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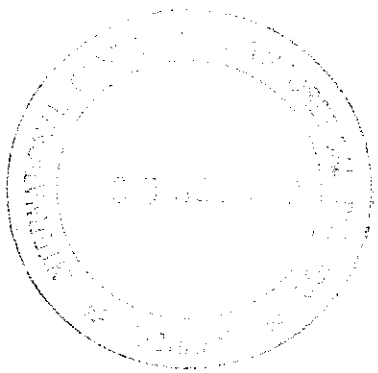
"Model Calculations and Evaluation of Nuclear Data for Isotope Production and Monitor Reactions"



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Submitted to the Workshop on Nuclear Data for Science and Technology: Medical Applications Trieste, 4-15 October 1999

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Introduction

Three large domain of activity may be singled in evaluation process:
1. Collecting, selecting, compiling , expert studying of experimental data with possible modifications.
2. Model calculations with the corresponding codes.
3. Using the selected and corrected information to generate the output, which is usually evaluated curve, its error band and covariance matrix of evaluated values.

The first stage is not easy to formalize and reduce to algorithms. The results of model calculations depending on models chosen and input parameters can serve often as a guide for estimations. On the final stage should be used the results of model calculations and various matematical methods.

Here we would like to demonstrate the abilities of nuclear models and mathematical methods for the case of development of reference charge particle cross section database for medical radioisotope production based on the investigations of the last several years in various laboratories.

CALCULATIONS AND EVALUATIONS

Creation of a Reference Charged Particle Cross Section Database for Medical Radioisotope Production requires the evaluation of both experimental and modeled cross sections for beam monitor reactions and for radionuclide (positron and gamma emitters) production reactions. It was recognized at the first meeting of this CRP in Vienna in 1995 that modeling will play an important role in predicting cross sections where measurements are either not available or have large discrepancies. Because of the volume of work involving about fifty reactions in the CRP, it was decided to use

modeling as a guide rather than for full evaluation. However in some cases the CRP used the modeled cross sections as the recommended values. Thus the modeling was done using global input parameters. In this chapter we describe the modeling by four different groups: Livermore, Obninsk, Beijing and Islamabad. First we give a general overview of nuclear reaction models that may be used in modeling cross sections below 100 MeV. This will be followed by a short description of the codes and calculations actually used by the participating groups. (We note that the codes have similar basic reaction physics, but they differ in details and in actual applications.) In the final section we give a discussion of the modeling with its successes and failures in reproducing experimental data using global input parameters.

NUCLEAR REACTION MODELS

The specific reactions involved in the CRP were chosen earlier for the most important monitor reactions and reactons for the radioisotope production. The energies for these reactions range from the threshold (several MeV) to about one hundred MeV with protons, deuterons, ^{3}He and alpha particles as projectiles, and targets ranging from light (nitrogen) to heavy (bismuth) masses. The nuclear reaction theories and models covering the target-projectile and energy ranges relevant to this CRP include various preequilibrium models (Blann, 1975; Gadioli and Hodgson, 1992) coupled with the Hauser-Feshbach theory (1952) or the Weisskopf-Ewing evaporation model (1940). Intranuclear cascade models (Bertini, 1963; Chen *et al.*, 1968; Gudima *et al.*, 1983; Cugnon *et al.*, 1997) could be used in this energy regime, but have not been used for this CRP. The quantum mechanical, multistep direct reaction theories (Feshbach *et al.*, 1980; Udagawa *et al.*, 1982; Nishioka *et al.*, 1988) have started to play a role in this energy range, but the modeling has not yet matured to the level of a routine application to data evaluations. Also R-matrix calculations (Lane and Thomas, 1958), which are quite complex but more appropriate for lighter targets, such as, ^{14,15}N and ^{16,18}O, are not done here. The CRP relied on evaluation of the experimental cross sections to obtain the recommended values for targets below A < 30. For other targets the cross sections were modeled using preequilibrium-evaporation formalisms, as described below and in the following section.

The commonly used preequilibrium models are the exciton model and the hybrid model (Gadioli and Hodgson, 1992; Blann, 1975). These semiclassical models both originate from the pioneering paper, "Statistical Model of Intermediate Structure", by J. J. Griffin (1966). The nuclear state is characterized by the excitation energy of the composite nucleus and the exciton number, which is the total number of particles above and holes below the Fermi surface. It is assumed that all possible ways of sharing the excitation energy between different particle-hole configurations with the same exciton number have equal a-priori probability. The exciton number changes

during the reaction process as a result of intranuclear two-body collisions. At each stage of the reaction there may be a non-zero probability that a particle is emitted. If this happens at an early stage, we speak of pre-equilibrium emission. If the emission does not occur at an early stage, the system eventually reaches the equilibrium or evaporation stage. This stage is described by the Weisskopf-Ewing formalism (1940) (which does not treat angular momentum and parity explicitly) or more rigorously by the Hauser-Feshbach formalism (1952) which explicitly treats vector coupling of spins and parities between compound and residual nuclei and ejectiles. Preequilibrium models have been widely used in modeling nuclear cross sections below 200 MeV and have provided an adequate description of the high-energy tails (i. e., the region between the evaporation peak and the discrete states) of the outgoing particle spectra (Blann *et al.*, 1994; Michel and Nagel, 1997).

Several formulations of PE decay are in use; these are the 'hybrid', the 'geometry dependent hybrid' (GDH) and the 'exciton' model formulations. These approaches rely on a quantity called the "partial state density," which is the number (per MeV) of energy partitions available for a Fermi gas where every partition of p particles and h holes is assumed to occur with equal a-priori probability. The first expression for this partial state density was due to Strutinsky (1958) ,

$$\rho_n(E) = g(gE)^{n-1}/(p!h!(n-1)!),$$

where n, the exciton number, equals the number of excited particles "p" plus holes "h," E is the excitation energy in MeV, and g is the single particle level density at the Fermi energy. PE decay models in use make the assumption that within each exciton hierarchy, all configurations are populated with equal a-priori probability.

Three groups and K. Gul (Islamabad, Pakistan) were involved in modeling cross sections for the last CRP. The group at Obninsk used the Alice-IPPE code (Dityuk *et al.*, 1998), the group from China used the Spec code (Shen and Zhang, 1993) and the Livermore group used HMS-Alice (Blann, 1996) for nucleon induced reactions and Alice-91 (Blann, 1991) for deuteron, ^{3}He and alpha induced reactions. The Alice family of codes are based on the hybrid, the geometry-dependent hybrid (GDH) or the HMS preequilibrium models and the Weisskopf-Ewing evaporation formalism. The Spec code is also constructed within the framework of the Weisskopf-Ewing evaporation formalism, but preequilibrium decay is calculated from the master equation exciton model (Blann, 1975). The HMS-Alice code uses a Monte Carlo precompound formulation with Weisskopf-Ewing evaporation. The lack of angular momentum and parity treatments in the Weisskopf-Ewing formalism used in these codes may be of some concern for certain aspects of reaction yields, (e.g., isomer yield calculations). But these codes are fast and convenient to use, i.e., when many natural isotopes are involved and many particles are emitted in the reaction process, and have

generally been found to be adequate when cross sections for isomeric states are not needed. Gul used codes, HFMOD (Gul, 1995) and PREMOD (Gul, 1996), in his calculations. The HFMOD code is based on the Hauser-Feshbach formalism and the PREMOD code is based on the concept of the geometry-dependent hybrid preequilibrium model generalized to include discrete levels, and to conserve angular momentum and parity. For complete formulations of the codes used in this CRP we refer to the appropriate references, but some of the highlights are given in the next section.

CODES AND CALCULATIONS

A variety of codes (Grogi, Stapre, Alice, Gnash, Spec, etc., and their modifications) have been developed on the basis of equilibrium and preequilibrium reaction mechanisms. These codes have similar physics with different degrees of complexity in input preparation and require different computing times. Some of them are used when detailed properties of nuclear reactions are needed, including population of discrete levels. For example, the Stapre and Gnash codes are good choices if one needs to have information on each channel participating in the reaction process, and when the excitation energy (and the number of open channels) is not too large. On the other hand, when the number of open channels is large and it is impossible or very time consuming to provide all the required input data with sufficient accuracy, the advantages of these detailed codes may be reduced. In such a case, the faster codes with less effort in input preparation are often more practical choices. The Alice family of codes developed by Blann and a recent modification by the Obninsk group fall in this class, and are used in the calculations of the reaction cross sections for medical radioisotope production for the present CRP. We refer to recent international code comparisons for further details on many of the codes in current use (Pearlstein, 1988; Blann *et al.*, 1994; Michel and Nagel, 1997).

ALICE-91 code

This is the latest released version of the standard Alice code at Livermore (Blann, 1991), which uses hybrid or geometry dependent hybrid precompound models and Weisskopf-Ewing evaporation for the equilibrium part of the reaction process. The basic physics has been widely described in the literature, but most physics can be found in (Blann, 1975; Blann and Vonach, 1983). Earlier versions of Alice did not include gamma ray competition with nucleon, deuteron and alpha emissions. The gamma competition is included since 1990. The gamma emission rate is calculated by microscopic reversibility based on the giant dipole with Lorentzian line shape (Blann *et al.*, 1988). The Alice code uses the Fermi gas level density and has the option of using the shell-dependent level densities from Katatria and Ramamurthy (1980). The code

includes multiple preequilibrium nucleon emission. Some of these features are described below.

HMS-ALICE code

The HMS-Alice code is based on a new precompound Monte Carlo simulation (HMS) model described in (Blann, 1996). The model does not rely upon exciton state densities beyond three excitons, permits unlimited multiple precompound emission for each interaction and may be used to calculate exclusive particle spectra and yields. The evaporation part of the calculation is done with the usual Weisskopf-Ewing formalism, as in the Alice–91 code.

The HMS precompound decay model is formulated to reduce several inconsistencies and limitations of earlier formulations, such as in the hybrid, GDH and exciton models. These precompound formulations have relied upon contributions from the entire exciton populations based on a sequence of two-body collisions. It is further assumed that all possible ways of sharing the excitation energy between different particle-hole configurations with the same exciton number have equal a-priori probability. It was clearly shown the equal a-priori population assumption may be valid only for states with the first exciton number (three excitons for nucleon induced reactions) (Blann and Vonach, 1983) and not for higher exciton states (Bisplinghoff, 1986). Additionally, existing precompound formulations were not suited for multiple PE emissions beyond two, yet this becomes important at energies above ~ 50 MeV. To overcome these problems, Blann developed the HMS Monte Carlo precompound model,which uses only the kinematically justified two and three exciton densities with unlimited precompound particle emission. The formulation otherwise follows the philosophy of the hybrid model. The new approach is therefore referred to as the hybrid Monte Carlo simulation (HMS) model. It should be valid up to the pion threshold.

In the HMS approach, incident nucleons that make only 3-exciton states are considered. For each nucleon energy (selected at weighted random from the possible range of energies) the nucleon will either be emitted, or will rescatter. If it is emitted, the emission probability is calculated from equations (6), (9), and (11) of the hybrid model, using the $n=n_0$ term only in Eq. (6). (The remaining two quasiparticles will share the balance of the excitation energy and will initiate their own 3-quasiparticle states and then either decay or rescatter.) If the initial nucleon rescatters, it will make a new 3-exciton state and the process of decy or rescatter continues. The hole energy is similarly allowed to initiate a 2hole–1particle state, etc. In this fashion each cascade treats only the physically justified 2 and 3 exciton states, and can treat any number of precompound decays for each cascade.

The HMS model enjoys another advantage over closed form decay models (e.g., exciton, hybrid or GDH models) for calculation of particle spectra and recoil distributions. Because it is preformed in an event mode, the velocity of the emitting nuclide may be modified according to the angle and energy of each nucleon previously emitted, giving proper laboratory/center of mass transformations. The two-body assumption necessary in closed form calculations may be seen to be quite poor when comparisons are made between the two models.

The Monte Carlo precompound formulation is available at present for neutron and proton induced reactions, but not for deuteron, ^{3}He or alpha particle induced reactions. The Livermore group therefore used HMS-Alice for proton induced reactions in this CRP, but used the Alice-91 code for all other reactions. Both codes used optical models for incident nucleons, and for all inverse reaction cross sections. The parameter sets used are described in (Blann and Vonach, 1983).

ALICE-IPPE code

The Alice-IPPE code is the Alice-91 code version modified by the Obninsk group (Dityuk *et al.*, 1998) to include the generalized superfluid level density model of Ignatyuk and colleagues (Ignatyuk, 1983; Ignatyuk *et al.*, 1979; Blokhin *et al.*, 1988; Ignatyuk *et al.*, 1993) and preequilibrium cluster emissions. For the preequilibrium nucleon emission the geometry dependent hybrid (GDH) model is used. Calculation of the alpha-particle spectra is performed taking into account both the pickup (Iwamoto and Harada, 1982; Sato *et al.*, 1983) and knockout processes (Milazzo-Colli and Braga-Marcazzan, 1973; Ferrero *et al.*, 1979; Oblozinsky and Ribansky, 1978). A phenomenological approach is used to describe direct emission of the deuteron (Dityuk *et al.*, 1998). The triton and ^{3}He spectra are calculated according to the coalescence pickup model of Sato, Iwamoto and Harada (1983). The level density formalism includes both collective and non-collective effects, and excitation-energy-dependent shell effects. These level density improvements over the Fermi gas model are described here. For details on the cluster emission models and calculations we refer to (Dityuk *et al.*, 1998) and references therein.

Generalized superfluid model of nuclear level density

The nuclear level density was calculated using the phenomenological approach[Ig83] based on the generalised superfluid model for all nuclei formed in evaporation cascade.

The level density in generalised superfluid model can be described if we subdivide the excited states into quasiparticle, coherent and colective ones. Then nuclear level density is presented as

$$\rho(U) = \rho_{qp}(U')\ K_{vib}(U')\ K_{rot}\ (U'), \tag{1}$$

where $\rho_{qp}(U')$ - is the density of quasiparticle (non-collective) nuclear excitations, $K_{vib}(U')$ and $K_{rot}(U')$ - are coefficients of level density enhancement due to vibrational and rotational states at the effective excitation energy U'.

The energy dependence of the quasiparticle level density has been calculated on the basis of superfluid nuclear model. The correlation function for the ground states of nuclei was defined as $\Delta_0 = 12.0/A^{1/2}$ MeV. This choice of Δ_0 is consistent with the systematics of nuclear masses and with the results of analysis of the experimental data on neutron resonances for heavy nuclei. The critical temperature of the phase transition from superfluid to normal state, the condensation energy, the critical energy of the phase transition and the effective excitation energy are connected with correlation function Δ_0 by the following equations:

$$\begin{aligned} t_{cr} &= 0.567\cdot\Delta_0 \\ U_{cr} &= 0.472\cdot a_{cr}\cdot\Delta_0^2 - n\,\Delta_0 \\ E_{con} &= 0.152\cdot a_{cr}\cdot\Delta_0^2 - n\cdot\Delta_0 \\ U' &= U + n\cdot\Delta_0 + \delta_{shift} \end{aligned} \tag{2}$$

where $n = 0, 1$ and 2 for even-even, odd and odd-odd nuclei, correspondingly, and the empirical value of the excitation energy shift δ_{shift} chosen on the base of consistent description of the level density of low lying collective levels and data on neutron resonances.

The shell effects were included into consideration using the energy dependence of nuclear level density parameter $a(U,A)$ determined phenomenologically:

$$\begin{aligned} a(U,Z,A) &= \tilde{a}(A)\cdot\left(1+\delta W(Z,A)\cdot\frac{\varphi(U'-E_{cond})}{U'-E_{cond}}\right), \quad U'>U_{cr} \\ a(U,Z,A) &= a(U_{cr},Z,A), \quad U'<U_{cr} \end{aligned} \tag{3}$$

where the asymptotic value of level density parameter at high excitation energy is equal to

$$\tilde{a}(A) = 0.073A + 0.115A^{2/3}, \tag{4}$$

where $\delta W(Z,A)$ is the shell correction to nuclear binding energy defined from the experimental values of nuclear masses or in the case of their lack with the help of the Mayers-Swiatecki formula, $\varphi(U)=\{1-exp(-\gamma U)\}$ is the dimensionless function which defines the energy dependence of the level density parameter at low excitation energies, value $\gamma = 0.4/A^{1/3}$ was chosen from the description of density of neutron resonances.

The vibrational enhancement of nuclear level density was presented in the following form

$$K_{vib} = exp[\delta S - (\delta U/t)] , \tag{5}$$

where δS, δU are the changes of entropy and excitation energy due to collective modes and defined from relations for Bose-particle gas

$$\begin{aligned} \delta S &= \sum_{i=1}^{\infty} (2\lambda_i + 1)\{(1+n_i)\ln(1+n_i) - n_i \ln(n_i)\} \\ \delta U &= \sum_{i=1}^{\infty} (2\lambda_i + 1)\omega_i n_i , \end{aligned} \tag{6}$$

where ω_i and λ_i are the energy and the multipolarity of collective excited state, n_i is its population for the corresponding temperature. The attenuation of vibrational enhancement of level density at high temperatures is taken into account with the following oqupation number dependence:

$$n_i = \frac{\exp\{-\gamma_i / (2\omega_i)\}}{\exp\{\omega_i / t\} - 1}, \tag{7}$$

through the parameter γ_i obtained empirically on consistent description of the low-lying levels and the data on neutron resonances

$$\gamma_i = 0.0075A^{1/3}(\omega_i^2 + 4\pi^2 t^2) . \tag{8}$$

The quadrupole and octupole states were considered in the calculations only. The position of the lowest state for the all nuclei, with exception of ^{208}Pb, was defined by phenomenological equations which reproduced the experimental data well enough for middle weight nuclei:

$$\omega_2 = 30A^{-1/3}; \qquad \omega_3 = 50A^{-1/3} . \tag{9}$$

For nucleus ^{208}Pb the position of 2^+ state was assumed to be equal to experimental value *4.1* MeV.

For all spherical nuclei the coefficient of vibrational enhacement of the level $K_{vibr}(U')$ was taken into account according equation (5) only. For deformed nuclei the enhancement of level density connected with rotational mode of collective excitation $K_{rot}(U')$ was taken into account according to Ref. [Ig83] :

$$K_{rot}(U) = \sigma_{\perp}^2 \cdot g(U) = \sigma^2 \cdot (1 + \beta/3) \cdot g(U) , \tag{10}$$

where σ is the spin cut-off factor, and $g(U)$ is the empirical function taking into account the attenuation of rotation modes at high energies

$$g(U) = \{1 + exp[(U - U_r)/d_r]\}^{-1} , \tag{11}$$

where the parameters of attenuation function are connected with the parameter of quadrupole nuclear deformation β by relations:

$$U_r = 120A^{-1/3}\beta^2 ; d_r = 1400A^{-2/3}\beta^2 . \tag{12}$$

The parameter of quadrupole deformation was defined from formulae for nuclear masses [My67].

The advantage of considered approach to obtain nuclear level density consists in calculation of cross-sections for magic and neighboring nuclei taking into account shell effects.

SPEC Code

SPEC (Shen and Zhang, 1993) is a program for calculating the neutron or charged particle (*p, d, t,* ^{3}He, α) induced reactions on medium-heavy nuclei in the incident energy range up to 60 MeV including up to 6 successive emission processes per nucleus. For those reaction channels contributed only by 1~5 emission processes the incident energy can go up to 100 MeV. This program is written in FORTRAN-77.

SPEC is constructed within the framework of the optical model, the master equation exciton model (Blann, 1975), and the Weisskopf-Ewing evaporation model (1940). For the first and second particle emission processes, the preequilibrium emission and evaporation are considered, but for 3-6 particle emission processes, only evaporation is considered. The preequilibrium and direct reaction mechanisms of γ emission (Akkermans *et al.*, 1985) are also included. The effect of the recoil nucleus is considered for calculating spectra.

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ACCURACY OF CALCULATED DATA

Accuracy of data calculated with the codes can not be stated beforehand. The analysis of the results of calculations for many reaction cross sections and the comparison with experimental data should be performed first.

EVALUATION OF CALCULATION METHODS FOR EXCITATION FUNCTIONS CALCULATIONS FOR MEDICAL RADIOISOTOPE PRODUCTION

During the last years new experimental data appeared for the regions Z=51-55 and Z=80-83. and also a revised version of the well-known computer code ALICE has been released by M. Blann. This version takes into account our observations described earlier (Kurenkov et al., 1993) in the paper in which we performed calculations and analysis of experimental excitation functions for many reactions in the region Z=51-

55. This version was developed further in IPPE, Obninsk, and includes now a set of further improvements. Thus it appeared interesting to compare the excitation functions calculated using the new code ALICE-IPPE with the known experimental data, including recently published ones, and calculated data.

The calculations of the excitation functions with the use of various versions of the ALICE code have been performed for some time, see e.g. ALICE 85/300 (Nortier et al., 1990, Steyn et al., 1991, 1992), OVERLAID ALICE (Zaitseva et al., 1991, 1992), ALICE 82 (Lagunas-Solar and Haff, 1993), ALICE 87 (Dovbenko et al., 1991, Kurenkov et al., 1992, 1993, 1994 and 1995). The popularity of this code is explained elsewhere (Blann 1988, Lagunas-Solar et al., 1993). But up to now the choice of the versions of this code has been chaotic and, as a rule, obsolete versions of the code are still in use. A critical analysis and selection criteria for a given version of the code are practically not available. This forms an additional reason to test the new version of the ALICE code in comparison with older and new experimental data and with results of the ALICE-87 version.

