucleon optical models have been obtained with χ^2 techniques, the experience at SPN is that the best results stem from optimization based on grid search techniques, especially when certain physical constraints are imposed on the parameters. A simple explanation is that a multi-dimensional search routine tries to optimize a certain optical model parameter which probably does not coincide with the parameter one would choose on the basis of the eye or physical knowledge. What is required is to somehow merge the knowledge of the optical model scientist with search routines (probably artificial intelligence is needed), a very interesting subject on its own but not further discussed here.

If one chooses to optimize by eye, one pays the price. Optical model "searchers" that do NOT use automatic optimization techniques may recognize the following working procedure:

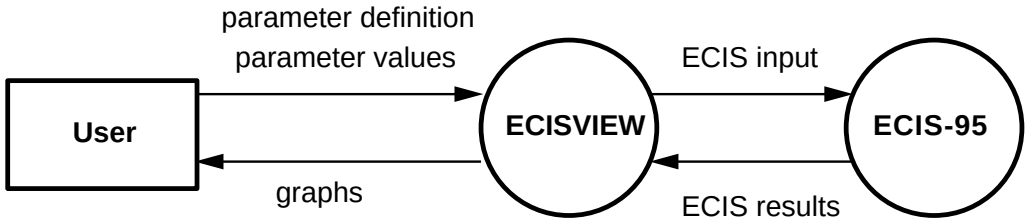

Figure 1: Data Flow Diagram of ECISVIEW.

1. Construct/change the input file, for several incident energies.
2. Run the optical model code.
3. Extract the relevant table of cross sections from the output file.
4. Run a graphical program to compare with experimental data (on screen or printer).
5. If the results are not satisfactory, change parameters and goto 1.

Depending on the degree of automatization, the duration of such a loop may vary from one to several minutes, certainly when the results must be compared with experimental data for several energies and different observables at the same time. As a result, the manual construction of an adequate optical model for one nuclide may take weeks or months. For once, such an exercise may be useful as education, but usually one is not too keen to take the second nuclide. To motivate gross-scale optical model research, we have developed ECISVIEW, which enables a researcher to perform the aforementioned loop within the blink of an eye. As its name already suggests, our software is entirely directed towards ECIS [1], arguably the best and most complete computer code for basic nuclear reaction processes.

The basis behind our method is called Computational Steering. This relatively new branch of computational science is conceptually simple, though technically non-trivial. For ECISVIEW the idea is illustrated in fig. 1. ECISVIEW is connected with the input file and output file of ECIS-95, while ECIS-95 itself is waiting in the background for the command to perform calculations. The user changes optical model (or other) parameters with the mouse or the keyboard via several dialogue boxes (as in a usual X-windows environment), ECISVIEW makes the associated ECIS input file and starts running ECIS-95, after which the calculated result is shown, together with the experimental data, on the screen. For the user, it seems as if this happens instantaneously! In general, this working method applies to any computer code that produces results within a relatively short time. It has been applied by one of us (JvW) in several other branches of physics and energy research.

It is obvious that a lot, if not all, unneccessary and boring overhead is removed by this method. Once the experimental database is installed, a spherical optical model can be created within one or a few hours, provided one has a decent starting point from previous analyses or personal experience. Moreover, ECISVIEW provides insights, by the possibility to try various functional forms for the parameters, that would otherwise be impossible or too time-consuming to attain.

The purpose of the present version of ECISVIEW is twofold: (a) for the construction of phenomenological optical models; (b) as an educational tool for students, and maybe also for experts, to get a feeling for the behaviour of predicted observables as a function of the parameters before they explore more sophisticated (microscopical) methods. As an illustration, we present a phenomenological spherical 0-200 MeV nucleon optical model for ^{90}Zr that we constructed with ECISVIEW just after the meeting.