Method of calculations

The importance to take into account gamma-ray competition in the calculations of excitation functions for the reactions induced by medium-energy nucleons on neutron-deficient nuclei, in particular ^{124}Xe, has been noted repeatedly earlier (Lunev et al., 1991, Dovbenko et al., 1991, Kurenkov et al., 1993, Blann et al., 1994). Accounting for gamma-ray competition enables to avoid spurious peaks in the near-threshold region when calculating the excitation functions for proton-induced (p,pxn)-reactions. In the new version of the ALICE-IPPE code the gamma-emission is taken into account at every decay step properly. The algorithm of level density calculations according to the generalised superfluid model was tested, corrected and improved. The corrections were made for the multiple precompound proton emission near the threshold, for gamma-emission and optical model parameters and some others. The list of the improvements is given by Shubin (Shubin et al., 1995). The new approach to the cluster emission calculation, which takes into account both pick-up and knock-out processes (Konobeyev et al., 1995) was included also. The optical potential parameters used in the calculations with both versions of the ALICE code were taken on basis of recommendations worked out using experimental data for many nuclei (Blann and Vonach., 1983). Preequilibrium nucleon emission was calculated within the framework of the geometry-dependent hybrid model (GDH), in which the initial exciton number was not varied and was determined according to the algorithm of the code. The mean free path of nucleons in a nucleus was determined through the imaginary part of the optical potential used in the calculations. The calculations were done from the reaction threshold energy up to 50 or 100 MeV. All calculations were performed under identical assumptions and conditions using a constant parameter set

based on values or options recommended for this code as optimal. No attempt was made to improve the agreement with experimental data by varying any parameters.

Results and discussion

The excitation functions for 52 various nuclear reactions induced by protons, deuterons and alpha-particles with the emission of several nucleons were calculated in this work using the ALICE-87 and ALICE-IPPE 96 codes. Only a selection of the results is graphically shown. In all figures the points are experimental data and the curves are the calculated excitation functions. The results of the calculations with the ALICE-87 code are shown in the figures with dashed lines, while the solid lines show the results calculated with the ALICE-IPPE 96 code.

The results of the excitation functions calculations for radioisotopes produced in the bombardment of tellurium, xenon, iodine, thallium and lead with protons were compared with experimental data for the following reactions: $^{123}Te(p,n)^{123}I$ and $^{123}Te(p,2n)^{122}I$ (Scholten et al., 1989); $^{124}Te(p,n)^{124}I$ reaction (Qaim et al., 1994, Scholten et al., 1995) and (Kondo et al., 1977); $^{124}Xe(p,2n)^{123}Cs$ and $^{124}Xe(p,pn)^{123}Xe$ (Kurenkov et al., 1989) and (Tarkányi et al., 1991); $^{124}Xe(p,p2n)^{122}Xe$ (Tarkányi et al., 1991); $^{126}Xe(p,2n)^{125}Cs$ and $^{126}Xe(p,pn)^{125}Xe$ (Venikov et al., 1993); for proton induced reactions on ^{127}I (Lagunas-Solar et al., 1986), (Diksic and Yaffe, 1977) and (West et al., 1993); $^{202}Hg(p,xn)Tl$ (Birratari et al., 1982); $^{203}Tl(p,xn)Pb$ (Lagunas-Solar et al., 1978), (Lagunas -Solar et al., 1980) and (Blue et al., 1978); $^{205}Tl(p,xn)Pb$ (Lagunas -Solar et al., 1980); Pb(p,xn) (Bell and Skarsgard, 1956); Tl(p,pxn) (Qaim et al., 1979).

The excitation functions for the reactions induced by protons as calculated with the ALICE-IPPE code show a shift of 1-3 MeV to the higher energy region in comparison with the corresponding calculations using the ALICE-87 code. For many cases the inclusion of gamma competition results in an effective shift of the threshold only and does not influence the energy dependence of the excitation functions. As a rule, the values of the calculated cross sections are consistently higher than the experimental ones at the maximum of the excitation functions. The excitation functions for proton induced reaction calculated with the ALICE-IPPE code are in better agreement with the experimental data than calculated with the ALICE-87 code. Generally, the calculated curves have maximum cross section values close to each other, but for the ALICE-IPPE version the maximum values are systematically less, and this can be seen for the reactions with the emission of several neutrons. The exception between 25 proton-induced reactions considered are only three to five reactions where the maximum values calculated with the ALICE-IPPE code are a little bit more than for the ALICE-87 code.

The possibility to show all calculations of the excitation functions for the reactions listed above is limited; therefore we present some of them. The large

discrepancy between calculated and experimental data for the cross section of the $^{124}Te(p,n)^{124}I$ reaction has been noted in our previous paper (Kurenkov et al., 1993). For this reaction the calculation exhibits a noticeable shift to the low energy region and the calculated cross section at the maximum is a little larger than the experimental value. The results of recent experiments for this reaction (Qaim et al., 1994, Scholten et al., 1995) are in better agreement with our calculations (see Fig. 1), than the data of Kondo et al.(Kondo et al., 1977), particularly near the threshold. The results of the excitation function calculations for the reaction $^{124}Xe(p,2n)^{123}Cs$ are shown in Figure 2 together with the experimental data (Kurenkov et al., 1989) and (Tarkányi et al., 1991). For proton-induced reactions on ^{127}I shown in Figure 3 the agreement between experimental data (Lagunas-Solar et al., 1986) and calculated ones can be considered as satisfactory or even good. But the data of West et al., (1993) for the reaction $^{127}I(p,n)^{127}Xe$ are in considerably better agreement with the calculated ones. For the $^{203}Tl(p,xn)Pb$ reaction the experimental data of Lagunas-Solar et al., (1978) disagree with those of Blue et al., (1978) (see Fig. 4). On the whole, however, the calculations with the ALICE-IPPE code reproduce better the tendencies of the experimental data of Lagunas-Solar et al., (1978) for the $^{203}Tl(p,3n)^{201}Pb$ reaction and of Blue et al., (1978) for the $^{203}Tl(p,4n)^{200}Pb$ reaction.

The excitation functions for proton-induced reactions that occur with the emission of a proton and one or several neutrons are shown in Figure 5. There are two sets of experimental data for the $^{124}Xe(p,pn)^{123}Xe$ reaction (Kurenkov et al., 1989) and (Tarkányi et al., 1991). The calculation results with the ALICE-IPPE code are in a better agreement with the data of Kurenkov (Kurenkov et al., 1989) (see Fig. 5). The excitation functions for the $^{124}Xe(p,p2n)^{122}Xe$ reaction, calculated with the same version of the code, are close to the experimental data (Tarkányi et al., 1991).

We considered in the present work a large number of reactions induced by deuterons. The experimental data for deuteron-induced reactions were taken from: $^{122}Te(d,n)^{123}I$, $^{122}Te(d,2n)^{122}I$ and $^{122}Te(d,3n)^{121}I$ (Beyer et al., 1988) and (Zaidi et al., 1983); $^{124}Te(d,2n)^{124}I$ and $^{124}Te(d,3n)^{123}I$ (Firouzbakht et al., 1993); $^{124}Xe(d,3n)^{123}Cs$ and $^{124}Xe(d,p2n)^{123}Xe$ (Kurenkov et al., 1992); $^{127}I(d,2n)^{127}Xe$ (West et al., 1993), $^{127}I(d,4n)^{125}Xe$ and $^{127}I(d,7n)^{122}Xe$ (Weinreich et al., 1974); $^{203}Tl(d,xn)Pb$ and $^{205}Tl(d,xn)$ (Blue et al., 1978). The results of the excitation function calculations for such reactions are shown in Figures 6 through Figure 8 in comparison with experimental data. For example, for the $^{122}Te(d,n)^{123}I$ reaction the calculations with the ALICE-IPPE code can be considered as describing the experimental data of Beyer et al., (1988) satisfactorily, but they do not agree with the data of Zaidi et al., (1983) for the same reaction near the threshold. There is also a discrepancy with the data on the $^{122}Te(d,2n)^{122}I$ and $^{122}Te(d,3n)^{121}I$ reactions (see Fig. 6). The comparison of experimental and calculated data for the $^{124}Te(d,2n)^{124}I$ and $^{124}Te(d,3n)^{123}I$ reactions is

presented in Figure 7. For the ^{124}Te(d,2n)^{124}I reaction the experimental cross section data of Firouzbakht et al., (1993) (open circles) are unreasonably less than the calculated results. For the ^{124}Te(d,3n)^{123}I reaction experimental data (open squares) below 14 MeV are probably erroneous because the reaction threshold is about 14 MeV. We have a small group of nuclear reactions induced by deuterons occurring with the emission of a charged particle (proton) and several neutrons. For example, the agreement between experimental and calculated data can be considered as satisfactory for the ^{124}Xe(d,p2n)^{123}Xe reaction (Fig. 8).

The excitation function for five nuclear reactions induced by alpha-particles were calculated also. The experimental data for alpha-particles induced reactions were taken from: Watson et al., (1973), Calboreanu et al., (1982) and Bhardway et al., (1986). The results of the excitation function calculations for alpha-particle induced reactions on ^{197}Au describe the experimental data better with the ALICE-IPPE code.

The quality of the description of available experimental data with the ALICE-87 and ALICE-IPPE codes was estimated on basis of statistical analysis. This was made by two methods, and the results of the analysis for the proton-induced reactions are presented in Table 1. Two quantities were calculated which determine the mean weighted deviation and the relative variance of theoretical and experimental data:

$$F = \left\{ 1/N \sum_{i=1}^{N} \left[\left(\sigma_i^{calc} - \sigma_i^{exp} \right) / \Delta\sigma_i^{exp} \right]^2 \right\}^{1/2} \qquad (1)$$

and:

$$D = \left\{ 1/N \sum_{i=1}^{N} \left| \sigma_i^{calc} - \sigma_i^{exp} \right| / \sigma_i^{exp} \right\}, \qquad (2)$$

where σ_i^{calc} is the calculated cross section, σ_i^{exp} and $\Delta\sigma_i^{exp}$ are the experimental cross section and its uncertainty, respectively, and N is the number of experimental data points. The number of excitation functions for proton-induced reactions is 25, the number of experimental data points is 680. The largest uncertainty occurs in threshold region, so additional analysis has been performed for the same data set but without the first one or first two points for every excitation function. It can be seen that the ALICE-IPPE code describes the excitation functions for proton-induced reactions better than ALICE-87. With the ALICE-IPPE code the relative variance drops to 55 % on average, and it decreases down to 45 % when we exclude the first two points near the reaction threshold for every experimental set.

The results of statistical analysis for the reactions induced by deuterons and alpha-particles are presented in Tables 2 and 3. The description of the experimental data for these reactions is not so good. This situation can be explained by two factors. First, global sets of the optical potential parameters for deuterons and α-particles are not so well defined as for nucleons. Second, the contribution of various reaction

mechanisms for complex charged particles is not so well understood and requires further investigation. Nevertheless, the description of experimental data with ALICE-IPPE code is better than with ALICE-87 version.

Conclusion

The excitation functions for 25 proton-induced nuclear reactions were calculated and analysed in the regions Z=51-55 and Z=79-83. For the most of the reactions the comparison of experimental and theoretical data was made and statistical analysis has been performed. It is shown that the new version of the computer code ALICE-IPPE, which includes a set of improvements, gives the better description of experimental data in a wide energy region up to 100 MeV. It should be mentioned that we compared the experimental and calculated data keeping in mind to use the latter for the prediction of unknown excitation functions and for the estimates of optimal conditions for radionuclide production and contamination levels. In connection with the above-mentioned the authors consider that the use of the new version of the ALICE code is preferable.

Table 1. The results of the statistical analysis for 25 proton-induced reactions.

Number of experimental points	F		D		Comments
	ALICE-IPPE	ALICE-87	ALICE-IPPE	ALICE-87	
680	8.12	23.66	0.55	1.11	All points
643	6.34	13.46	0.47	0.88	First energy point excluded
606	6.14	13.15	0.45	0.81	First two energy points excluded

Table 2. The same as in Table 1 for 19 deuteron induced reactions.

Number of experimental points	F		D		Comments
	ALICE-IPPE	ALICE-87	ALICE-IPPE	ALICE-87	
364	107.24	234.57	2.82	7.05	All points
343	103.16	115.09	2.24	3.68	First energy points excluded
322	104.69	107.36	1.81	2.58	First two energy points excluded

Table 3. The same as in Table 1 for 5 alpha-particle induced reactions.

Number of experimental points	F		D		Comments
	ALICE-IPPE	ALICE-87	ALICE-IPPE	ALICE-87	
179	64.67	84.12	1.76	1.94	All points
171	65.19	85.13	1.24	1.29	First energy points excluded
162	66.26	86.56	1.01	1.05	First two energy points excluded

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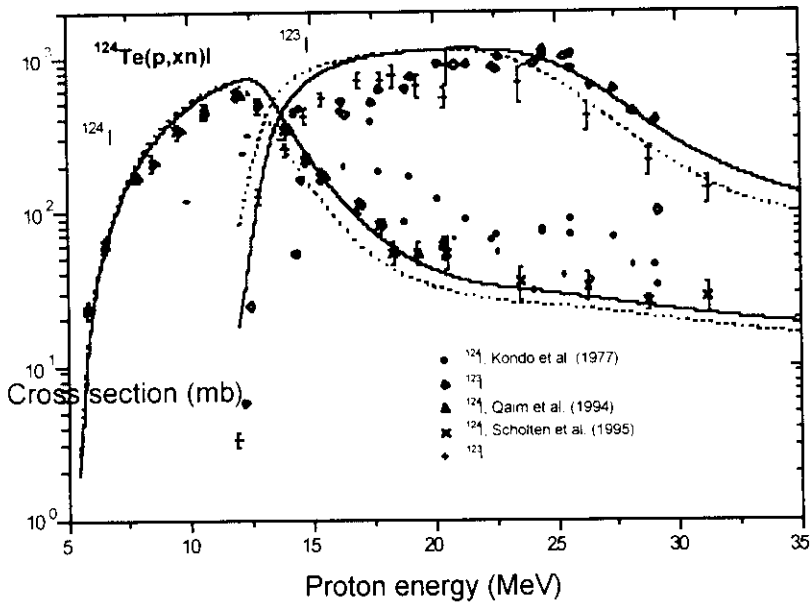

Fig. 1. Calculated and experimentally measured ^{124}Te(p,xn)I excitation functions. The points are experimental results reported by Kondo *et al.*, (1977), Qaim *et al.*, (1994) and Scholten *et al.*, (1995). The dashed curve results from the ALICE-87 code, the solid from the ALICE-IPPE code.

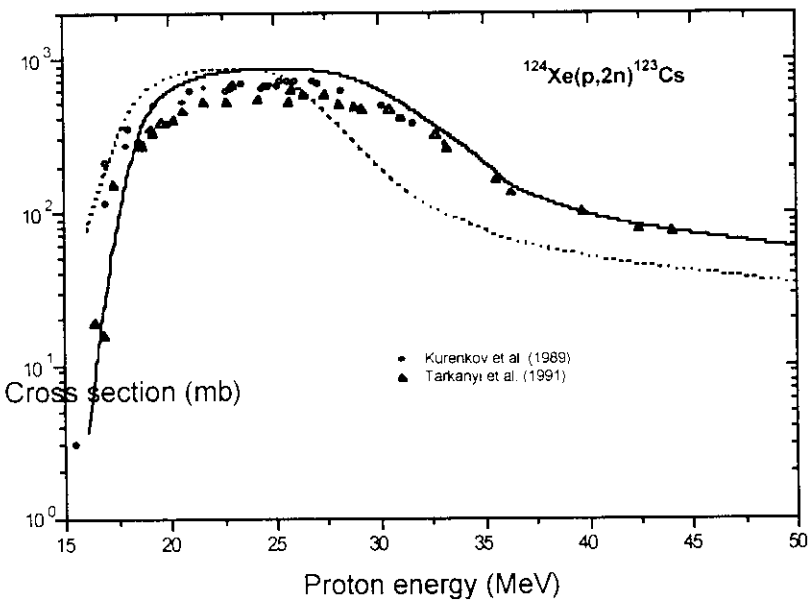

Fig. 2. As in Fig. 1 for the ^{124}Xe(p.2n)^{123}Cs reaction. The open points and triangles are experimental data of Kurenkov *et al.*, (1989) and Tarkanyi *et al.* (1991), respectively.

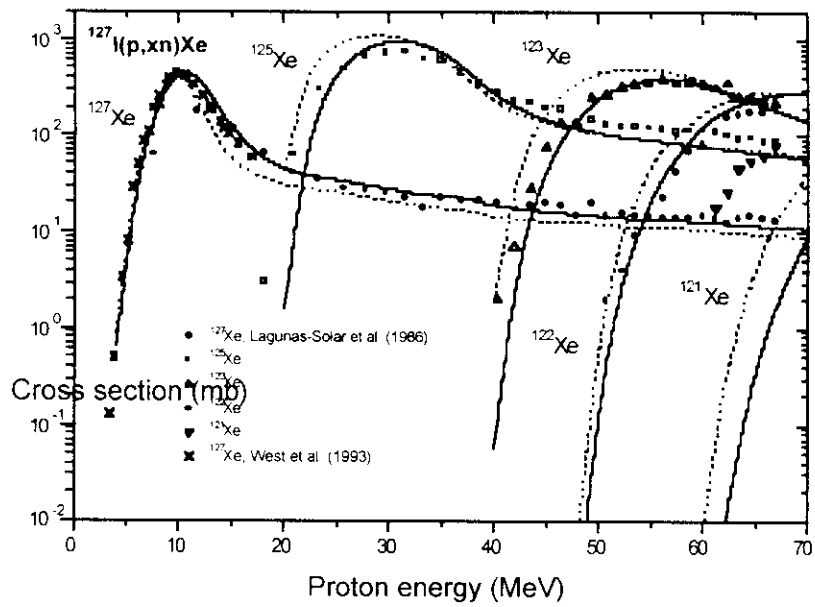

Fig. 3. As in Fig. 1 for the ^{127}I(p,xn)Xe reactions. The experimental data are of Lagunas-Solar *et al.*, (1986) and West *et al.*, (1993).

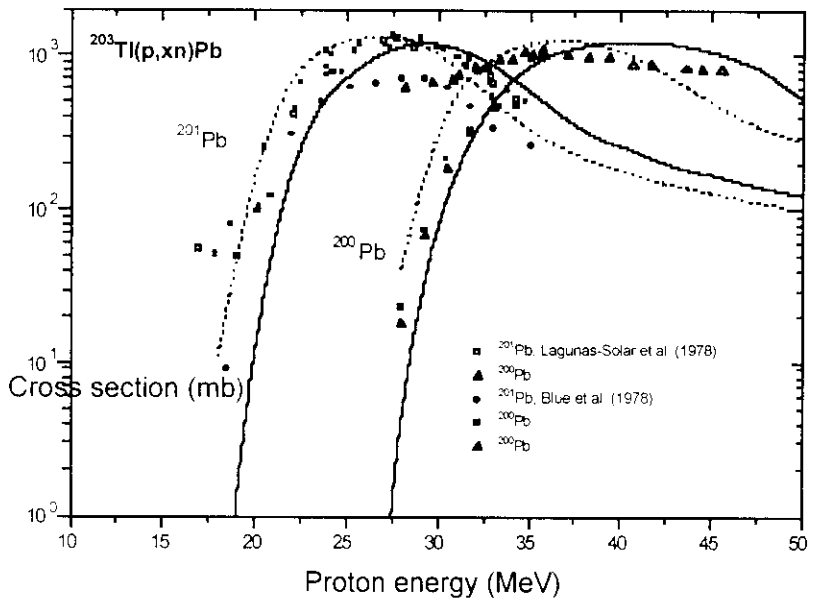

Fig. 4. As in Fig. 1 for the ^{203}Tl(p,xn)Pb reactions. The experimental data are of Lagunas-Solar *et al.*, (1978) and Blue *et al.*, (1978).

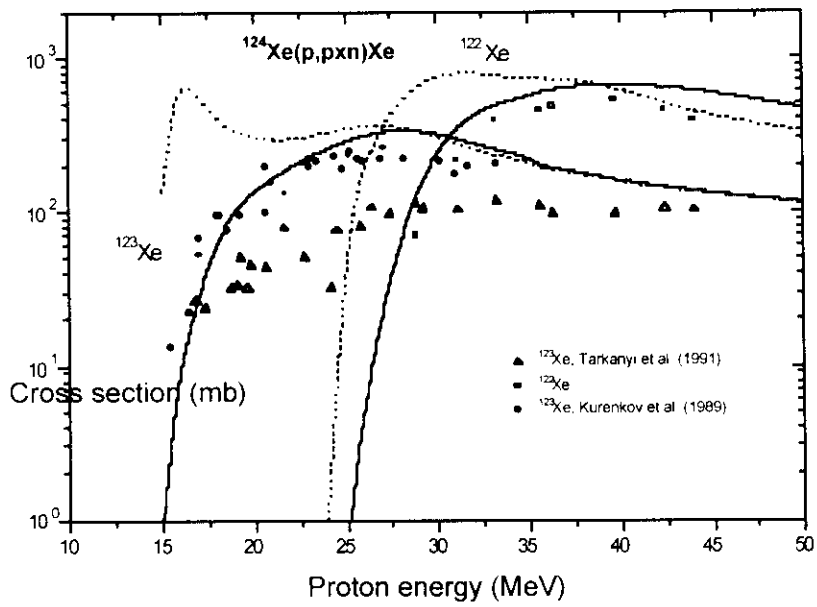

Fig. 5. As in Fig. 1 for the ^{124}Xe(p,pxn)Xe reactions. The open points and triangles are the experimental data of Kurenkov *et al.*, (1989) and Tarkanyi *et al.*, (1991).

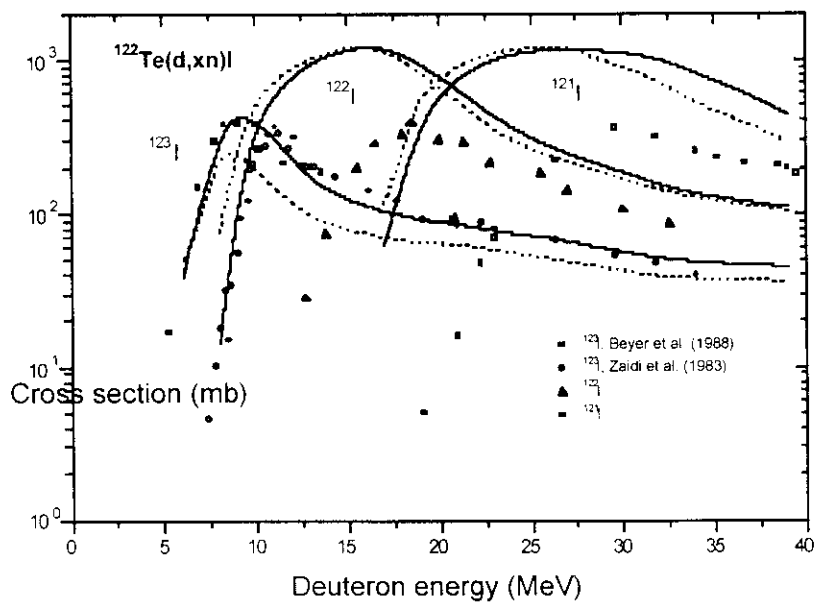

Fig. 6. As in Fig. 1 for the ^{122}Te(d,xn)I reactions. The experimental data are of Beyer *et al.* (1988) and Zaidi *et al.*, (1983).

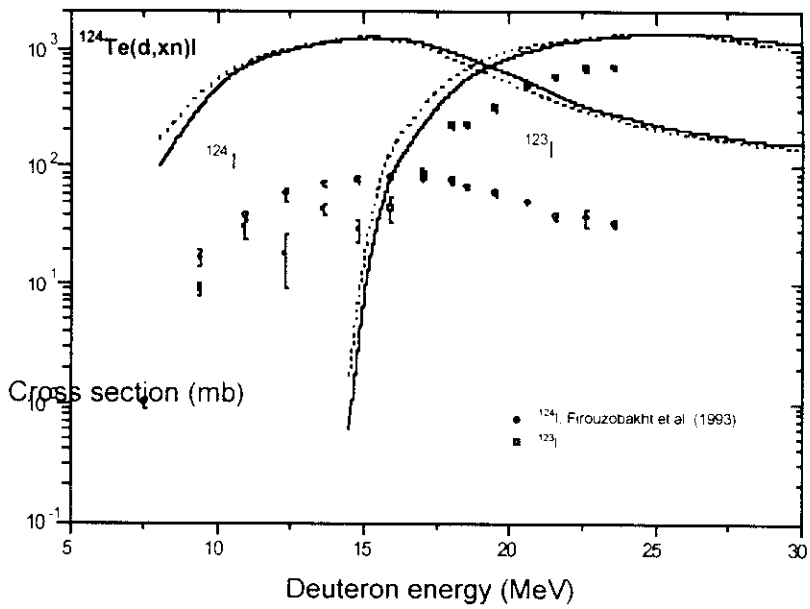

Fig. 7. As in Fig. 1 for the ^{124}Te(d,2n)^{124}I and ^{124}Te(d,3n)^{123}I reactions. The open points are experimental data of Firouzbakht *et al.*, (1993)

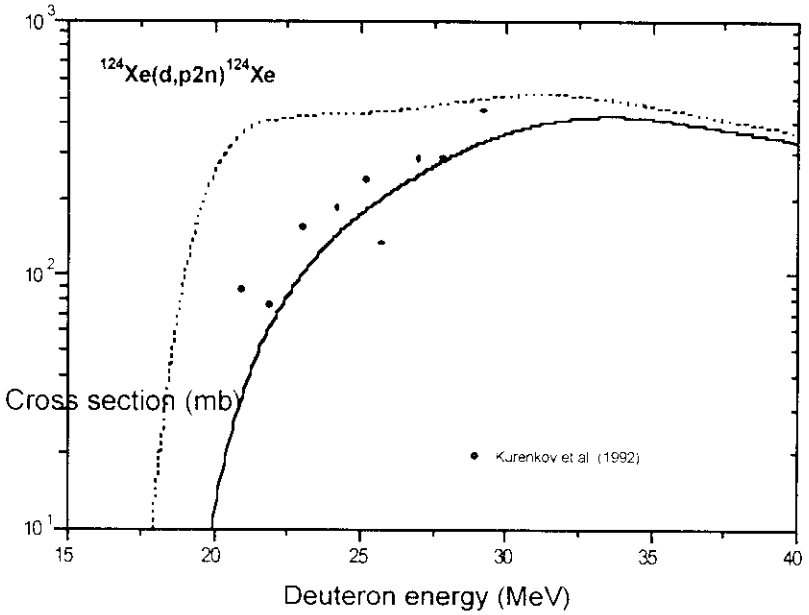

Fig. 8. As in Fig. 1 for the ^{124}Xe(d,p2n)^{123}Xe reaction. The experimental data are of Kurenkov *et al.*, (1992).

EXAMPLES OF THE MODEL CALCULATIONS FOR THE REFERENCE DATA BASE

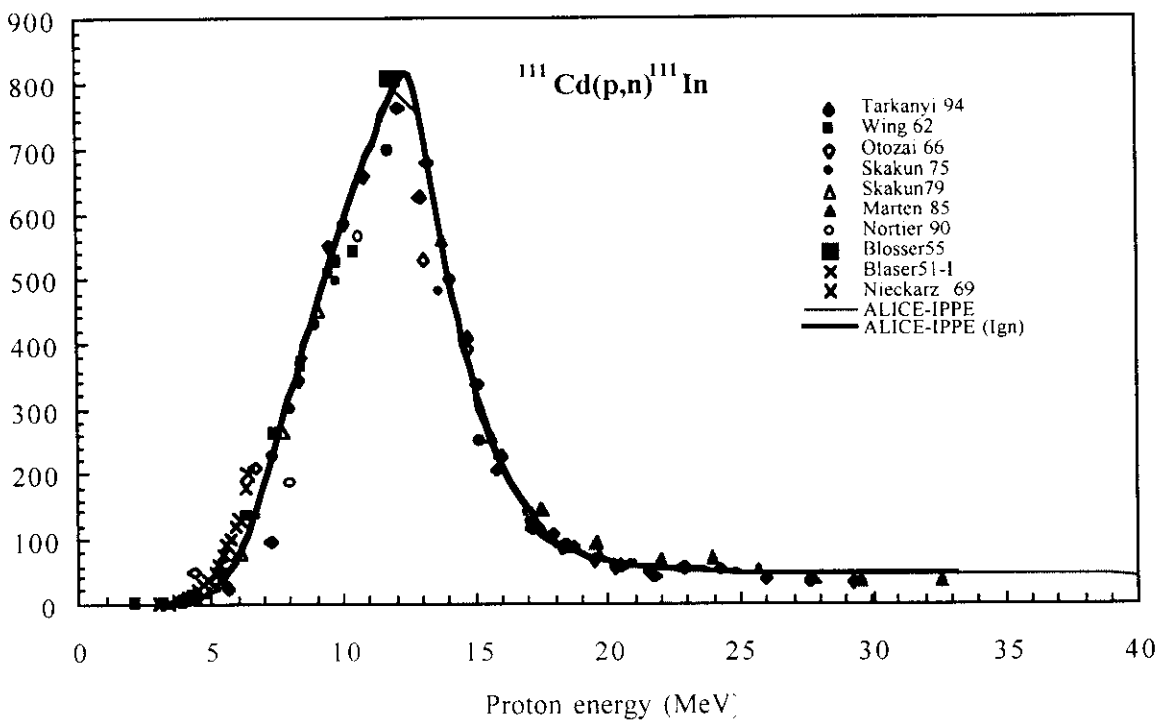

Fig. 9. Calculated ^{111}Cd(p,n)^{111}In reaction cross section (mb).

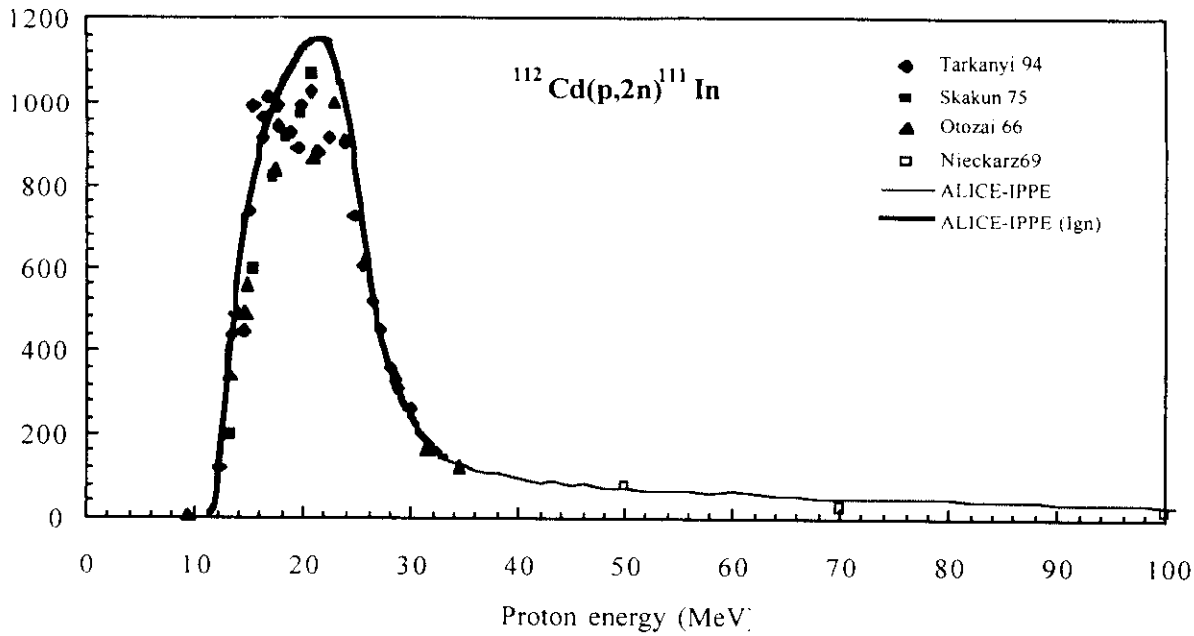

Fig.10. Calculated ^{112}Cd(p,2n)^{111}In reaction cross section (mb).

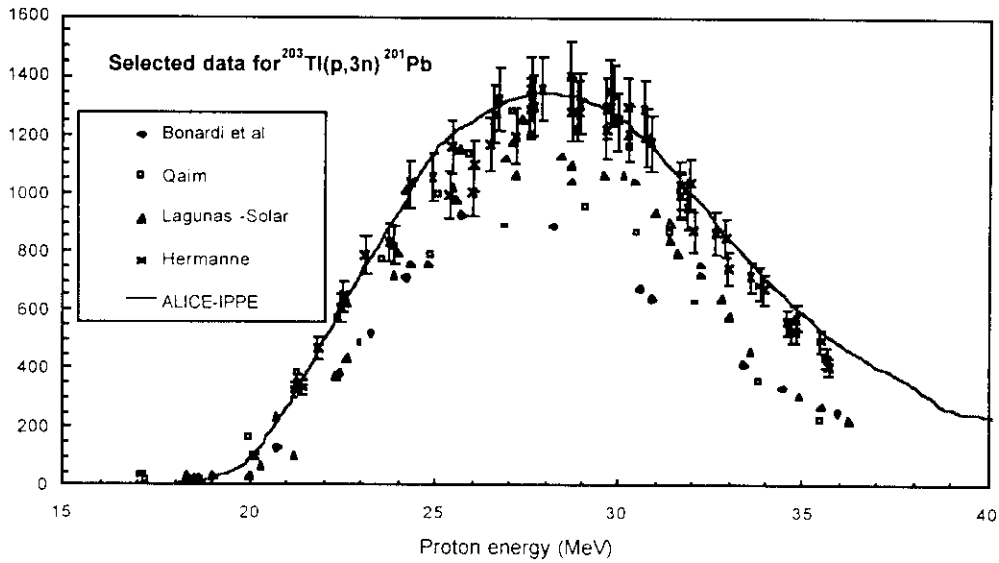

Fig. 11. Calculated ^{203}Tl(p,3n)^{201}Pb reaction cross section.

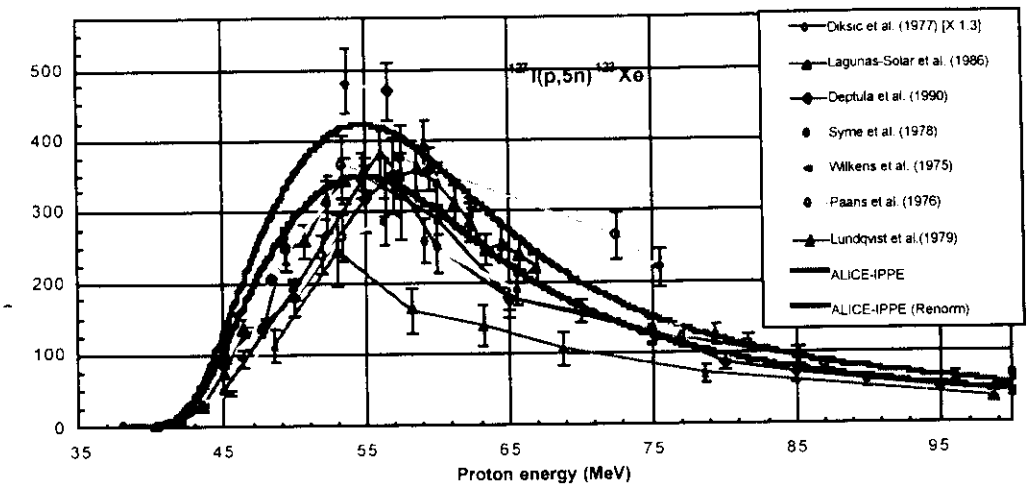

Fig. 12. Calculated the $^{127}I(p,5n)^{123}Xe$ reaction cross section normalised to 350 mb at 55 MeV.

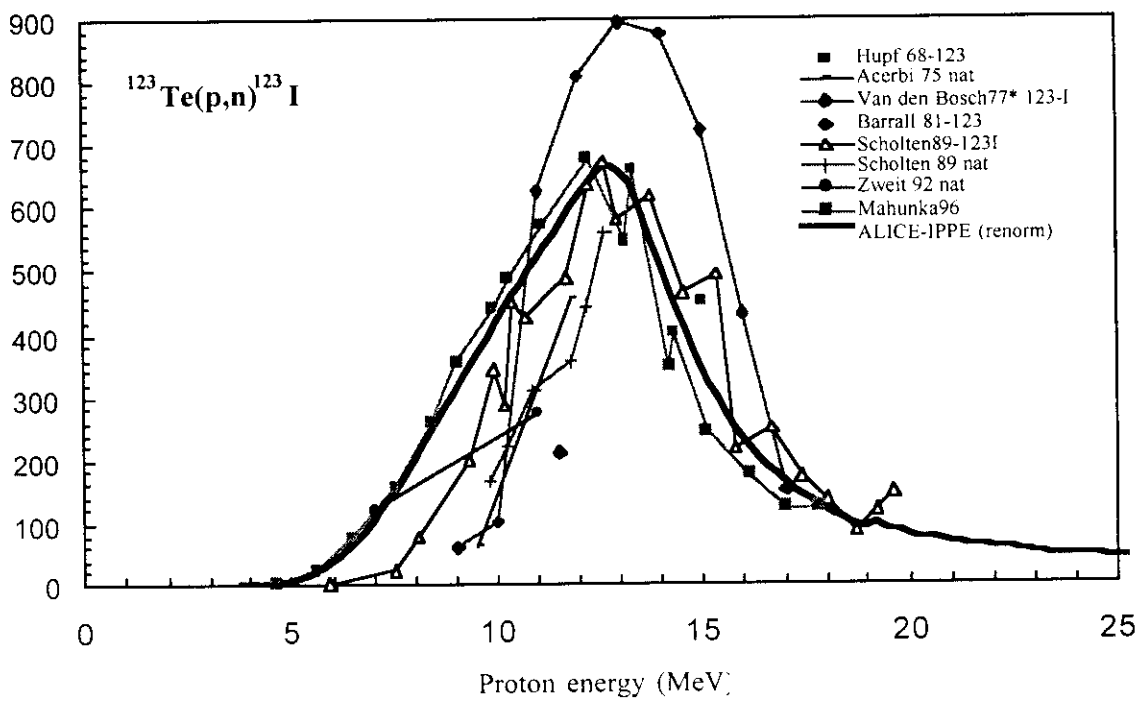

Fig. 13. Calculated $^{123}Te(p,n)^{123}I$ reaction cross section normalised to the experimental peak value of 665 mb.

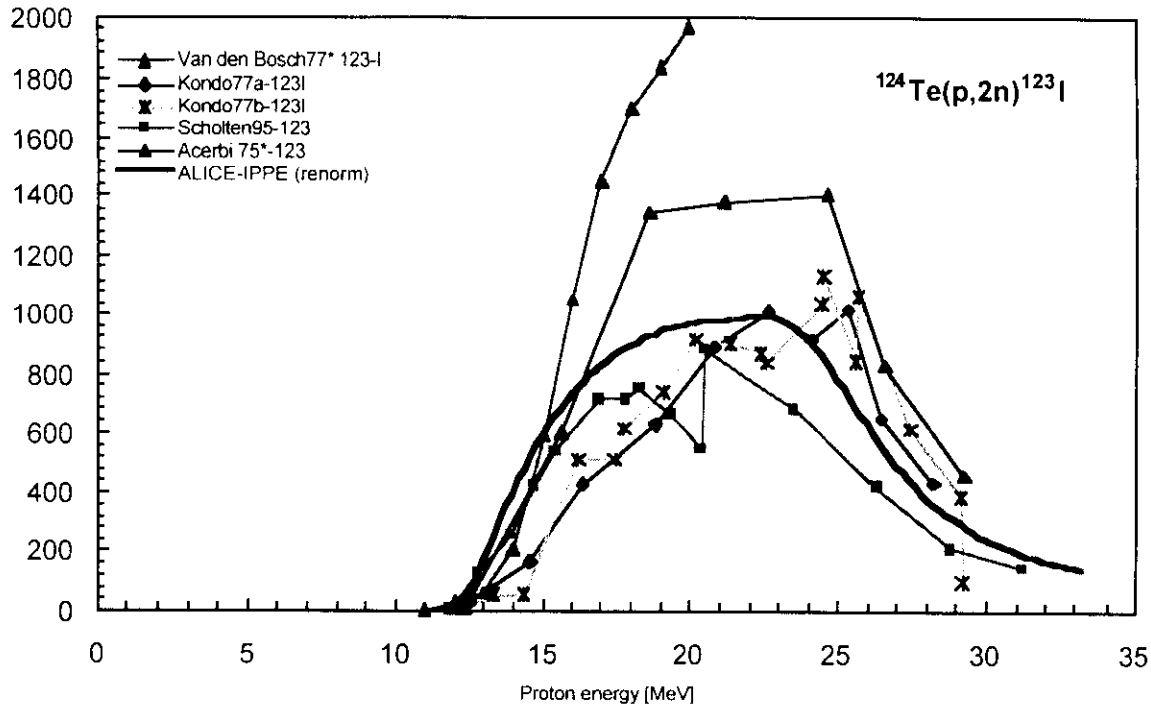

Fig. 14 Calculated $^{124}Te(p,2n)^{123}I$ reaction cross section normalised to the experimental peak value of 995 mb.