2 Possibilities: Physics

The first version of ECISVIEW has the possibility to compare calculated elastic angular distributions and polarizations with experimental data for an arbitrary number of incident energies and a simultaneous comparison of the total elastic, reaction and total cross section with measurements. As an illustration, a typical case is shown in fig. 2: eleven experimental neutron elastic angular distributions for ^{90}Zr with energies ranging from 4.5 to 24 MeV as well as the experimental total cross section up to 200 MeV are displayed, together with results from ECIS-95. Energy dependent potentials have been postulated in advance. When we change a parameter, within about 0.4 seconds eleven angular distributions are calculated, at the exact incident energies of the measurements, and plotted. On the Silicon Graphics workstation we use, a single ECIS-95 calculation takes about 0.04 seconds and produces one differential cross section, one polarization, the reaction cross section and, in the case of neutrons, the total elastic and total cross sections. Of course, for the total cross section curve we need one ECIS-calculation for only one point. Therefore, for the total cross section first the two endpoints of the energy region are used for calculation, followed by successive midpoints of increasingly smaller intervals, i.e. the calculated total cross section curve will get smoother and smoother. This will produce a sufficiently smooth total cross section for the whole energy range within about 4-5 seconds. The complete process will be interrupted and started again when a parameter is changed. Fig. 3 shows a case that involves polarizations.

We feel that the *most important* technical feature of ECISVIEW is that *any* functional form of the potential parameters can be specified, as a function of energy, Z and A or as a function of user-defined parameters. This should be clear from fig. 2: for example, the volume absorption W_V is a function of E, E_f, a_1 and b_1 and the latter two parameters can be varied. Also here, the functional form can be changed and immediately the new results are shown.

Here is a list of the other possibilities of ECISVIEW that concern physics:

- Use of neutrons up to alpha's as incident particles.
- Choice between relativistic (default) and non-relativistic kinematics.
- User-defined maximum angular momentum (for educational purposes only; we always use a safe, big value).
- User-defined matching radius (for educational purposes only).
- For charged particles, the possibility to either display differential cross sections or the ratio between differential cross-sections and the Rutherford cross section (default).
- Easy inclusion of older and newer versions of ECIS. In fact, the code can be treated as a black box since all graphical operations are done outside ECIS.

We stress again that the figures presented in this paper are not merely the usual display of calculated vs. measured observables (for a publication one would use a more fancy layout, whereas this is a working tool). They are in fact snapshots and, for the moment, final results of a manual optimization process. Not shown in these figures are dialogue boxes and communication windows with all kinds of options and sliders for all user-defined adjustable parameters. When a slider is pulled, all calculated curves change according to the new parameters.

3 Possibilities: Graphics

Although not directly related to the procedure of obtaining the best parameters, we also list the various graphical options for completeness. There are many ways to display the data. The options are:

- Inclusion of many sets of experimental data. For example, for the total cross section many complementary experimental data sets can be shown in the same graph. Every experimental data set has a different colour, which is equal to the colour of the corresponding calculated curve.

- The range for each slider can easily be set. For every parameter there is a default button, so one can always return to the starting value if the result is not satisfactory.

- Zooming-in: Possibility to set the range of both the x-axis (energy) and the y-axis (total cross section). This enables fine-tuning at parts of the figure that the user considers important, see fig. 4. At the other extreme, the high-energy limit can easily be set at 600 MeV or higher if the user wishes to create an optical model for these energies (we mention here that the option of Dirac phenomenology is not yet included).

- User-defined angle-step (default 1 degree) for the differential cross sections and polarizations.

- Possibility to look at only one observable at the time, e.g. total cross section only, see fig. 4.

- A communication window with all the potential parameters. One can choose an energy with a slider and the values of each parameter (which follows from the more general A, Z, E-dependent parametrization as that of Eq. (4)) at that energy are shown.

- Several additional cosmetical features: black/white or colour, possibility to show graphs from left to right (as in this paper) or from top to bottom, option to turn the display of the parametrization off or on (as in fig. 2) and the possibility to switch legends on or off. In the process of searching, we usually put all these features off, to obtain a maximal stretching of the graphs on the screen.

As an obvious extra option, at any moment during the process all settings concerning the optical model parameters, graphics, experimental data, etc. can be saved for future use.