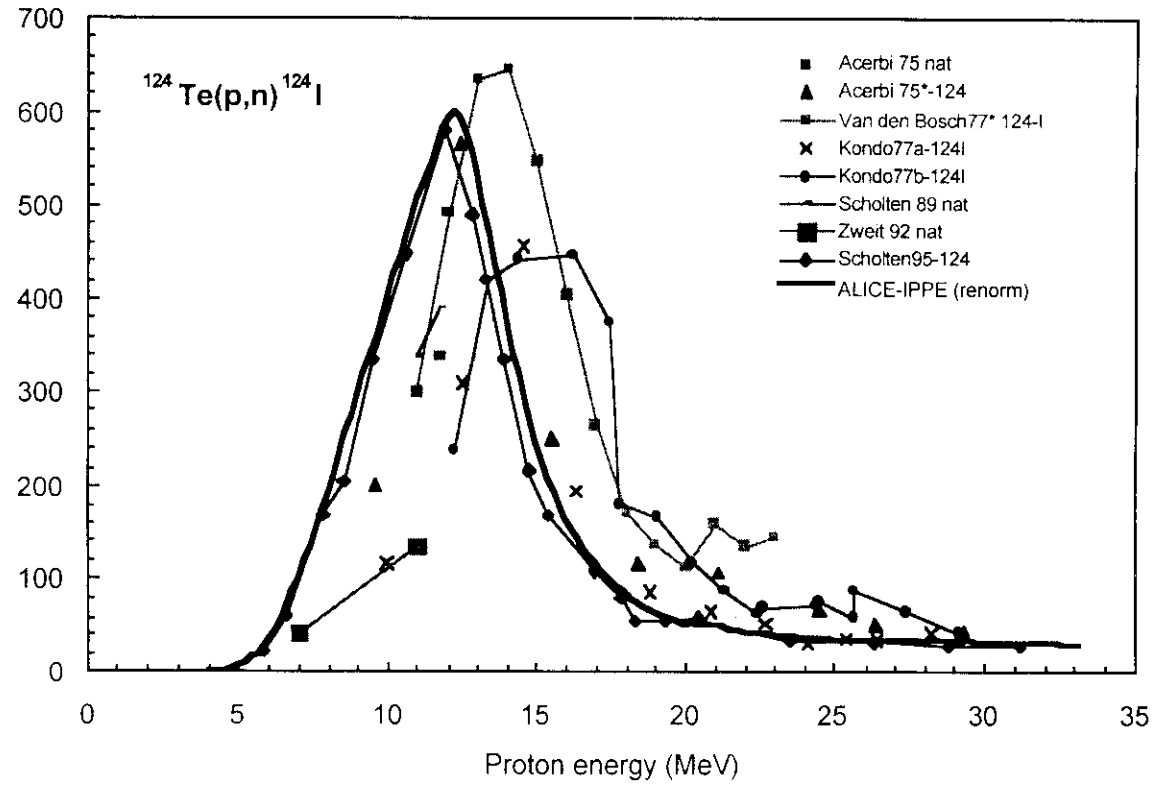

Fig. 15. Calculated $^{124}Te(p,n)^{124}I$ reaction cross section normalised to the experimental peak value of 600 mb.

EXAMPLES OF THE MODEL CALCULATIONS FOR THE CROSS SECTION PREDICTIONS AND A SEARCH OF NEW ROUTS OF THE ISOTOPE PRODUCTION.

POSSIBILITY OF THALLIUM-199 PRODUCTION BY PROTON BOMBARDMENT OF MERCURY-200

A possibility to produce thallium-199 via the proton induced reaction $^{200}Hg(p,2n)^{199}Tl$ in the energy range 10-35 MeV was investigated. The excitation functions for the $^{200}Hg(p,2n)^{199}Tl$ reaction and also for the interfering $^{200}Hg(p,n)^{200}Tl$ and $^{200}Hg(p,3n)^{198}Tl$ reactions were calculated with ALICE-IPPE code. Thick target yields for thallium-199, thallium-200 and thallium-198 and the radionuclidic purity of thallium-199 were estimated using the excitation functions obtained. The estimations showed that the Tl-199 yield via the $^{200}Hg(p,2n)^{199}Tl$ reaction for proton energy of 30 MeV exceeds its yield via the $^{197}Au(\alpha,2n)$ reaction almost 100 times.

Introduction

In nuclear medicine ^{201}Tl ($T_{1/2}$ 73 h) has found a wide application for myocardial studies, while occasionally also ^{199}Tl ($T_{1/2}$ 7.4 h) is used (Lishmanov et al., 1990 and Chernov et al., 1995). ^{199}Tl decays via EC and emits X-rays with an average energy of 72.5 keV and gamma rays of 158, 208, 247, and 455 keV. The emission characteristics of ^{199}Tl for imaging are not worse than those of ^{201}Tl (Lishmanov et al., 1990), but associated equivalent dose is 10 times less per unit of activity in comparison with that of ^{201}Tl (see Table 1, Tultaev et al., 1989). The short-lived ^{199}Tl is produced already during almost ten years on α-particle beam of Tomsk Politechnical University U-120 cyclotron in Russia (Glukhov et al., 1989, and Skuridin et al., 1996). The attempts to make the routine production of ^{199}Tl on Moscow (Kurenkov et al., 1996) and St.-Petersburg University cyclotrons are undertaken (Alexeyev et al., 1991).

^{199}Tl is produced by a-particle bombardment of gold, but this route has a low yield (Nagame et al., 1979). Purpose of this study is evaluation of an alternative production route for ^{199}Tl with a higher yield, so that ^{199}Tl may become more attractive to be applied for myocardial studies in addition to application of ^{201}Tl, which is produced via the reaction $^{203}Tl(p,3n)^{201}Pb®^{201}Tl$.

Calculations

Excitation functions for reactions on mercury isotopes yielding ^{199}Tl have not been not investigated experimentally so far. Mercury consists of seven stable isotopes: ^{204}Hg - 6.85%; ^{202}Hg - 29.80%; ^{201}Hg - 13.22%; ^{200}Hg - 23.13%; ^{199}Hg - 16.84%; ^{198}Hg -

10.02% and ^{196}Hg - 0.14%. Proton induced nuclear reactions resulting in formation of ^{199}Tl are possible in five of them. The reactions induced with protons on natural mercury and enriched with ^{202}Hg isotope were investigated earlier (Dmitriev, et al., 1976, Dmitriev, et al., 1988, and Birratari, et al., 1982). The yields of thallium radioisotopes, in particular ^{201}Tl, have been measured. Subject of our study was the ^{200}Hg(p,2n)^{199}Tl reaction. In previous work it was shown that the modified ALICE-IPPE code may give a reasonable estimate for the excitation functions for proton-induced reactions (Kurenkov et al., in press, ARI 1409). This code was used for the estimation of the excitation functions for the reactions ^{200}Hg(p,2n)^{199}Tl, ^{200}Hg(p,n)^{200}Tl and ^{200}Hg(p,3n)^{198}Tl.

Results and discussion

Fig. 1 shows the excitation functions for the reaction ^{200}Hg(p,2n)^{199}Tl and for the two interfering reactions ^{200}Hg(p,n)^{200}Tl and ^{200}Hg(p,3n)^{198}Tl. Thick target yields as function of proton energy have been calculated using stopping power values of mercury metal for protons (Janni, 1982). Table 2 lists the thick target yields for the required product ^{199}Tl as well as for the impurities ^{198}Tl and ^{200}Tl.

From Table 2 it is clear that the formation of ^{198}Tl may be suppressed by setting an upper limit to the incident proton energy. However, the threshold for formation of ^{200}Tl is lower than that of ^{199}Tl. Both impurities are unwanted because of the equivalent dose per unit of activity administered and/or the radiation properties. In particular the ^{200}Tl impurity should be reduced as much as possible. On one hand it contributes per unit of activity strongly to the equivalent dose and it has high-energy gamma rays. Its longer half life implies that the ^{200}Tl impurity level in a ^{199}Tl preparation increases with time. At present an ^{200}Tl impurity below 1.5-2% is considered as acceptable, without substantial deterioration of the image quality due to high-energy gamma-ray penetration of the collimator septa.

The optimum energy interval in the target is a trade off between ^{199}Tl yield on one hand and impurity levels due to ^{198}Tl and ^{200}Tl on the other. The impurity levels are not only determined by the energy interval, but also by the duration of the irradiation and the time elapsed after EOB until administration. As is obvious from Fig. 1 and Table 2, there is no possibility to produce ^{199}Tl without radionuclidic impurities. The calculation results for ^{199}Tl, ^{198}Tl and ^{200}Tl activities induced by proton bombardment of ^{200}Hg with the enrichment 100% with current 1 μA in the energy range of 21.5-16.5 MeV as a function of the irradiation time are presented in Fig. 2.

For instance, for an energy interval from 21.5 MeV to 16.5 MeV, an irradiation period of 1 h and a current of 50 mA, the ^{199}Tl yield is ca 1050 mCi and the ^{200}Tl yield is ca 21.7 mCi and the ^{198}Tl yield is ca 29 mCi. The ^{198}Tl yield becomes insignificant at

proton energy below 20.5 MeV. For an energy interval from 20.5 MeV to 15.5 MeV and the mentioned above irradiation conditions , ^{199}Tl yield is ca 935 mCi, ^{200}Tl yield is ca 22.7 mCi.

. When administered to patients 7.4 h after EOB, the activity amounts to 467 mCi and 18.8 mCi respectively, and the associated equivalent doses after a single administration of 2 mCi of ^{199}Tl are 0.5 mSv and 0.44 mSv respectively. This implies that almost half of the equivalent such dose received stems from the ^{200}Tl impurity. Nevertheless, this impure product may still be attractive, since the dose is still a factor 5 lower compared to that when using ^{201}Tl. Furthermore, ^{199}Tl permits to carry out several tests in a short time interval. Extraction of ^{199}Tl from the irradiated target and preparation of the product takes not more than 2 hours. The preparation of ^{201}Tl requires more than 2 days, from which 32 hours is the optimal cooling time of ^{201}Pb to accumulate maximum quantity of ^{201}Tl. On the other hand, the ten times lower half life of ^{199}Tl demands faster logistics and also a need for more local production sites.

In this work, the possibility for ^{199}Tl production was investigated and the excitation functions and thick target yields were calculated. The calculations assume the use of mercury isotopically enriched to almost 100% ^{200}Hg and a nearly quantitative recovery of this expensive material. When still substantial amounts of other mercury isotopes are present in the target material, the formation of other thallium radioisotopes will increase. Use of mercury as a target material entails special difficulties. The technology of thallium separation from mercury targets for nuclear medicine has already been developed (P.P. Dmitriev et al., 1976 and 1988).

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Table 1. Equivalent doses from radiothallium after a single administration of 2 mCi thallium chloride.

Radionuclide	^{199}**Tl**	^{200}**Tl**	^{201}**Tl**	^{202}**Tl**
Physical half-life	7.4 h	26.1 h	73.1 h	293.5 h
Effective half-life	7.3 h	24.8 h	63.4 h	182.1 h
Mode of decay	EC	EC	EC	EC, β^-
Equivalent dose, mSv				
1. Thyroid	12	64	110	230
2. Kidney	10	79	110	330
3. Liver	2.2	26	19	100
4. Ovaries	0.67	19	11	150
5. Total body	0.5	11	4.7	53

Table 2. Thick target yields of ^{198}Tl, ^{199}Tl and ^{200}Tl as a function of proton energy.

Proton energy, MeV	^{200}Tl yield, mCi/mAh	^{199}Tl yield, mCi/mAh	^{198}Tl yield, mCi/mAh
10.5	0.16	-	
11.5	0.35	-	
12.5	0.63	0.156	
13.5	0.91	0.75	
14.5	1.1	2.1	
15.5	1.3	4.2	
16.5	1.4	7.0	
17.5	1.5	10.4	
18.5	1.6	14.4	
19.5	1.7	18.8	
20.5	1.76	23.8	0.07
21.5	1.84	29.0	0.55
22.5	1.9	34.2	2.1
23.5	1.98	38.8	5.2
24.5	2.05	42.6	9.9
25.5	2.1	45.6	16.1
26.5	2.18	47.9	23.5
27.5	2.24	49.8	32.1
28.5	2.3	51.4	41.5
29.5	2.36	52.7	51.3
30.5	2.42	53.9	61.0
31.5	2.48	55.0	70.1
32.5	2.53	56.0	77.9
33.5	2.59	57.0	84.7

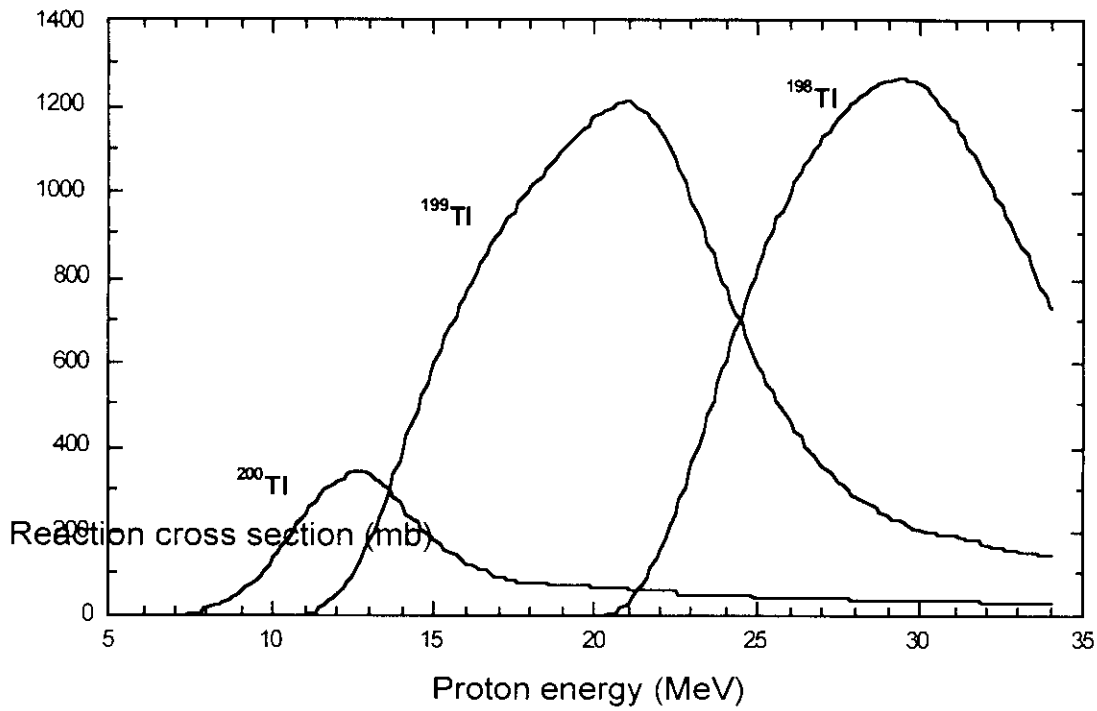

Fig. 16. Excitation functions of proton induced reactions ^{200}Hg(p,xn) calculated with the ALICE-IPPE code.

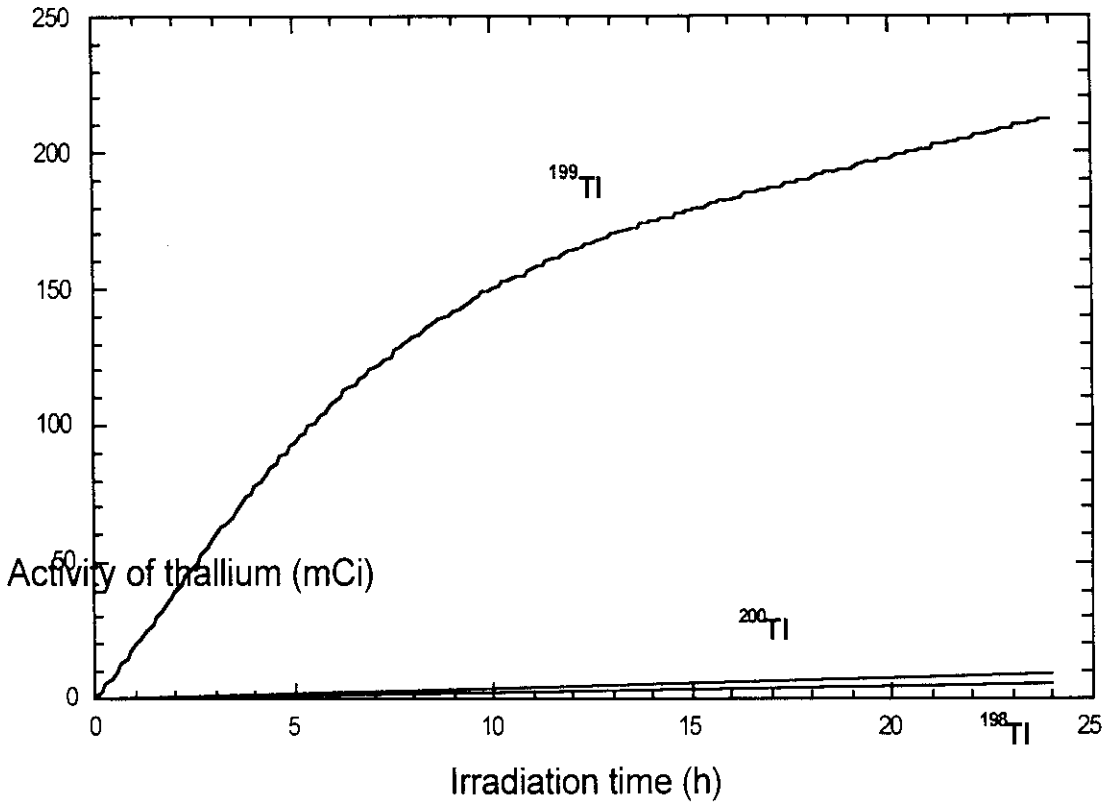

Fig. 17. The calculation results of ^{199}Tl, ^{198}Tl, and ^{200}Tl activities induced by proton bombardment of ^{200}Hg with enrichment up to 100%, with beam current 1 μA in the energy interval 21.5 MeV - 16.5 MeV, as a function of the irradiation time.

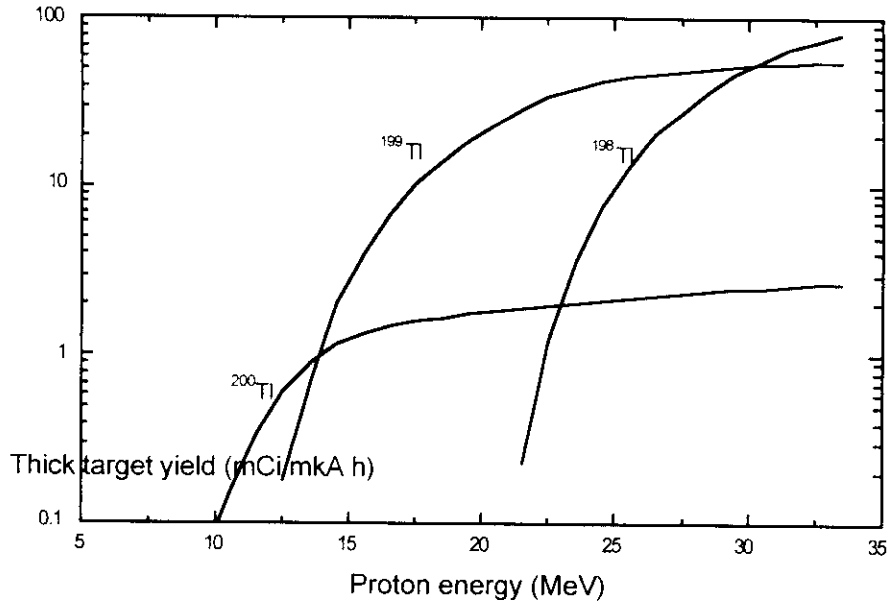

Fig. 18. Thick target yields of 200Tl, 199Tl and 198Tl plotted as a function of proton energy on 200Hg. Data were calculated using the solid curves given in Fig. 1.

METHODS OF STATISTICAL OPTIMISATION AND APPROXIMATION OF EXPERIMENTAL DATA WITH RATIONAL FUNCTIONS.

The methodology of excitation function evaluation, developed in Theory Division of IPPE , was proposed and used for the evaluation of the excitation functions for medical radioisotope production and monitor reactions. The method is based on the statistical optimisation and approximation of experimental data with rational functions (Pade -approximation).

When the status of the experimental data is appropriate, meaning that a reasonable amount of independent measurements have been published that do not show inexplicable discrepancies between them and that for all points reliable estimations are available, a purely statistical fit over the selected data points can be performed. For the approximation of experimental data various analytical functions can be used. The polynomial approximation is the simplest, best developed and most popular one. Well-known Spline fit method is based on the approximation by polynomials. However, the physics of the problem often dictates the necessity to use more complicated functions having special analytical features. Rational functions (ratio of two polynomials) represent the more general class of analytical functions as compared with polynomials. In particular, these functions enable to describe in a natural way the nuclear reaction cross sections in resonance region, which are determined by the positions of poles of the corresponding S-matrix and, consequenttly, are well approximated with the polar expansion, that is, with rational function of the energy.

Although the approximation with rational functions (Pade- approximation) has been proposed at the end of last century [1], only in the last decades is extensively used in mathematical physics [2-7].

A Pade-approximant of the first kind (Pade-I) of an order L=N+M+1 for a function f(z) is a rational function, which have the first L terms of the Taylor expansion in power series equal to the corresponding the Taylor series of f(z). Using of Pade-I approximation enables to go out of the convergency limits of the Taylor series. For the construction of Pade-I approximation it is necessary to be able to calculate the high order derivatives of an approximating function. This method is practically not applicable when a function is in a tabular form, particularly when there are significant uncertainties. For the functions set pointwize the Pade-II approximation is used.

For the evaluation of the excitation functions for the reactions producing radioisotopes and monitor reactions the method of descrete optimisation of approximants (Pade-II) was used. A Pade-approximant of the second kind (Pade-II) of an order L=N+M+1 for a function f(z) is a rational function determined by a set of equations

$$f_L(z) = P_N^{(L)}(z) / Q_M^{(L)}(z); \qquad f_L(z_i) = f(z_i), \qquad i = 1,2,\ldots L \qquad \textbf{(1)}$$

where P and Q are polynomials of degrees N and M. In some cases there is no need to show the power of a numerator and denominator, because they are determined by the initial approximation, the recurrent chain and approximation rank L uniquely. In these cases we use the denotation

$$f_L(z) = P^{(L)}(z) / Q^{(L)}(z).$$

The applications of well known methods of Pade-approximation in data processing and analysis was hindered until recently by two obstacles. First is the difficulty of realisation. Rational approximants unlike polynomials lead to complicated non-linear systems of equations in the least squares method (LSM). Second is a special form of approximant's instability - possible real pole-zero pairs (noise doublets). The method to circumvent both difficulties is based on the recursive calculation of many approximants differing by the choice of interpolation knots with their statistical optimisation by discrete sorting.

Eqs. (1) result in the linear sistem of equations for coefficients which may be solved either with determinants or with the recurrent formulae. The simplest of the latter is:

$$f_L(\gamma,z) = \frac{P^{(L-2)}(z) + \gamma_L(z - z_{L-1})P^{(L-2)}(z)}{Q^{(L-2)}(z) + \gamma_L(z - z_{L-1})Q^{(L-2)}(z)} \qquad (2)$$

In the equation (2) an index (L) in the right side is not the order of the polinomials P and Q, but is the approximation rank.

In practice we use the diagonal and nearly diagonal approximants with N=M or N=M-1 only, in accordance with the initial conditions:

$$P_0^{(0)} = 0; \qquad P_0^{(1)} = f(z_1);$$
$$Q_0^{(0)} = 1; \qquad Q_0^{(1)} = 1.$$

That gives the next recurrent chain:

$$f_2(\gamma_2,z) = \frac{P_0^{(1)} + \gamma_2(z - z_1)P_0^{(0)}}{Q_0^{(1)} + \gamma_2(z - z_1)Q_0^{(0)}(z)} =$$

$$= \frac{f_1 + \gamma_2(z - z_1) \cdot 0}{1 + \gamma_2(z - z_1) \cdot 1} \equiv P_0^{(2)}/Q_1^{(2)};$$

$$f_3(\gamma_3, z) = \frac{P_0^{(2)} + \gamma_3(z - z_2)P_0^{(1)}}{Q_1^{(2)} + \gamma_3(z - z_2)Q_0^{(1)}(z)} = P_1^{(3)} / Q_1^{(3)};$$

and so on.

The coefficients of the recurrent formula γ_L are defined from the equation:

$$f_L(z_L) = f(z_L), \quad \text{namely}$$

$$\gamma_L = \frac{f(z_L)Q^{(L-1)}(z_L) - P^{(L-1)}(z_L)}{(z_L - z_{(L-1)})(P^{(L-2)}(z_L) - f(z_L)Q^{(L-2)}(z_L))}$$

Essential stages of the proposed and realised method of Pade-approximation of experimental data sets are: for $N_{ex} >> L$ (N_{ex} is the number of experimental points) we choose an initial set of L "supporting" points z_k, F_k (F_k is experimental value in the point z_k); $1 \leq k \leq N_{ex}$ and recursive algorithm (2) interpolate them with a rational function. Then the values $f_L(z_i)$ for all experimental points are computed and inserted in the functional to be minimised, usually

$$S = \sum_{i=1}^{N_{ex}} (f_L(z_i) - F_i)^2 / 2\sigma_i^2, \qquad (3)$$

defining a starting interpolation. Then iteration process begins. On its n-th stage one of the supporting points is replaced by another experimental point, new approximant and its functional's value S^n are calculated. If $S^n < S^{n-1}{}_{min} = \min(S^1, S^2, \ldots S^{n-1})$, then n-th set of supporting points is stored as current optimum and so on.

One of the advantages of discrete optimisation as compared with continuous least squares method (LSM) is the possibility to use a variety of statistical functionals. Theoretical estimates show that mean quadratic deviation of the approximant, found by discrete optimisation, from continuous LSM solution in the case $L << N_{ex}$ is $\cong (N_{ex}/L)^{1/2}$ times less then deviation of the last from exact curve, so the approximant is statistically equivalent to LSM solution.

The approximant's polar expansion

$$f^L(z) = C + \sum_{i=1}^{l} \frac{a_i}{z - p_i} + \sum_{k=1}^{m} \frac{\alpha_k(z - \varepsilon_k) + \beta_k}{(z - \varepsilon_k)^2 + \gamma_k{}^2} \qquad (4)$$

may be called resonance expansion because for a cross section approximant in resonance region ε_k and γ_k are energy and total half-width of a k-th resonance level, α_k and β_k may be expressed in terms of partial widths and interference parameters. The first sum corresponds to real poles, the second sum - to complex poles.

A prominent disturbing feature of numerically generated rational approximants is appearance of real poles (denominator zeros) **inside** the approximation interval which is physically senseless and makes the approximant unusable. The poles are closely accompanied by real zeros of the numerator. These couples constitute so called "noise doublets" (NDs). It was the NDs that prevented wide use of Pade-approximants in data handling.

But in the proposed method they not only are neutralised but become in a sense useful. The NDs correspond to the terms with p_i inside the interval of approximation and with relatively small a_i in the first sum of Eq. (4). In our method they are just cancelled, eliminated from the sum and that regularization gives satisfactory results. Normally NDs appear with increasing L on the final stages of approximation and indicate (together with statistical criteria) that analytical information is exhausted.

Situation may be different if some points in the input data deviate abnormally from the general trend. In this case NDs appear at relatively low L near those "bad points" describing them by local singularities rather than by smooth components. When the singularities are eliminated the resulting regularised curve practically ignores the "marked" bad points. This is a way to identify them automatically.

From the point of view of mathematical statistics the method is equivalent to LSM, so experimental data set must be statistically consistent. In the case when there are a few sets of experimental data and discrepancies between different sets are significantly larger than their declared errors, statistical processing of the data by the method is possible only after their preliminary preparing (selection) by expert.

The simple version of Pade-2 code is applicable in the cases when number of experimental points $N_{ex} \leq 500$, number of approximant's parameters $L \leq 40$ and $(F_i)_{max}/(F_i)_{min} \leq 10^6$. The method is also very convenient for calculation of approximant's error band and covariational matrix. The method is described in detail in a book [5] (in Russian) and generally outlined in [6-7].

References

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PADEMIN code system

The PADEMIN code system consist of the PADE2 CODE realizing the construction of rational function, approximating the given set of experimental points, calculates covariance matrix of parameter errors and mean square deviation of the approximant, and the AUXILI-2 code, which enables to prepare the input file of the energies where the approximant should be calculated. The parameters of the rational function are defined in the form of the sets of the coefficients in the polar series.

Main possibilities and limitations of the code:

a) It is assumed that experimental errors are independent and normally distributed with zero average mean deviaton.

b) The algorithm used and his realization do not limit to the number of experimental points NEP and the number of the approximant parameters.

c) The assumed interval of variations of experimental values is no more than six orders of magnitude.

The PADEMIN code is written using FORTRAN-4.

SELECTION OF CODE'S REGIME:

Input data for the PADEMIN system

1. IN.DAT file:

LMIN (the lower limit of the number of rational function's coefficients)
LMAX (the upper limit of the number of rational function's coefficients)
NEP (the total number of measured cross-sections)
LR (step of parametric mesh)
IND1 (parameter, usually IND1=0)
IND2 (parameter, usually IND2=2)
IFOR (parameter, regulating the format of data input, usually IFOR=3)
ICOR (parameter, points out whether the correlations measured cross-sections are taken into account
(ICOR=1) or not (ICOR=0))
IPOLE (parameter, usually IPOLE=0)
IFILE (parameter, points out whether the preparation of the estimated data files in the ENDF format is required (IFILE=1) or not (IFILE=0))
NEXP (the number of experiments)
MINCOR (parameter, points out whether the minimized functional is calculated with taking covariations of experimental data into account (MINCOR=1) or not (MINCOR=0))
MAXL (the number of rows of the COV-matrix as declared in the main subroutine)
INAVCO (parameter, points out whether the average correlation coefficients are entered (INAVCO=1) or not (INAVCO=0))
ICALAC (parameter,points out whether the average correla tion coefficients are calculated (ICALAC=1) or not used at all (ICALAC=0))
NSYST (the number of components of systematical error)

2. CR-SECT.DAT file:

Contains energies, cross sections and uncertainties.
Format **3F15.5.**

3. ADDZ.DAT file:
This file contains the array of energies (different from experimental), where should be calculated the approximant.
Format:
1st line **-I5**-Number of energies, next lines: **6F10.0** -the energies, (or see below).

4. AUXIL2.IN file:
The energies where should be calculated the approximant can be set with the help of the **AUXIL2.FOR**.
(PADE2\AUXILI-2)

Input set **auxil2.in** :

1. Minimum energy,
2. Maximum energy,
3. Eenergy step.

Format: **3F5.2.**

AUXIL2.BAT

The results of work **auxil2.out** should be written in **addz.dat** and put to directory **PADE2\PADEMIN.**

CALCULATION:

PADEMIN.BAT

Results are given in two files:

OUT.DAT file is the main set of resulting data and contains the following information:

1. Paramaters of calculations given in **IN.DAT** file .
2. Table of the input data (energy, reacton cross section, uncertainties).
3. Table of output data (energy, input reaction cross section, output reaction cross section, χ^2).
4. The results of the statistical analysis.
5. Array of the parameters of complex and real poles.

ADDF.DAT contains the energies and output reaction cross sections at these energies. The values of the energies is taken from ADDZ.DAT, which represents the array with constant energy step.

RESULTS OF STATISTICAL ANALYSIS

The results of statistical analysis for the 16O(p,α)13N reaction is presented below. Complete numerical information on the Pade-approximation of O^{16}(p,alpha) cross section for 6.508 — 17.77 MeV energy range split into three subranges: 6.508-9.488; 9.488-12.149; 12.149-17.77 MeV

THE RESULTS OF STATISTICAL ANALYSIS

IR= 8 IER= 0

SUM3= 0.36066E+00

SUM1= 0.33946E+00 SUM2= 0.33946E+00

THE NOISE POLES

-0.17018E-01 0.89937E+01
0.12763E-01 0.72658E+01

SUM1= 0.35379E+00 ERR= 0 IERR= 0

NEP= 119 **L= 17** K1= 6 K2= 6 **CON= 0.167557125E+02**

ARRAYS ZNEP, FNEP, FAPR, XI-SQ CONTR.

0.6508E+01 0.5200E-01 0.6217E-01 0.3827E-01
0.6510E+01 0.5000E-01 0.6003E-01 0.4028E-01
0.6623E+01 0.5300E-01 0.5939E-01 0.1453E-01
0.6640E+01 0.5000E-01 0.8087E-01 0.3812E+00
0.6660E+01 0.1000E+00 0.1138E+00 0.1897E-01
0.6667E+01 0.2710E+00 0.1273E+00 0.2813E+00
0.6685E+01 0.6310E+00 0.1667E+00 0.5414E+00
0.6703E+01 0.2460E+00 0.2131E+00 0.1784E-01
0.6710E+01 0.2500E+00 0.2331E+00 0.4578E-02
0.6739E+01 0.2600E+00 0.3272E+00 0.6677E-01
0.6769E+01 0.3230E+00 0.4443E+00 0.1409E+00
0.6778E+01 0.1540E+01 0.4833E+00 0.4708E+00
0.6780E+01 0.3300E+00 0.4923E+00 0.2418E+00
0.6791E+01 0.1490E+01 0.5430E+00 0.4039E+00
0.6864E+01 0.1540E+01 0.9507E+00 0.1464E+00
0.6875E+01 0.1207E+01 0.1023E+01 0.2327E-01
0.6890E+01 0.1100E+01 0.1126E+01 0.5532E-03
0.6893E+01 0.3093E+01 0.1147E+01 0.3958E+00
0.6910E+01 0.1160E+01 0.1271E+01 0.9227E-02
0.6915E+01 0.2398E+01 0.1309E+01 0.2061E+00
0.6990E+01 0.4507E+01 0.1948E+01 0.3225E+00

0.6991E+01	0.2520E+01	0.1957E+01	0.4991E-01
0.6995E+01	0.2506E+01	0.1995E+01	0.4160E-01
0.7010E+01	0.2630E+01	0.2140E+01	0.3470E-01
0.7012E+01	0.2500E+01	0.2160E+01	0.1851E-01
0.7048E+01	0.3233E+01	0.2531E+01	0.4710E-01
0.7074E+01	0.2738E+01	0.2818E+01	0.8582E-03
0.7101E+01	0.5500E+01	0.3132E+01	0.1853E+00
0.7110E+01	0.2820E+01	0.3241E+01	0.2226E-01
0.7111E+01	0.2800E+01	0.3253E+01	0.2616E-01
0.7116E+01	0.3580E+01	0.3314E+01	0.5521E-02
0.7145E+01	0.4979E+01	0.3679E+01	0.6813E-01
0.7185E+01	0.4924E+01	0.4214E+01	0.2082E-01
0.7198E+01	0.7926E+01	0.4395E+01	0.1985E+00
0.7210E+01	0.4920E+01	0.4565E+01	0.5207E-02
0.7241E+01	0.4980E+01	0.5019E+01	0.6160E-04
0.7260E+01	0.3125E+01	0.5307E+01	0.4877E+00
0.7274E+01	0.7095E+01	0.5524E+01	0.4900E-01
0.7300E+01	0.1093E+02	0.5938E+01	0.2084E+00
0.7305E+01	0.1168E+02	0.6019E+01	0.2347E+00
0.7310E+01	0.1160E+02	0.6101E+01	0.2247E+00
0.7340E+01	0.6200E+01	0.6601E+01	0.4180E-02
0.7365E+01	0.7170E+01	0.7031E+01	0.3766E-03
0.7398E+01	0.8285E+01	0.7617E+01	0.6505E-02
0.7411E+01	0.1069E+02	0.7853E+01	0.7031E-01
0.7438E+01	0.1069E+02	0.8354E+01	0.4764E-01
0.7462E+01	0.4875E+01	0.8811E+01	0.6519E+00
0.7490E+01	0.7990E+01	0.9357E+01	0.2927E-01
0.7510E+01	0.1155E+02	0.9756E+01	0.2413E-01
0.7519E+01	0.1540E+02	0.9937E+01	0.1258E+00
0.7532E+01	0.1506E+02	0.1020E+02	0.1041E+00
0.7560E+01	0.9400E+01	0.1078E+02	0.2169E-01
0.7615E+01	0.1490E+02	0.1197E+02	0.3864E-01
0.7627E+01	0.2345E+02	0.1224E+02	0.2286E+00
0.7654E+01	0.1290E+02	0.1285E+02	0.1249E-04
0.7672E+01	0.2294E+02	0.1328E+02	0.1774E+00
0.7710E+01	0.1380E+02	0.1422E+02	0.9225E-03
0.7726E+01	0.1778E+02	0.1465E+02	0.3112E-01
0.7740E+01	0.1310E+02	0.1504E+02	0.2201E-01
0.7780E+01	0.1646E+02	0.1642E+02	0.5576E-05
0.7781E+01	0.9250E+01	0.1646E+02	0.6076E+00
0.7790E+01	0.1590E+02	0.1687E+02	0.3705E-02
0.7793E+01	0.1965E+02	0.1702E+02	0.1791E-01
0.7838E+01	0.5034E+02	0.2122E+02	0.3347E+00
0.7865E+01	0.1890E+02	0.3102E+02	0.4113E+00
0.7883E+01	0.1081E+03	0.5764E+02	0.2177E+00
0.7892E+01	0.1000E+03	0.9996E+02	0.1280E-06
0.7933E+01	0.1348E+03	0.1348E+03	0.6845E-07
0.7990E+01	0.1010E+03	0.3933E+02	0.3729E+00
0.7991E+01	0.8285E+02	0.3908E+02	0.2791E+00

0.8000E+01 0.5130E+02 0.3723E+02 0.7527E-01
0.8018E+01 0.2318E+02 0.3491E+02 0.2566E+00
0.8027E+01 0.4457E+02 0.3420E+02 0.5412E-01
0.8045E+01 0.5562E+02 0.3331E+02 0.1608E+00
0.8114E+01 0.4340E+02 0.3302E+02 0.5716E-01
0.8122E+01 0.3059E+02 0.3315E+02 0.6985E-02
0.8149E+01 0.3572E+02 0.3368E+02 0.3253E-02
0.8160E+01 0.3453E+02 0.3394E+02 0.2980E-03
0.8208E+01 0.2860E+02 0.3522E+02 0.5365E-01
0.8220E+01 0.3260E+02 0.3557E+02 0.8293E-02
0.8266E+01 0.3692E+02 0.3689E+02 0.9576E-06
0.8293E+01 0.4507E+02 0.3761E+02 0.2734E-01
0.8365E+01 0.4880E+02 0.3908E+02 0.3969E-01
0.8369E+01 0.4608E+02 0.3913E+02 0.2273E-01
0.8419E+01 0.3093E+02 0.3939E+02 0.7480E-01
0.8450E+01 0.2950E+02 0.3914E+02 0.1067E+00
0.8464E+01 0.4311E+02 0.3890E+02 0.9545E-02
0.8490E+01 0.2860E+02 0.3826E+02 0.1140E+00
0.8541E+01 0.3860E+02 0.3619E+02 0.3889E-02
0.8550E+01 0.4035E+02 0.3572E+02 0.1320E-01
0.8581E+01 0.5623E+02 0.3387E+02 0.1581E+00
0.8614E+01 0.4110E+02 0.3159E+02 0.5351E-01
0.8663E+01 0.3652E+02 0.2782E+02 0.5668E-01
0.8680E+01 0.3550E+02 0.2647E+02 0.6477E-01
0.8685E+01 0.4079E+02 0.2607E+02 0.1303E+00
0.8694E+01 0.1991E+02 0.2535E+02 0.7471E-01
0.8739E+01 0.3640E+02 0.2183E+02 0.1602E+00
0.8751E+01 0.3686E+02 0.2093E+02 0.1868E+00
0.8789E+01 0.1248E+02 0.1825E+02 0.2140E+00
0.8792E+01 0.1100E+02 0.1805E+02 0.4116E+00
0.8798E+01 0.1610E+02 0.1766E+02 0.9404E-02
0.8863E+01 0.1320E+02 0.1390E+02 0.2797E-02
0.8900E+01 0.1630E+02 0.1218E+02 0.6392E-01
0.8902E+01 0.1726E+02 0.1209E+02 0.8964E-01
0.8907E+01 0.1880E+02 0.1189E+02 0.1351E+00
0.8911E+01 0.1194E+02 0.1172E+02 0.3200E-03
0.8989E+01 0.1280E+02 0.9168E+01 0.8052E-01
0.8998E+01 0.4995E+01 0.8940E+01 0.6238E+00
0.9015E+01 0.7752E+01 0.8543E+01 0.1042E-01
0.9110E+01 0.6400E+01 0.6997E+01 0.8715E-02
0.9119E+01 0.5878E+01 0.6900E+01 0.3021E-01
0.9178E+01 0.5813E+01 0.6418E+01 0.1082E-01
0.9228E+01 0.7499E+01 0.6184E+01 0.3073E-01
0.9242E+01 0.6080E+01 0.6142E+01 0.1043E-03
0.9309E+01 0.5749E+01 0.6049E+01 0.2729E-02
0.9320E+01 0.5100E+01 0.6049E+01 0.3460E-01
0.9390E+01 0.6080E+01 0.6117E+01 0.3691E-04
0.9422E+01 0.6566E+01 0.6182E+01 0.3428E-02
0.9488E+01 0.6890E+01 0.6362E+01 0.5876E-02

ARRAY OF THE PARAMETERS OF THE COMPLEX POLES

Alpha	**beta**	**eps**	**gamma**
0.69442E+01	**-0.57281E+02**	**0.69017E+01**	**0.15810E+01**
0.53916E+00	**0.50278E-01**	**0.79119E+01**	**0.10209E-01**
-0.11543E+02	**0.40742E+01**	**0.85819E+01**	**0.40604E+00**

ARRAY OF PARAMETERS FOR REAL POLES

-0.17018313E-01	0.89936954E+01
0.12763191E-01	0.72658225E+01

SUPPORTING ARGUMENTS AND ORDINATES

0.93900003E+01	0.60800023E+01
0.79330001E+01	0.13483690E+03
0.82659998E+01	0.36924015E+02
0.92419996E+01	0.60800023E+01
0.72740002E+01	0.70950069E+01
0.68899999E+01	0.11000007E+01
0.78920002E+01	0.10000005E+03
0.73649998E+01	0.71700029E+01
0.76539998E+01	0.12899997E+02
0.65100002E+01	0.50000634E-01
0.89110003E+01	0.11938005E+02
0.66599998E+01	0.99999860E-01
0.89890003E+01	0.12800002E+02
0.77800002E+01	0.16456984E+02
0.72600002E+01	0.31249506E+01
0.89980001E+01	0.49942575E+01
0.90150003E+01	0.77519932E+01

****
****

THE RESULTS OF STATISTICAL ANALYSIS

IR= 3 IER= 0

SUM3= 0.23355E+00

SUM1= 0.22259E+00 SUM2= 0.22259E+00

THE NOISE POLES

0.10994E+00 0.99066E+01

SUM1= 0.22969E+00 ERR= 0 IERR= 0

NEP= 65 **L= 6** K1= 1 K2= 2 **CON= 0.000000000E+00**

ARRAYS ZNEP, FNEP, FAPR, XI-SQ CONTR.