4 An application: 0-200 MeV optical models

As a direct application, we present here a 0-200 MeV nucleon optical model for ^{90}Zr. All illustrations in this paper concern snapshots of ECISVIEW for these potentials. The phenomenological optical model potential U has the following form:

$$\begin{aligned} U(r) &= -Vf_v(r) - iWf_w(r) + 4ia_{w_D}W_D\frac{\mathrm{d}f_{w_D}(r)}{\mathrm{d}r} \\ &- \left(\frac{\hbar}{m_\pi c}\right)^2 \mathbf{L}.\sigma(V_{so}+iW_{so})\frac{1}{r}\frac{\mathrm{d}f_{so}(r))}{\mathrm{d}r}, \end{aligned} \tag{1}$$

where the form factors of each component are of the Woods-Saxon type

$$f_i(r) = \frac{1}{1+\exp((r-R_i)/a_i)}, \tag{2}$$

where a_i is the diffuseness and the radius is given by

$$R_i = r_i A^{1/3}. \tag{3}$$

For all nuclei we have under study, we attempt to use the same functional form for the parametrization, in which we try to minimize the number of adjustable parameters and avoid dependencies of our parameters for which we have no physical justification. We adopt an exponential decrease of the real central and spin-orbit potential depths, an imaginary volume potential depth of the form proposed by Jeukenne and Mahaux [2] and an imaginary surface potential depth of the form proposed by Delaroche et al. [3]. All geometries are energy independent and we impose as further constraints equal real and imaginary volume geometries and equal real and imaginary spin-orbit geometries. Finally, we take a linear decrease of the (small) imaginary spin-orbit potential.

In sum, we have

$$
\begin{aligned}
V(E) &= V_0 \exp(-\lambda(E-E_f)) \\
r_v &= \text{constant} \\
a_v &= \text{constant} \\
W_V(E) &= a_1 \frac{(E-E_f)^m}{(E-E_f)^m + b_1^m}, \qquad \text{where} \quad m=4 \\
r_w &= r_v \\
a_w &= a_v \\
W_D(E) &= d_1 \exp(-d_2(E-E_f)) \frac{(E-E_f)^n}{(E-E_f)^n + d_3^n}, \qquad \text{where} \quad n=4 \\
r_{w_D} &= \text{constant} \\
a_{w_D} &= \text{constant} \\
V_{so}(E) &= V_0^{so} \exp(-\lambda_{so} E) \\
r_{v_{so}} &= \text{constant} \\
a_{v_{so}} &= \text{constant} \\
W_{so}(E) &= W_0^{so} - c_{wso} E \\
r_{w_{so}} &= r_{v_{so}} \\
a_{w_{so}} &= a_{v_{so}}, \qquad (4)
\end{aligned}
$$

where the Fermi energy E_f for neutrons is given by

$$E_f({}^N_Z A) = -\frac{1}{2}[S_n({}^N_Z A) + S_n({}^{N+1}_Z A + 1)] \qquad (5)$$

with S_n the neutron separation energy, and for protons by

$$E_f({}^N_Z A) = -\frac{1}{2}[S_p({}^N_Z A) + S_p({}^N_{Z+1} A + 1)] \qquad (6)$$

with S_p the proton separation energy.

In table 1, the obtained parameters for both neutrons and protons incident on ^{90}Zr are given and the results are presented in the ECISVIEW panels of figs. 2-4. We use relativistic kinematics. It is obvious from fig. 2 that compound nucleus contributions are not included. We note that our results are preliminary and that table 1 does not yet represent the final answer. In particular, the prediction of the proton reaction cross section and the angular distributions at the highest energies are not yet satisfactory. However, we may still allow ourselves some more freedom in our parametrization that keeps it physically justified. We can introduce an energy-dependent radius of the real volume potential, which simulates dispersive effects. Parametrizations with this option are presently under study.

In conventional phenomenological optical models, straight line segments are often used to represent the absorption potentials. Here, the smooth functional forms for W_V and W_D incorporate essentially the same number of parameters but provide more flexibility. They help to attain a parametrization over the whole 0-200 MeV range, without any discontinuity. This is very important for nuclear model calculations that take the optical model as a starting point. The problem one generally faces is that for complete spectrum calculations reliable optical potentials for all outgoing energies are required, but a complete parametrization is usually missing. Typically, one is forced to take optical model potential A in the first energy region, optical model potential B in the second energy region, etc., which leads to undesired discontinuities, not only for the predicted standard observables, but also for other outgoing channels. The parametrization of Eq. (4) cures this problem.