0.9488E+01 0.6890E+01 0.5903E+01 0.2050E-01
0.9509E+01 0.4824E+01 0.6112E+01 0.7124E-01
0.9518E+01 0.1134E+02 0.6203E+01 0.2052E+00
0.9550E+01 0.5900E+01 0.6540E+01 0.1176E-01
0.9607E+01 0.5941E+01 0.7187E+01 0.4396E-01
0.9656E+01 0.7926E+01 0.7795E+01 0.2729E-03
0.9682E+01 0.8750E+01 0.8139E+01 0.4873E-02
0.9694E+01 0.8250E+01 0.8303E+01 0.4168E-04
0.9699E+01 0.7843E+01 0.8373E+01 0.4560E-02
0.9719E+01 0.8070E+01 0.8656E+01 0.5275E-02
0.9738E+01 0.1077E+02 0.8935E+01 0.2904E-01
0.9770E+01 0.8600E+01 0.9425E+01 0.9195E-02
0.9780E+01 0.1515E+02 0.9583E+01 0.1350E+00
0.9847E+01 0.8875E+01 0.1072E+02 0.4324E-01
0.9882E+01 0.1012E+02 0.1137E+02 0.1516E-01
0.9915E+01 0.2506E+02 0.1202E+02 0.2710E+00
0.9946E+01 0.1994E+02 0.1266E+02 0.1334E+00
0.9986E+01 0.2590E+02 0.1354E+02 0.2279E+00
0.1000E+02 0.2080E+02 0.1386E+02 0.1114E+00
0.1003E+02 0.1232E+02 0.1470E+02 0.3732E-01
0.1004E+02 0.1305E+02 0.1472E+02 0.1642E-01
0.1017E+02 0.2036E+02 0.1843E+02 0.9004E-02
0.1018E+02 0.1781E+02 0.1858E+02 0.1915E-02
0.1018E+02 0.2992E+02 0.1880E+02 0.1381E+00
0.1023E+02 0.1610E+02 0.2024E+02 0.6616E-01
0.1024E+02 0.1683E+02 0.2067E+02 0.5216E-01
0.1025E+02 0.3180E+02 0.2097E+02 0.1160E+00
0.1025E+02 0.2480E+02 0.2100E+02 0.2342E-01
0.1035E+02 0.2872E+02 0.2453E+02 0.2127E-01
0.1036E+02 0.2259E+02 0.2514E+02 0.1280E-01
0.1043E+02 0.3269E+02 0.2768E+02 0.2353E-01

0.1050E+02	0.3360E+02	0.3061E+02	0.7942E-02
0.1051E+02	0.3200E+02	0.3102E+02	0.9305E-03
0.1053E+02	0.3541E+02	0.3174E+02	0.1074E-01
0.1056E+02	0.2635E+02	0.3333E+02	0.7005E-01
0.1067E+02	0.3244E+02	0.3761E+02	0.2542E-01
0.1073E+02	0.3987E+02	0.3974E+02	0.1124E-04
0.1079E+02	0.4320E+02	0.4168E+02	0.1236E-02
0.1087E+02	0.4059E+02	0.4366E+02	0.5729E-02
0.1089E+02	0.5466E+02	0.4403E+02	0.3784E-01
0.1104E+02	0.5360E+02	0.4504E+02	0.2552E-01
0.1106E+02	0.4741E+02	0.4495E+02	0.2697E-02
0.1106E+02	0.4825E+02	0.4493E+02	0.4718E-02
0.1116E+02	0.4918E+02	0.4367E+02	0.1253E-01
0.1126E+02	0.4941E+02	0.4162E+02	0.2484E-01
0.1128E+02	0.3672E+02	0.4116E+02	0.1459E-01
0.1132E+02	0.4150E+02	0.3998E+02	0.1335E-02
0.1136E+02	0.2726E+02	0.3876E+02	0.1781E+00
0.1139E+02	0.4529E+02	0.3798E+02	0.2609E-01
0.1145E+02	0.3037E+02	0.3594E+02	0.3367E-01
0.1146E+02	0.4447E+02	0.3578E+02	0.3816E-01
0.1155E+02	0.2408E+02	0.3283E+02	0.1322E+00
0.1160E+02	0.2750E+02	0.3143E+02	0.2043E-01
0.1164E+02	0.3733E+02	0.3039E+02	0.3452E-01
0.1168E+02	0.3802E+02	0.2903E+02	0.5589E-01
0.1172E+02	0.2673E+02	0.2811E+02	0.2687E-02
0.1185E+02	0.3000E+02	0.2463E+02	0.3203E-01
0.1186E+02	0.3116E+02	0.2442E+02	0.4688E-01
0.1187E+02	0.3279E+02	0.2413E+02	0.6972E-01
0.1189E+02	0.1686E+02	0.2365E+02	0.1617E+00
0.1198E+02	0.2918E+02	0.2181E+02	0.6367E-01
0.1198E+02	0.2812E+02	0.2179E+02	0.5060E-01
0.1209E+02	0.1962E+02	0.1957E+02	0.6573E-05
0.1211E+02	0.3000E+02	0.1925E+02	0.1284E+00
0.1215E+02	0.2294E+02	0.1858E+02	0.3608E-01

ARRAY OF THE PARAMETERS OF THE COMPLEX POLES

Alpha	beta	eps	gamma
0.93257E+01	0.29113E+02	0.10911E+02	0.81026E+00

ARRAY OF PARAMETERS FOR REAL POLES

0.10993681E+00 0.99065740E+01

SUPPORTING ARGUMENTS AND ORDINATES

0.10729000E+02 0.39869999E+02
0.12092000E+02 0.19621000E+02
0.99150000E+01 0.25063059E+02
0.96990004E+01 0.78429966E+01
0.97189999E+01 0.80700006E+01
0.98470001E+01 0.88749990E+01

****
****

THE RESULTS OF STATISTICAL ANALYSIS

IR= 28 IER= 0

SUM3= 0.37647E-01

SUM1= 0.28623E-01 SUM2= 0.28623E-01

THE NOISE POLES

0.35328E-01 0.13287E+02
-0.10707E-01 0.13280E+02
0.44542E-02 0.14528E+02
-0.43942E-02 0.12626E+02
-0.20438E-02 0.13839E+02
0.10664E-02 0.14053E+02
-0.56931E-03 0.17120E+02
-0.19724E-03 0.17749E+02

SUM1= 0.36501E-01 ERR= 0 IERR= 0

NEP= 307 L= 56 K1= 19 K2= **20** **CON= 0.000000000E+00**

ARRAYS ZNEP, FNEP, FAPR, XI-SQ CONTR.

0.1215E+02 0.2294E+02 0.2295E+02 0.3435E-06
0.1221E+02 0.2349E+02 0.2306E+02 0.3325E-03
0.1223E+02 0.2294E+02 0.2304E+02 0.2061E-04
0.1226E+02 0.2330E+02 0.2297E+02 0.2056E-03

0.1228E+02	0.2312E+02	0.2287E+02	0.1207E-03
0.1230E+02	0.2213E+02	0.2271E+02	0.6830E-03
0.1232E+02	0.2226E+02	0.2251E+02	0.1246E-03
0.1235E+02	0.2220E+02	0.2221E+02	0.2712E-06
0.1237E+02	0.2201E+02	0.2194E+02	0.1071E-04
0.1238E+02	0.2145E+02	0.2182E+02	0.2876E-03
0.1241E+02	0.2115E+02	0.2154E+02	0.3556E-03
0.1242E+02	0.2115E+02	0.2150E+02	0.2830E-03
0.1244E+02	0.2153E+02	0.2154E+02	0.9685E-07
0.1245E+02	0.2139E+02	0.2160E+02	0.9873E-04
0.1246E+02	0.2189E+02	0.2178E+02	0.2589E-04
0.1249E+02	0.2232E+02	0.2227E+02	0.4474E-05
0.1253E+02	0.2263E+02	0.2297E+02	0.2213E-03
0.1253E+02	0.2282E+02	0.2298E+02	0.5550E-04
0.1255E+02	0.2300E+02	0.2325E+02	0.1197E-03
0.1255E+02	0.2312E+02	0.2336E+02	0.1084E-03
0.1256E+02	0.2300E+02	0.2345E+02	0.3889E-03
0.1257E+02	0.2367E+02	0.2363E+02	0.2754E-05
0.1258E+02	0.2385E+02	0.2380E+02	0.5135E-05
0.1258E+02	0.2397E+02	0.2388E+02	0.1572E-04
0.1260E+02	0.2379E+02	0.2420E+02	0.2888E-03
0.1262E+02	0.2671E+02	0.2447E+02	0.6992E-02
0.1263E+02	0.2306E+02	0.2453E+02	0.4076E-02
0.1263E+02	0.2301E+02	0.2456E+02	0.4488E-02
0.1264E+02	0.2560E+02	0.2466E+02	0.1352E-02
0.1264E+02	0.2470E+02	0.2470E+02	0.7187E-08
0.1267E+02	0.2452E+02	0.2495E+02	0.3065E-03
0.1269E+02	0.2588E+02	0.2507E+02	0.9791E-03
0.1269E+02	0.2464E+02	0.2508E+02	0.3095E-03
0.1269E+02	0.2531E+02	0.2508E+02	0.8130E-04
0.1270E+02	0.2580E+02	0.2515E+02	0.6418E-03
0.1271E+02	0.2580E+02	0.2521E+02	0.5270E-03
0.1272E+02	0.2568E+02	0.2526E+02	0.2631E-03
0.1275E+02	0.2574E+02	0.2538E+02	0.1939E-03
0.1277E+02	0.2616E+02	0.2542E+02	0.8108E-03
0.1279E+02	0.2568E+02	0.2542E+02	0.1003E-03
0.1281E+02	0.2513E+02	0.2540E+02	0.1115E-03
0.1284E+02	0.2586E+02	0.2531E+02	0.4573E-03
0.1286E+02	0.2489E+02	0.2516E+02	0.1184E-03
0.1287E+02	0.2683E+02	0.2510E+02	0.4184E-02
0.1288E+02	0.2592E+02	0.2500E+02	0.1273E-02
0.1290E+02	0.2592E+02	0.2484E+02	0.1747E-02
0.1291E+02	0.2464E+02	0.2472E+02	0.1088E-04
0.1292E+02	0.2476E+02	0.2452E+02	0.9830E-04
0.1293E+02	0.2483E+02	0.2445E+02	0.2290E-03
0.1293E+02	0.2458E+02	0.2438E+02	0.7003E-04
0.1296E+02	0.2355E+02	0.2386E+02	0.1702E-03
0.1297E+02	0.2343E+02	0.2366E+02	0.1011E-03
0.1299E+02	0.2220E+02	0.2321E+02	0.2100E-02

0.1300E+02 0.2300E+02 0.2310E+02 0.1817E-04
0.1301E+02 0.2170E+02 0.2286E+02 0.2839E-02
0.1302E+02 0.2127E+02 0.2273E+02 0.4742E-02
0.1306E+02 0.2071E+02 0.2141E+02 0.1150E-02
0.1307E+02 0.2059E+02 0.2110E+02 0.6213E-03
0.1311E+02 0.1917E+02 0.1991E+02 0.1490E-02
0.1312E+02 0.1948E+02 0.1939E+02 0.2179E-04
0.1314E+02 0.1873E+02 0.1864E+02 0.2294E-04
0.1316E+02 0.1805E+02 0.1812E+02 0.1165E-04
0.1318E+02 0.1700E+02 0.1742E+02 0.6120E-03
0.1318E+02 0.1708E+02 0.1736E+02 0.2684E-03
0.1319E+02 0.1694E+02 0.1689E+02 0.8999E-05
0.1320E+02 0.1608E+02 0.1673E+02 0.1653E-02
0.1322E+02 0.1577E+02 0.1626E+02 0.9881E-03
0.1324E+02 0.1502E+02 0.1553E+02 0.1137E-02
0.1325E+02 0.1465E+02 0.1528E+02 0.1836E-02
0.1328E+02 0.1502E+02 0.1473E+02 0.3948E-03
0.1331E+02 0.1521E+02 0.1420E+02 0.4395E-02
0.1333E+02 0.1459E+02 0.1404E+02 0.1437E-02
0.1335E+02 0.1465E+02 0.1396E+02 0.2230E-02
0.1337E+02 0.1465E+02 0.1397E+02 0.2156E-02
0.1340E+02 0.1416E+02 0.1414E+02 0.2684E-05
0.1342E+02 0.1453E+02 0.1428E+02 0.2972E-03
0.1344E+02 0.1441E+02 0.1451E+02 0.4850E-04
0.1346E+02 0.1496E+02 0.1471E+02 0.2940E-03
0.1347E+02 0.1515E+02 0.1486E+02 0.3497E-03
0.1350E+02 0.1546E+02 0.1534E+02 0.5393E-04
0.1354E+02 0.1601E+02 0.1606E+02 0.1053E-04
0.1355E+02 0.1645E+02 0.1636E+02 0.2930E-04
0.1356E+02 0.1632E+02 0.1654E+02 0.1778E-03
0.1360E+02 0.1700E+02 0.1711E+02 0.3924E-04
0.1361E+02 0.1694E+02 0.1738E+02 0.6779E-03
0.1364E+02 0.1731E+02 0.1794E+02 0.1295E-02
0.1365E+02 0.1927E+02 0.1811E+02 0.3613E-02
0.1366E+02 0.1775E+02 0.1830E+02 0.9782E-03
0.1367E+02 0.1855E+02 0.1839E+02 0.7657E-04
0.1368E+02 0.1873E+02 0.1856E+02 0.9055E-04
0.1370E+02 0.2000E+02 0.1894E+02 0.2806E-02
0.1371E+02 0.1836E+02 0.1907E+02 0.1493E-02
0.1373E+02 0.1886E+02 0.1940E+02 0.8254E-03
0.1374E+02 0.1972E+02 0.1966E+02 0.1016E-04
0.1376E+02 0.1991E+02 0.1999E+02 0.1521E-04
0.1378E+02 0.1960E+02 0.2034E+02 0.1413E-02
0.1381E+02 0.2077E+02 0.2068E+02 0.2052E-04
0.1383E+02 0.2133E+02 0.2116E+02 0.6616E-04
0.1384E+02 0.1951E+02 0.2133E+02 0.8720E-02
0.1387E+02 0.2244E+02 0.2203E+02 0.3411E-03
0.1388E+02 0.2263E+02 0.2215E+02 0.4480E-03
0.1389E+02 0.2288E+02 0.2240E+02 0.4275E-03

0.1390E+02	0.2129E+02	0.2273E+02	0.4547E-02
0.1390E+02	0.2355E+02	0.2284E+02	0.8914E-03
0.1392E+02	0.2385E+02	0.2347E+02	0.2514E-03
0.1393E+02	0.2519E+02	0.2383E+02	0.2935E-02
0.1399E+02	0.2641E+02	0.2641E+02	0.6063E-07
0.1400E+02	0.2641E+02	0.2698E+02	0.4735E-03
0.1403E+02	0.2732E+02	0.2861E+02	0.2240E-02
0.1405E+02	0.2988E+02	0.3035E+02	0.2507E-03
0.1405E+02	0.2529E+02	0.3049E+02	0.4224E-01
0.1407E+02	0.3121E+02	0.3143E+02	0.4867E-04
0.1409E+02	0.3310E+02	0.3329E+02	0.3107E-04
0.1410E+02	0.3401E+02	0.3396E+02	0.2217E-05
0.1412E+02	0.3462E+02	0.3491E+02	0.6976E-04
0.1412E+02	0.3523E+02	0.3521E+02	0.4744E-06
0.1413E+02	0.3645E+02	0.3581E+02	0.3060E-03
0.1414E+02	0.3675E+02	0.3630E+02	0.1503E-03
0.1416E+02	0.3669E+02	0.3693E+02	0.4153E-04
0.1416E+02	0.3657E+02	0.3710E+02	0.2146E-03
0.1418E+02	0.3730E+02	0.3757E+02	0.5406E-04
0.1419E+02	0.3736E+02	0.3779E+02	0.1322E-03
0.1420E+02	0.3791E+02	0.3801E+02	0.7591E-05
0.1421E+02	0.3839E+02	0.3806E+02	0.7567E-04
0.1422E+02	0.3821E+02	0.3814E+02	0.3799E-05
0.1423E+02	0.3833E+02	0.3814E+02	0.2629E-04
0.1426E+02	0.3852E+02	0.3803E+02	0.1579E-03
0.1426E+02	0.3949E+02	0.3802E+02	0.1377E-02
0.1426E+02	0.3888E+02	0.3799E+02	0.5266E-03
0.1429E+02	0.3772E+02	0.3768E+02	0.1298E-05
0.1429E+02	0.3754E+02	0.3767E+02	0.1127E-04
0.1429E+02	0.3827E+02	0.3761E+02	0.2984E-03
0.1432E+02	0.3687E+02	0.3722E+02	0.8778E-04
0.1433E+02	0.3764E+02	0.3693E+02	0.3521E-03
0.1434E+02	0.3596E+02	0.3686E+02	0.6312E-03
0.1435E+02	0.3626E+02	0.3669E+02	0.1391E-03
0.1436E+02	0.3639E+02	0.3644E+02	0.2180E-05
0.1437E+02	0.3651E+02	0.3628E+02	0.4050E-04
0.1440E+02	0.3614E+02	0.3588E+02	0.5355E-04
0.1442E+02	0.3602E+02	0.3556E+02	0.1654E-03
0.1443E+02	0.3596E+02	0.3544E+02	0.2066E-03
0.1444E+02	0.3590E+02	0.3540E+02	0.1951E-03
0.1445E+02	0.3590E+02	0.3529E+02	0.2875E-03
0.1446E+02	0.3499E+02	0.3525E+02	0.5548E-04
0.1448E+02	0.3517E+02	0.3526E+02	0.6067E-05
0.1449E+02	0.3529E+02	0.3532E+02	0.6216E-06
0.1451E+02	0.3547E+02	0.3543E+02	0.1504E-05
0.1453E+02	0.2872E+02	0.3588E+02	0.6217E-01
0.1454E+02	0.3669E+02	0.3614E+02	0.2236E-03
0.1455E+02	0.3669E+02	0.3643E+02	0.4995E-04
0.1456E+02	0.3748E+02	0.3656E+02	0.5978E-03