5 Conclusions and possible extensions

The present version of ECISVIEW is an interactive optical model toolbox that can be used to obtain the optimal parameters for the phenomenological spherical optical model. It works on Silicon Graphics

Table 1: Optical model potential parameters for nucleons incident on ^{90}Zr. Preliminary results.

	Neutrons	Protons
V_0	54.0	60.0
λ	0.0077	0.0080
r_v	1.23	1.23
a_v	0.665	0.68
a_1	11.2	14.2
b_1	52.0	57.0
d_1	10.5	15.0
d_2	0.024	0.0256
d_3	11.0	10.0
r_{w_D}	1.24	1.294
a_{w_D}	0.58	0.607
V_0^{so}	7.00	6.00
λ_{so}	0.0045	0.0040
$r_{v_{so}}$	1.14	1.05
$a_{v_{so}}$	0.50	0.60
W_0^{so}	0.	0.875
c_{wso}	0.	0.0175
r_C	0.	1.25
E_f	-9.60	-6.80

(SGI), DEC-ALPHA and SUN (SPARC-4 and higher) workstations and mainframes. Several extensions are possible:

- Compound elastic cross sections for low incident energies. ECIS-95 has full compound nucleus capabilities and inclusion of the compound contribution would make the phenomenological optical model for spherical nuclides complete within ECISVIEW. A connection with a discrete level file is required.

- Coupled-channels calculations for deformed nuclei. It can be imagined that besides the elastic angular distribution also the angular distributions for the first few inelastic states are displayed, again for several incident energies simultaneously. Deformation parameters would then also be adjustable. Of course, this will slow down the calculations somewhat (vibrational nuclei) or significantly (rotational nuclei). Still, interactive optimization would be preferable over the conventional method.

- Features requiring the external input model of ECIS. The two aforementioned mechanisms could probably be included within the present set-up of ECISVIEW, i.e. it is still relatively easy to generate the associated ECIS-input file. From the graphical point of view, there is even no technical barrier to include more sophisticated optical models, such as the JLM method [5]: for spherical nuclei the interactive set-up is already there. The practical difficulty consists mainly of generating the input. The potential, resulting from microscopic folding models, has to be read in the so-called external input mode of ECIS, and although drivers that automatically generate this input exist, inclusion in ECISVIEW is not straightforward, though certainly not impossible.

- Display of other quantities: panels with transmission coefficients and S-matrix elements for several l-values. Other simple but important quantities are the s-wave and p-wave strength functions and the potential scattering radius for adequate parametrizations at very low energies.

- Possibility to handle several different nuclei at the same time. A method to do this is to use several different windows of ECISVIEW at the same time. This would then facilitate the construction of global optical models. It can be imagined that a parameter is changed, after which in all different windows (i.e. nuclei) the predicted observables change. We note that on our Silicon Graphics workstation, it is already possible to start up five *independent* sessions of ECISVIEW simultaneously. This gives the possibility to study the behaviour of predictions over a wide mass range. In the present version, the parameters then have to be changed to the same values for each ECISVIEW session.

- Search. Shortly after this meeting, a preliminary search option has been included in ECISVIEW. Parameter search merged with this graphical tool is particularly interesting since it leads to a "sit-down and watch" scenario, where the improvements can be followed directly on the screen. The overall χ^2 value is also continuously printed and every parameter can be included in the optimization process if desired. This preliminary version has been tested and worked for some simple parametrizations. It was not used, however, for the more involved parametrization given in this paper. We think it is too early to make global statements about its robustness. Anyway, it is clear that with ECISVIEW it is easier and more adequate, at a certain moment during the manual optimization process, to decide *which* parameter should be optimized with χ^2-techniques, and again this is based on eye and optical model experience. This enables to keep a search process much better under control.

In sum, we feel that ECISVIEW is a valuable addition to the optical model toolbox. Although we have only scratched the surface of ECIS, an important contribution to nuclear data projects can be made. For each spherical nucleus for which enough experimental data exist, a phenomenological optical model potential can be created in a way that is unprecedented in terms of convenience, speed and insight. Finally, we wish to emphasize that we do not mean to abandon χ^2-optimization completely. It can be imagined that alternating between manual and automatic search, in a careful and responsible way, provides the best result.

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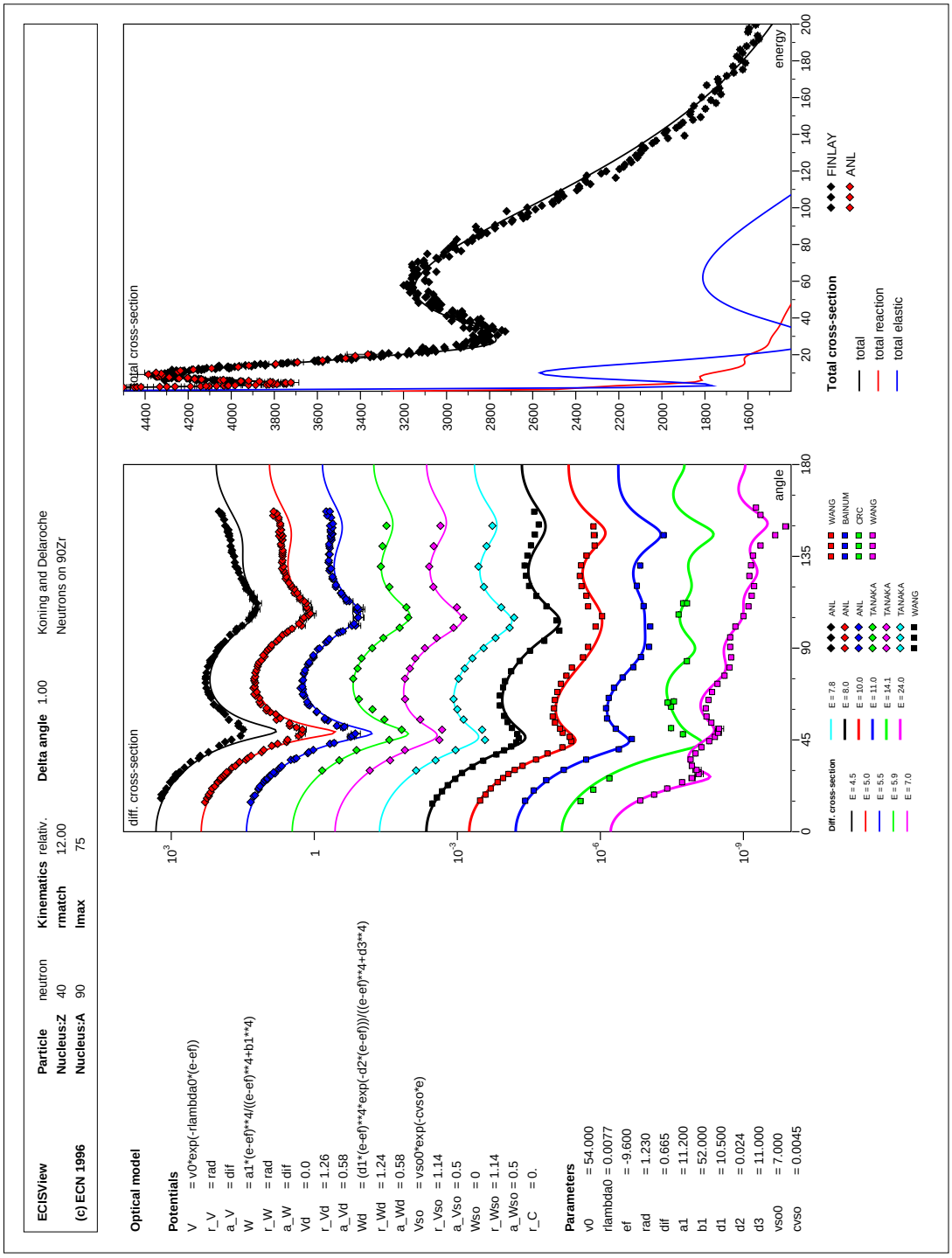

Figure 2: ECISVIEW-window for neutrons on ^{90}Zr. Displayed are the differential, total elastic, reaction and total cross section together with their legends, the optical model parametrization and the general info.