0.1456E+02 0.3724E+02 0.3646E+02 0.4310E-03
0.1456E+02 0.3657E+02 0.3642E+02 0.1598E-04
0.1457E+02 0.3499E+02 0.3596E+02 0.7665E-03
0.1457E+02 0.3499E+02 0.3555E+02 0.2605E-03
0.1458E+02 0.3395E+02 0.3292E+02 0.9190E-03
0.1458E+02 0.3389E+02 0.3261E+02 0.1437E-02
0.1458E+02 0.3097E+02 0.3228E+02 0.1797E-02
0.1459E+02 0.3231E+02 0.3129E+02 0.1002E-02
0.1459E+02 0.3207E+02 0.3095E+02 0.1207E-02
0.1459E+02 0.3042E+02 0.3062E+02 0.4158E-04
0.1459E+02 0.3030E+02 0.3129E+02 0.1057E-02
0.1459E+02 0.2945E+02 0.2965E+02 0.4604E-04
0.1459E+02 0.2896E+02 0.2934E+02 0.1713E-03
0.1460E+02 0.2720E+02 0.2712E+02 0.7835E-05
0.1460E+02 0.2708E+02 0.2694E+02 0.2430E-04
0.1460E+02 0.2695E+02 0.2678E+02 0.4292E-04
0.1462E+02 0.2568E+02 0.2561E+02 0.6546E-05
0.1463E+02 0.2501E+02 0.2545E+02 0.3121E-03
0.1463E+02 0.2464E+02 0.2545E+02 0.1078E-02
0.1464E+02 0.2501E+02 0.2560E+02 0.5547E-03
0.1464E+02 0.2513E+02 0.2561E+02 0.3663E-03
0.1465E+02 0.2525E+02 0.2563E+02 0.2194E-03
0.1466E+02 0.2568E+02 0.2580E+02 0.2318E-04
0.1468E+02 0.2604E+02 0.2600E+02 0.2933E-05
0.1468E+02 0.2586E+02 0.2603E+02 0.4124E-04
0.1470E+02 0.2635E+02 0.2608E+02 0.1062E-03
0.1471E+02 0.2623E+02 0.2608E+02 0.2961E-04
0.1473E+02 0.2531E+02 0.2604E+02 0.8382E-03
0.1477E+02 0.2550E+02 0.2585E+02 0.1913E-03
0.1479E+02 0.2574E+02 0.2571E+02 0.1454E-05
0.1482E+02 0.2562E+02 0.2549E+02 0.2528E-04
0.1484E+02 0.2429E+02 0.2537E+02 0.1976E-02
0.1486E+02 0.2489E+02 0.2522E+02 0.1818E-03
0.1488E+02 0.2537E+02 0.2505E+02 0.1665E-03
0.1493E+02 0.2531E+02 0.2479E+02 0.4196E-03
0.1496E+02 0.2489E+02 0.2474E+02 0.3276E-04
0.1497E+02 0.2476E+02 0.2474E+02 0.8346E-06
0.1499E+02 0.2476E+02 0.2480E+02 0.1992E-05
0.1500E+02 0.2543E+02 0.2482E+02 0.5790E-03
0.1505E+02 0.2556E+02 0.2519E+02 0.2084E-03
0.1506E+02 0.2531E+02 0.2529E+02 0.6643E-06
0.1507E+02 0.2537E+02 0.2545E+02 0.8756E-05
0.1514E+02 0.2507E+02 0.2505E+02 0.5595E-06
0.1515E+02 0.2476E+02 0.2481E+02 0.4054E-05
0.1517E+02 0.2379E+02 0.2429E+02 0.4436E-03
0.1523E+02 0.2336E+02 0.2306E+02 0.1723E-03
0.1525E+02 0.2288E+02 0.2264E+02 0.1032E-03
0.1528E+02 0.2207E+02 0.2229E+02 0.9694E-04
0.1530E+02 0.2176E+02 0.2217E+02 0.3575E-03

0.1532E+02	0.2164E+02	0.2204E+02	0.3493E-03
0.1534E+02	0.2201E+02	0.2199E+02	0.5484E-06
0.1537E+02	0.2220E+02	0.2199E+02	0.8544E-04
0.1539E+02	0.2183E+02	0.2200E+02	0.6794E-04
0.1541E+02	0.2207E+02	0.2206E+02	0.4564E-06
0.1549E+02	0.2238E+02	0.2224E+02	0.3831E-04
0.1550E+02	0.2226E+02	0.2224E+02	0.3903E-06
0.1555E+02	0.2232E+02	0.2207E+02	0.1206E-03
0.1556E+02	0.2263E+02	0.2204E+02	0.6782E-03
0.1556E+02	0.2282E+02	0.2200E+02	0.1274E-02
0.1561E+02	0.2115E+02	0.2138E+02	0.1214E-03
0.1564E+02	0.2090E+02	0.2100E+02	0.2426E-04
0.1566E+02	0.1972E+02	0.2058E+02	0.1892E-02
0.1566E+02	0.2077E+02	0.2044E+02	0.2519E-03
0.1568E+02	0.1997E+02	0.1996E+02	0.4618E-06
0.1570E+02	0.1929E+02	0.1940E+02	0.3109E-04
0.1571E+02	0.1941E+02	0.1926E+02	0.6416E-04
0.1573E+02	0.1855E+02	0.1854E+02	0.4619E-06
0.1575E+02	0.1799E+02	0.1790E+02	0.2582E-04
0.1577E+02	0.1793E+02	0.1728E+02	0.1309E-02
0.1580E+02	0.1589E+02	0.1647E+02	0.1315E-02
0.1581E+02	0.1502E+02	0.1600E+02	0.4178E-02
0.1583E+02	0.1620E+02	0.1565E+02	0.1145E-02
0.1583E+02	0.1608E+02	0.1549E+02	0.1302E-02
0.1585E+02	0.1527E+02	0.1503E+02	0.2513E-03
0.1586E+02	0.1490E+02	0.1472E+02	0.1430E-03
0.1587E+02	0.1478E+02	0.1424E+02	0.1333E-02
0.1590E+02	0.1342E+02	0.1350E+02	0.3621E-04
0.1590E+02	0.1403E+02	0.1347E+02	0.1628E-02
0.1592E+02	0.1335E+02	0.1290E+02	0.1169E-02
0.1593E+02	0.1199E+02	0.1249E+02	0.1673E-02
0.1594E+02	0.1206E+02	0.1219E+02	0.1281E-03
0.1594E+02	0.1193E+02	0.1217E+02	0.3821E-03
0.1599E+02	0.1120E+02	0.1109E+02	0.1146E-03
0.1601E+02	0.1079E+02	0.1068E+02	0.1004E-03
0.1601E+02	0.1067E+02	0.1059E+02	0.5739E-04
0.1602E+02	0.9967E+01	0.1042E+02	0.2103E-02
0.1603E+02	0.1009E+02	0.1035E+02	0.6693E-03
0.1605E+02	0.1026E+02	0.1006E+02	0.3687E-03
0.1611E+02	0.9613E+01	0.9602E+01	0.1216E-05
0.1616E+02	0.9377E+01	0.9225E+01	0.2611E-03
0.1619E+02	0.8787E+01	0.8903E+01	0.1755E-03
0.1621E+02	0.8610E+01	0.8600E+01	0.1418E-05
0.1635E+02	0.6428E+01	0.6729E+01	0.2195E-02
0.1642E+02	0.6428E+01	0.5990E+01	0.4636E-02
0.1643E+02	0.6133E+01	0.5891E+01	0.1555E-02
0.1646E+02	0.5662E+01	0.5652E+01	0.3170E-05
0.1648E+02	0.4954E+01	0.5450E+01	0.1002E-01
0.1654E+02	0.5367E+01	0.5122E+01	0.2081E-02

0.1654E+02 0.5308E+01 0.5103E+01 0.1491E-02
0.1654E+02 0.5072E+01 0.5099E+01 0.2921E-04
0.1658E+02 0.4777E+01 0.5026E+01 0.2718E-02
0.1661E+02 0.5072E+01 0.5063E+01 0.3098E-05
0.1664E+02 0.5956E+01 0.5186E+01 0.1672E-01
0.1673E+02 0.6428E+01 0.6480E+01 0.6461E-04
0.1676E+02 0.7195E+01 0.7186E+01 0.1717E-05
0.1676E+02 0.7549E+01 0.7310E+01 0.1002E-02
0.1681E+02 0.8433E+01 0.8424E+01 0.1133E-05
0.1682E+02 0.8787E+01 0.8636E+01 0.2942E-03
0.1686E+02 0.9672E+01 0.9366E+01 0.1002E-02
0.1692E+02 0.9731E+01 0.9781E+01 0.2652E-04
0.1695E+02 0.1020E+02 0.9956E+01 0.5882E-03
0.1700E+02 0.1026E+02 0.1025E+02 0.1275E-05
0.1705E+02 0.1115E+02 0.1091E+02 0.4483E-03
0.1706E+02 0.1156E+02 0.1120E+02 0.9747E-03
0.1709E+02 0.1193E+02 0.1186E+02 0.3406E-04
0.1712E+02 0.1280E+02 0.1256E+02 0.3457E-03
0.1712E+02 0.1249E+02 0.1271E+02 0.3035E-03
0.1714E+02 0.1329E+02 0.1317E+02 0.8651E-04
0.1717E+02 0.1422E+02 0.1422E+02 0.8266E-07
0.1719E+02 0.1515E+02 0.1519E+02 0.7087E-05
0.1721E+02 0.1577E+02 0.1577E+02 0.2644E-08
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0.1726E+02 0.1694E+02 0.1776E+02 0.2338E-02
0.1728E+02 0.1799E+02 0.1830E+02 0.2905E-03
0.1729E+02 0.1898E+02 0.1880E+02 0.8730E-04
0.1730E+02 0.1725E+02 0.1896E+02 0.9862E-02
0.1737E+02 0.2077E+02 0.2058E+02 0.9175E-04
0.1737E+02 0.2022E+02 0.2063E+02 0.4180E-03
0.1738E+02 0.2152E+02 0.2064E+02 0.1651E-02
0.1738E+02 0.2040E+02 0.2068E+02 0.1841E-03
0.1741E+02 0.2195E+02 0.2081E+02 0.2712E-02
0.1744E+02 0.1997E+02 0.2065E+02 0.1147E-02
0.1745E+02 0.2071E+02 0.2060E+02 0.3142E-04
0.1745E+02 0.2059E+02 0.2059E+02 0.3731E-07
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0.1759E+02 0.1805E+02 0.1713E+02 0.2595E-02
0.1761E+02 0.1669E+02 0.1669E+02 0.1406E-06

0.1764E+02	0.1540E+02	0.1591E+02	0.1132E-02
0.1765E+02	0.1533E+02	0.1547E+02	0.7971E-04
0.1767E+02	0.1465E+02	0.1500E+02	0.5707E-03
0.1770E+02	0.1416E+02	0.1415E+02	0.3763E-06
0.1774E+02	0.1298E+02	0.1305E+02	0.2219E-04
0.1775E+02	0.1403E+02	0.1276E+02	0.8227E-02
0.1775E+02	0.1237E+02	0.1274E+02	0.8978E-03
0.1775E+02	0.1366E+02	0.1264E+02	0.5669E-02
0.1777E+02	0.1305E+02	0.1226E+02	0.3610E-02

ARRAY OF THE PARAMETERS OF THE COMPLEX POLES

Alpha	beta	eps	gamma
-0.15276E+00	-0.81923E-01	0.12421E+02	0.14801E+00
-0.41012E+01	-0.16335E+01	0.13239E+02	0.36213E+00
0.26474E+01	0.31273E+00	0.14104E+02	0.20771E+00
-0.37955E+02	0.12507E+03	0.14398E+02	0.19992E+01
-0.30542E+00	0.12936E-02	0.14586E+02	0.31132E-01
-0.29144E-01	0.44305E-01	0.15117E+02	0.11167E+00
0.64939E+00	0.10995E+01	0.15577E+02	0.33878E+00
0.25084E+00	-0.89264E-02	0.16085E+02	0.14515E+00
0.69836E+00	0.12934E+00	0.16806E+02	0.18784E+00
0.35075E+01	0.19425E+01	0.17332E+02	0.34055E+00

ARRAY OF PARAMETERS FOR REAL POLES

0.35327959E-01	0.13286579E+02
-0.10707276E-01	0.13279679E+02
0.44542331E-02	0.14527621E+02
-0.43941737E-02	0.12625935E+02
-0.20437736E-02	0.13838897E+02
0.10664312E-02	0.14053205E+02
-0.56931316E-03	0.17120467E+02
-0.19723617E-03	0.17749156E+02

SUPPORTING ARGUMENTS AND ORDINATES

0.17697001E+02	0.14158995E+02
0.13554000E+02	0.16445997E+02
0.17610001E+02	0.16694008E+02
0.13990000E+02	0.26406979E+02
0.12577000E+02	0.23851982E+02
0.16107000E+02	0.96129951E+01
0.12149000E+02	0.22937992E+02

0.12345000E+02	0.22195999E+02
0.12567000E+02	0.23668989E+02
0.13251000E+02	0.14653069E+02
0.12629000E+02	0.23061230E+02
0.12438000E+02	0.21530996E+02
0.12907000E+02	0.24642998E+02
0.13000000E+02	0.23000000E+02
0.17122999E+02	0.12489003E+02
0.17749001E+02	0.14034471E+02
0.13497000E+02	0.15457000E+02
0.13313000E+02	0.15210063E+02
0.13277000E+02	0.15026544E+02
0.15144000E+02	0.25068790E+02
0.12624000E+02	0.26705616E+02
0.13744000E+02	0.19722994E+02
0.13805000E+02	0.20773989E+02
0.13241000E+02	0.15024042E+02
0.13840000E+02	0.19512005E+02
0.14051000E+02	0.29875992E+02
0.14122000E+02	0.35229916E+02
0.14485000E+02	0.35168934E+02
0.17209999E+02	0.15765914E+02
0.14602000E+02	0.27197845E+02
0.14562000E+02	0.36568989E+02
0.14546000E+02	0.36689919E+02
0.14617000E+02	0.25677032E+02
0.14536000E+02	0.36689976E+02
0.14679000E+02	0.26041979E+02
0.15503000E+02	0.22258205E+02
0.14791000E+02	0.25737860E+02
0.15056000E+02	0.25311668E+02
0.14969000E+02	0.24764946E+02
0.15682000E+02	0.19969175E+02
0.15344000E+02	0.22010393E+02
0.15410000E+02	0.22073080E+02
0.15733000E+02	0.18547813E+02
0.17447001E+02	0.20590218E+02
0.14053000E+02	0.25290003E+02
0.16457001E+02	0.56615281E+01
0.17750000E+02	0.12507689E+02
0.16995001E+02	0.10262373E+02
0.16212999E+02	0.86099720E+01
0.16756001E+02	0.71950665E+01
0.16806999E+02	0.84336576E+01
0.17118000E+02	0.12798077E+02
0.17169001E+02	0.14219495E+02
0.13333000E+02	0.14591017E+02
0.14527000E+02	0.28720371E+02
0.16608999E+02	0.50724936E+01

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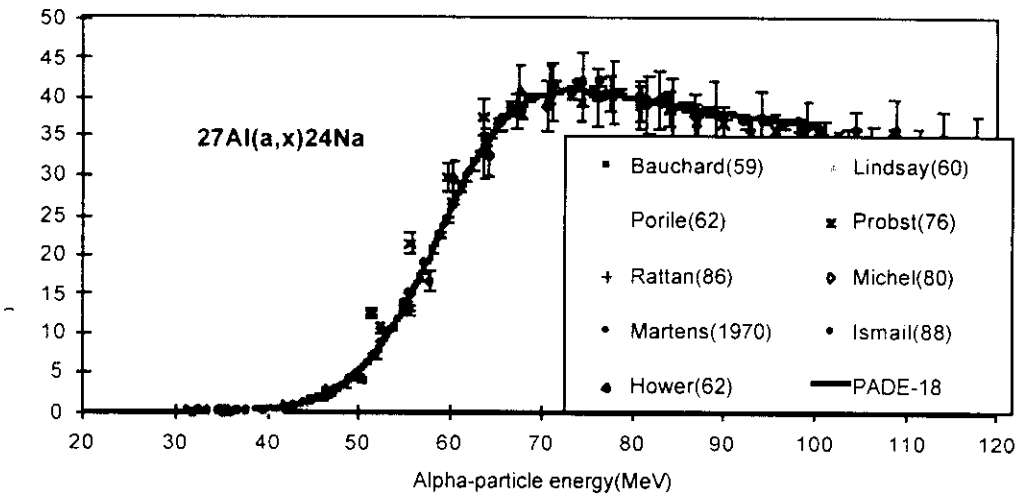
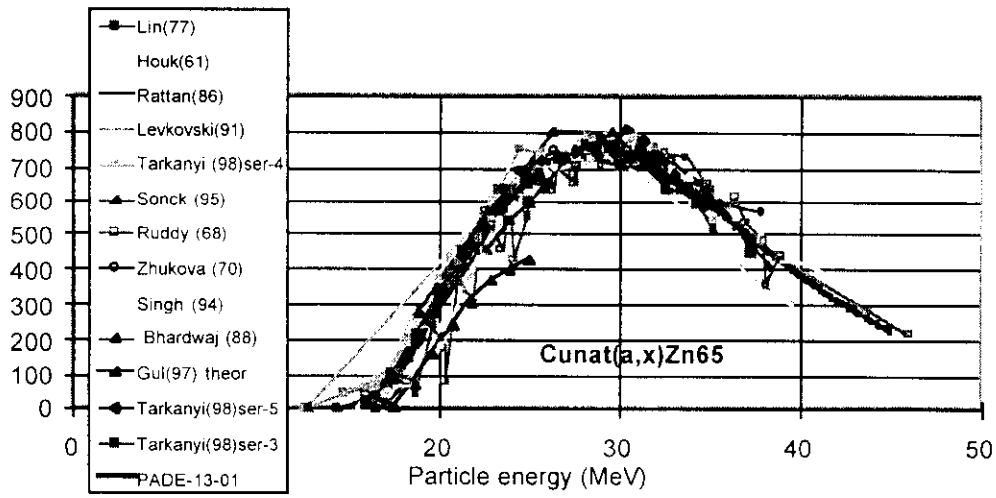
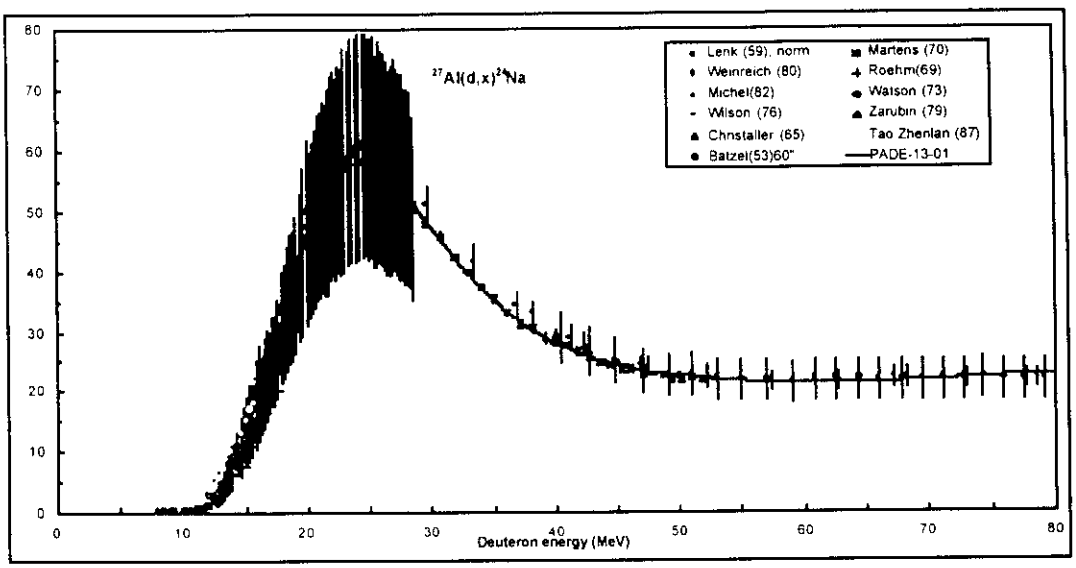
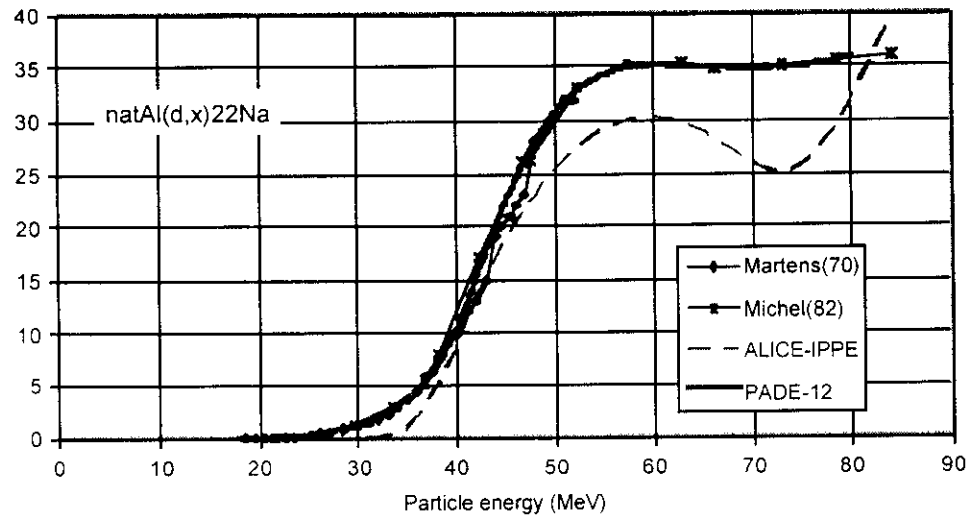
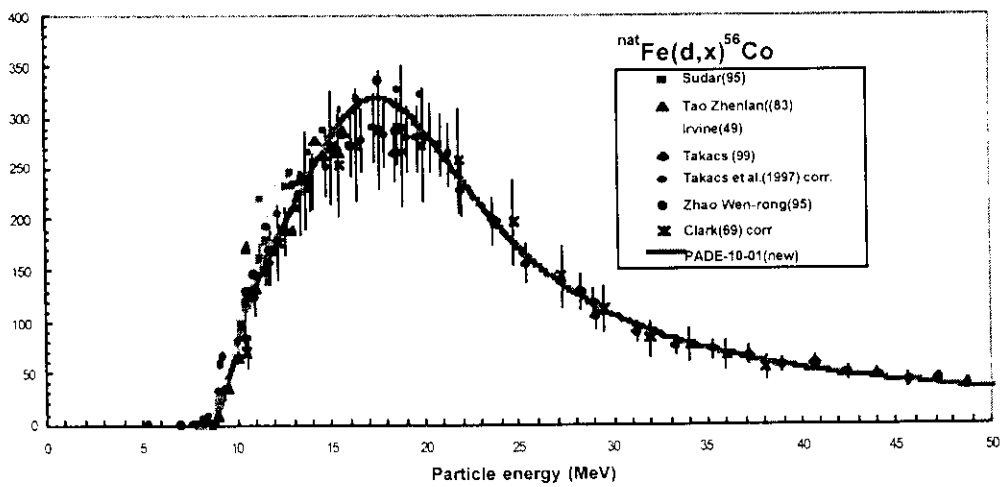
EXAMPLES OF EVALUATIONS USING STATISTICAL OPTIMISATION WITH PADE APPROXIMATION METHOD TOGETHER WITH MODEL CALCULTIONS.