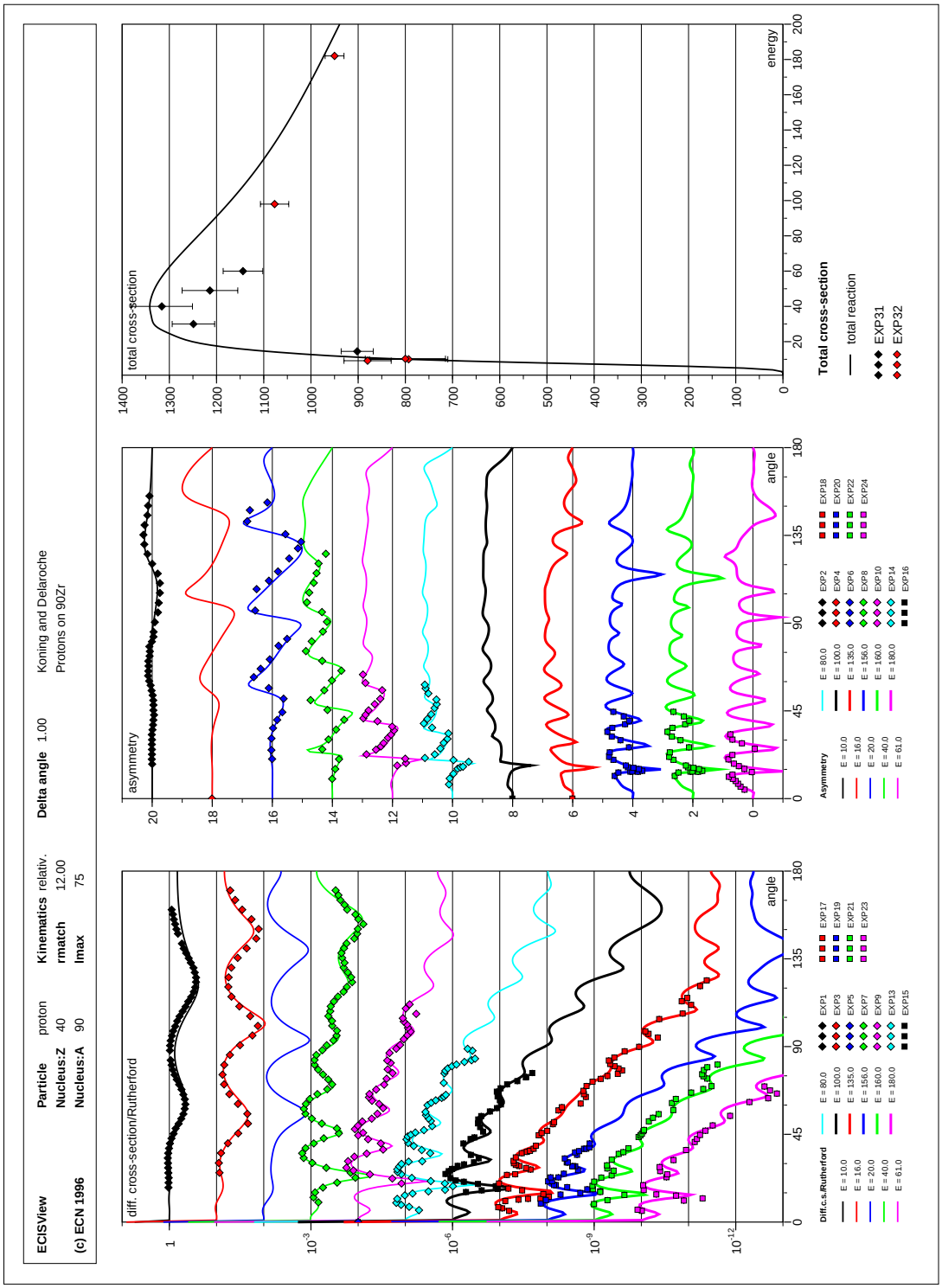

Figure 3: ECISVIEW-window for protons on ^{90}Zr. Displayed are the differential cross sections, the polarizations and the reaction cross section together with their legends and the general info.

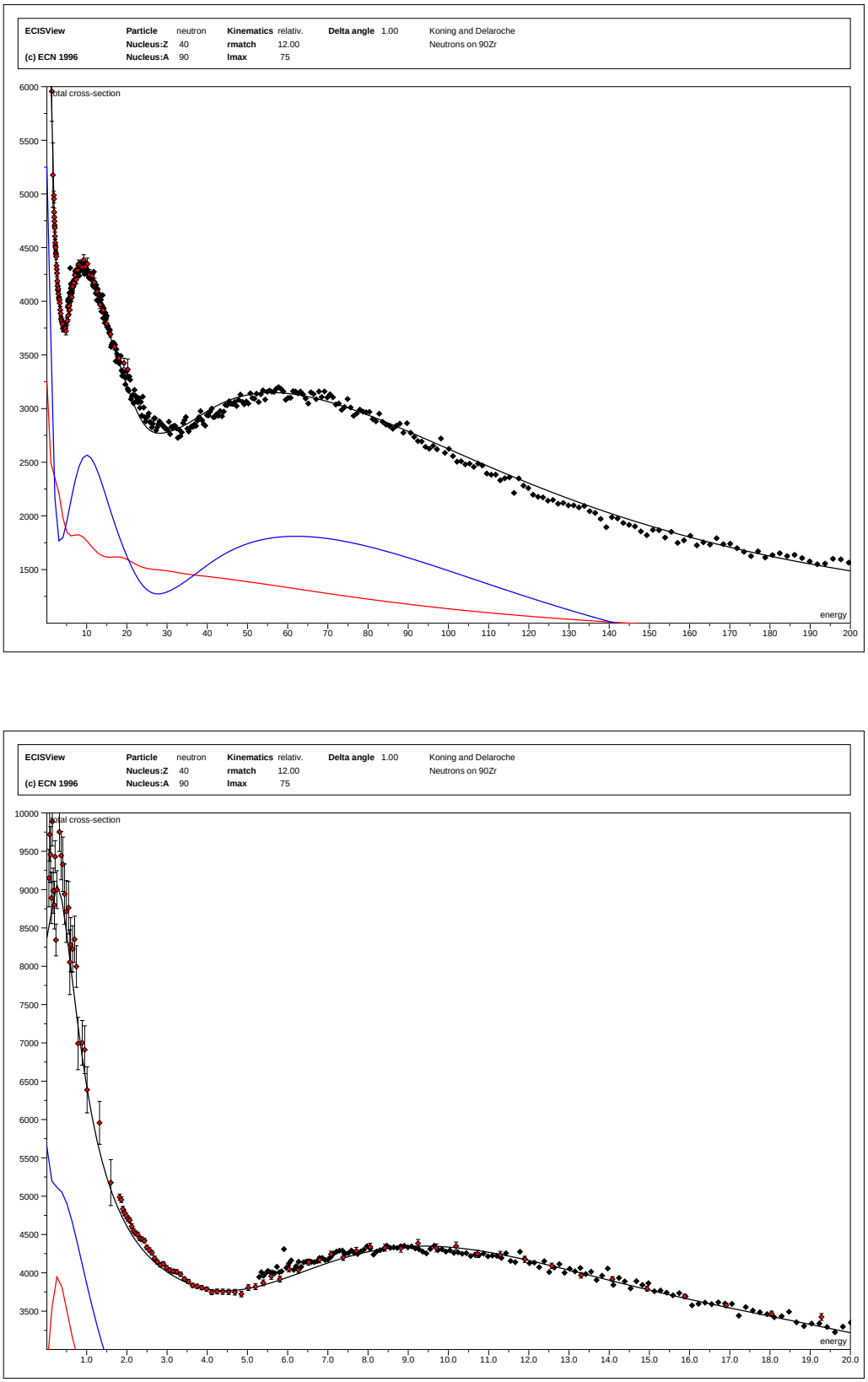

Figure 4: ECISVIEW-window for neutrons on ^{90}Zr. Displayed is the total cross section (and the total elastic and reaction cross section) for 0-200 MeV and for 0-20 MeV.