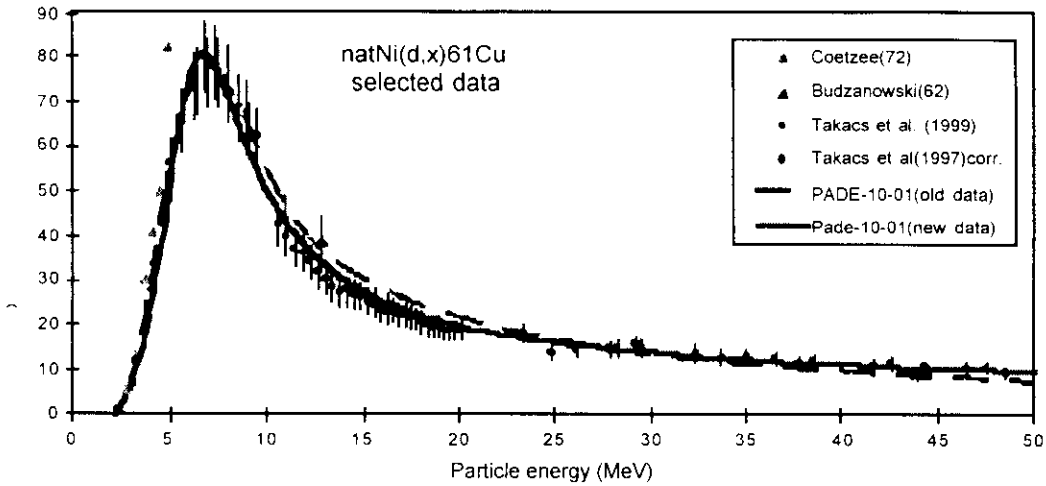


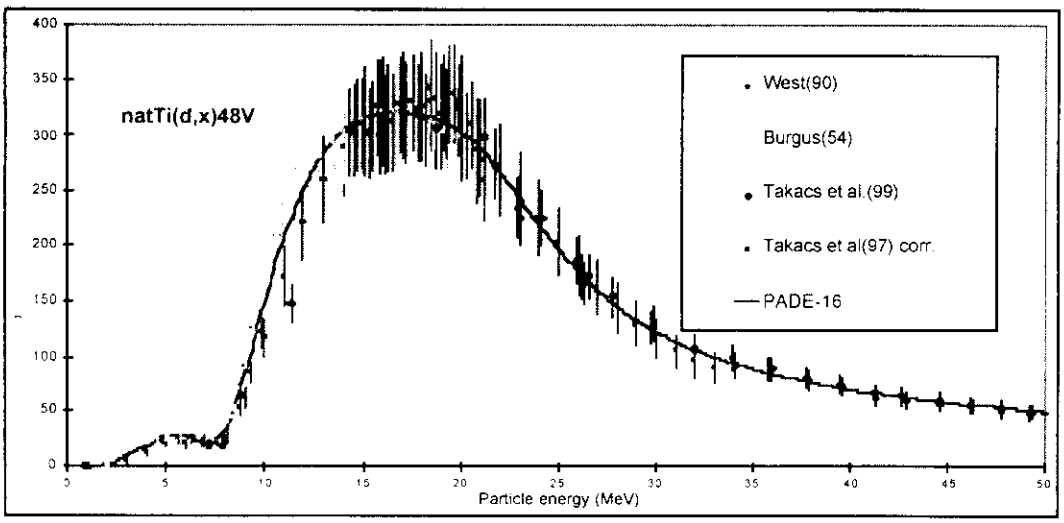


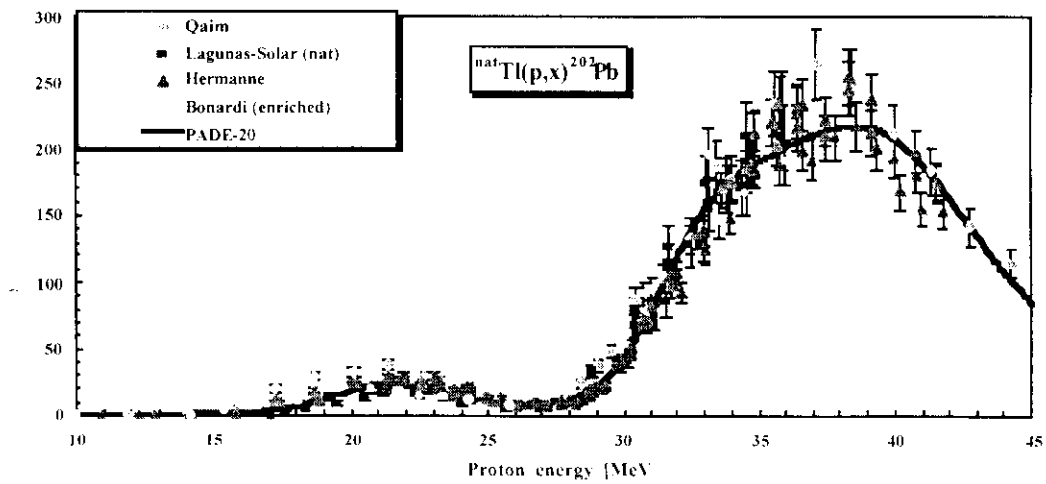

^{27}Al(d,x)^{24}Na
Lenk (59), norm
Weinreich (80)
Michel(82)
Wilson (76)
Chnstaller (65)
Batzel(53)60"
Martens (70)
Roehm(69)
Watson (73)
Zarubin (79)
Tao Zhenlan (87)
PADE-13-01
Deuteron energy (MeV)

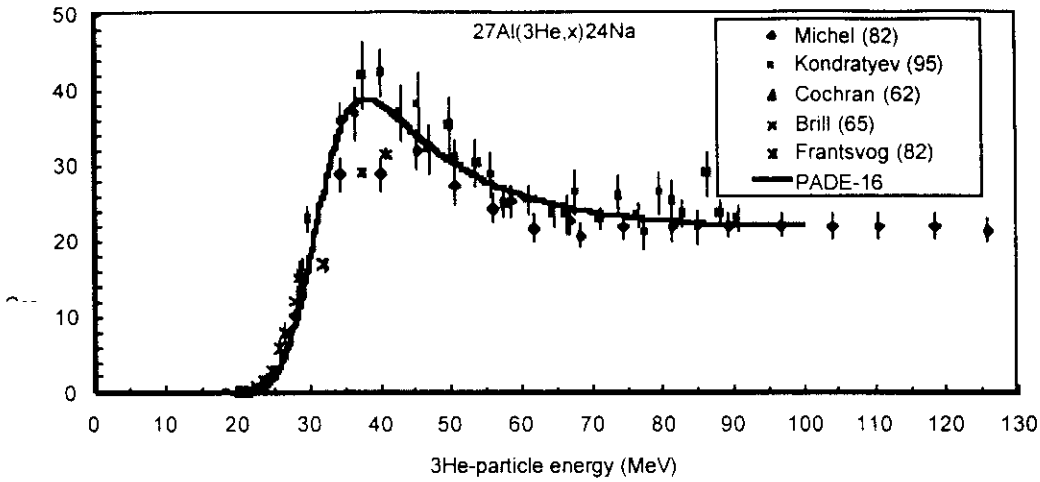

natAl(d,x)22Na
Martens(70)
Michel(82)
ALICE-IPPE
PADE-12
Particle energy (MeV)

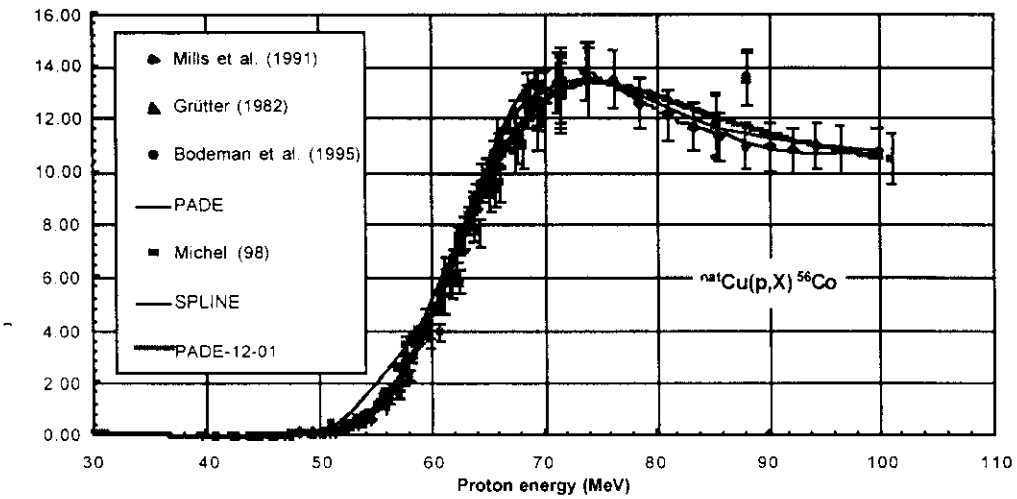

^{nat}Fe(d,x)^{56}Co
Sudar(95)
Tao Zhenlan((83)
Irvine(49)
Takacs (99)
Takacs et al.(1997) corr.
Zhao Wen-rong(95)
Clark(69) corr
PADE-10-01(new)
Particle energy (MeV)

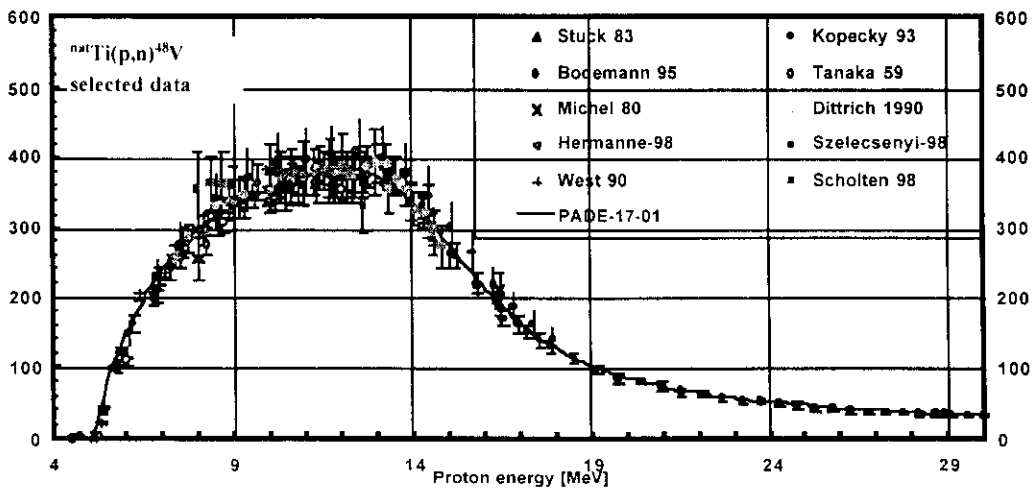

natNi(d,x)61Cu
selected data
Coetzee(72)
Budzanowski(62)
Takacs et al. (1999)
Takacs et al(1997)corr.
PADE-10-01(old data)
Pade-10-01(new data)
Particle energy (MeV)

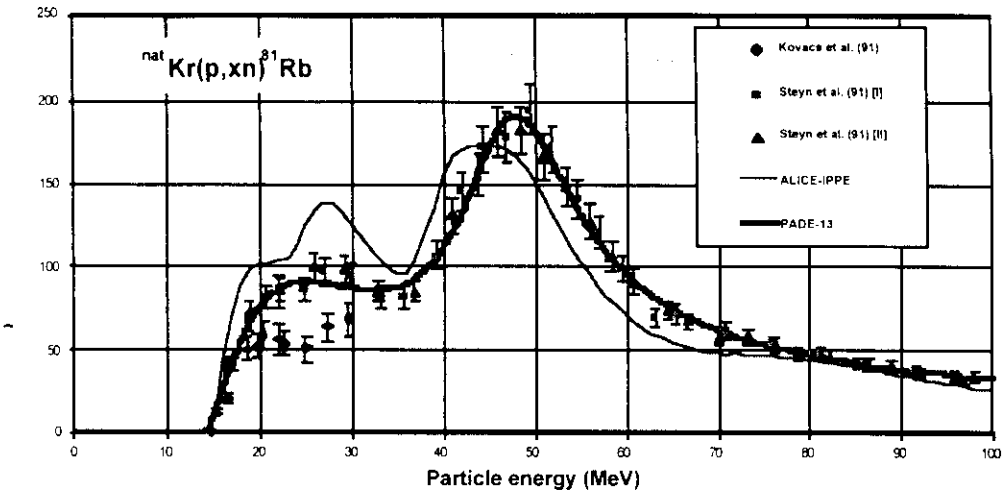

natTi(d,x)48V
West(90)
Burgus(54)
Takacs et al.(99)
Takacs et al(97) corr.
PADE-16
Particle energy (MeV)

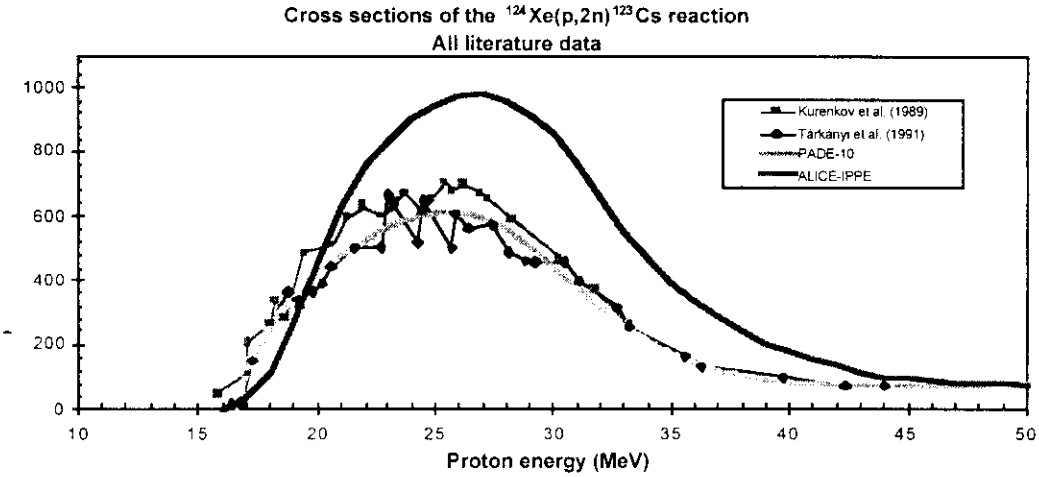

Qaim
Lagunas-Solar (nat)
Hermanne
Bonardi (enriched)
PADE-20
$^{nat}Tl(p,x)^{202}Pb$
Proton energy [MeV]

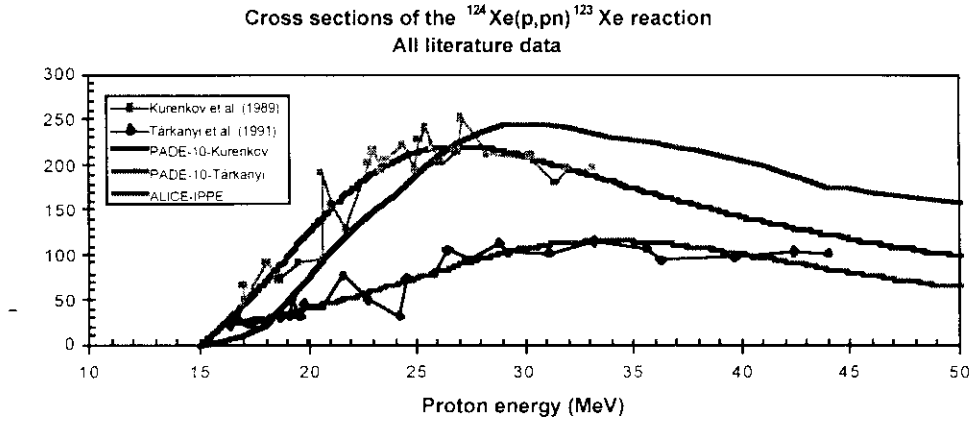

27Al(3He,x)24Na
Michel (82)
Kondratyev (95)
Cochran (62)
Brill (65)
Frantsvog (82)
PADE-16
3He-particle energy (MeV)

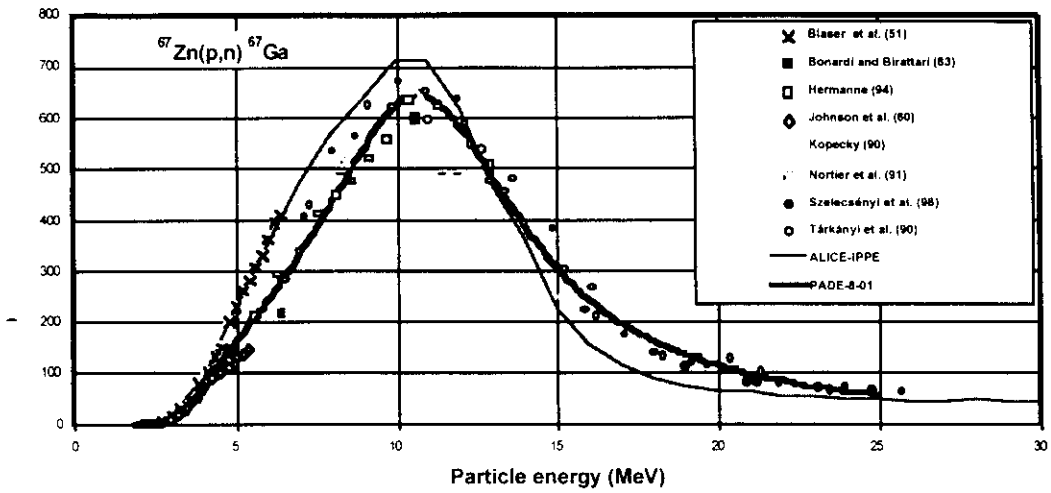

Mills et al. (1991)
Grütter (1982)
Bodeman et al. (1995)
PADE
Michel (98)
SPLINE
PADE-12-01
natCu(p,X)56Co
Proton energy (MeV)

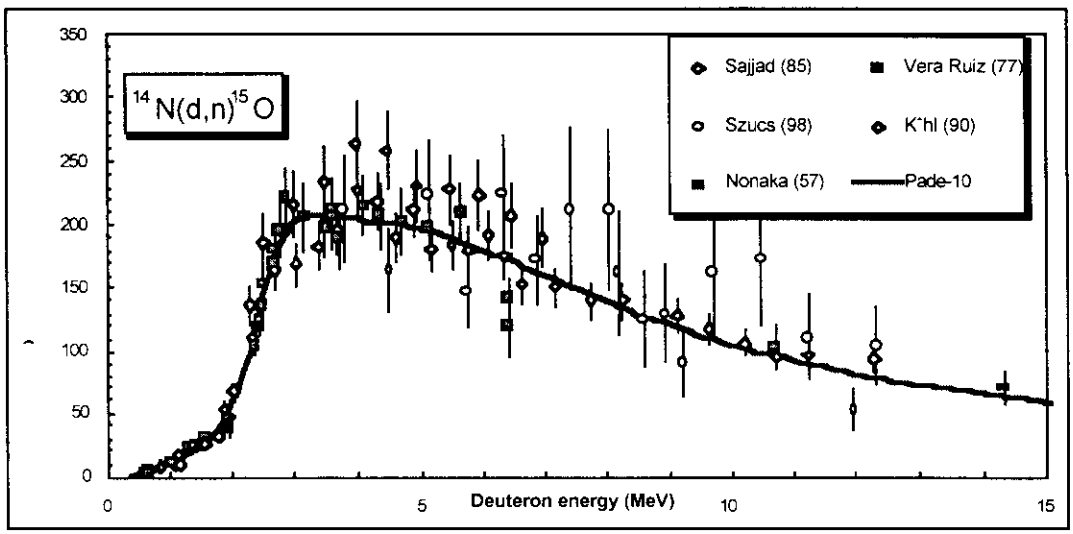

natTi(p,n)48V
selected data
Stuck 83
Bodemann 95
Michel 80
Hermanne-98
West 90
PADE-17-01
Kopecky 93
Tanaka 59
Dittrich 1990
Szelecsenyi-98
Scholten 98
Proton energy [MeV]

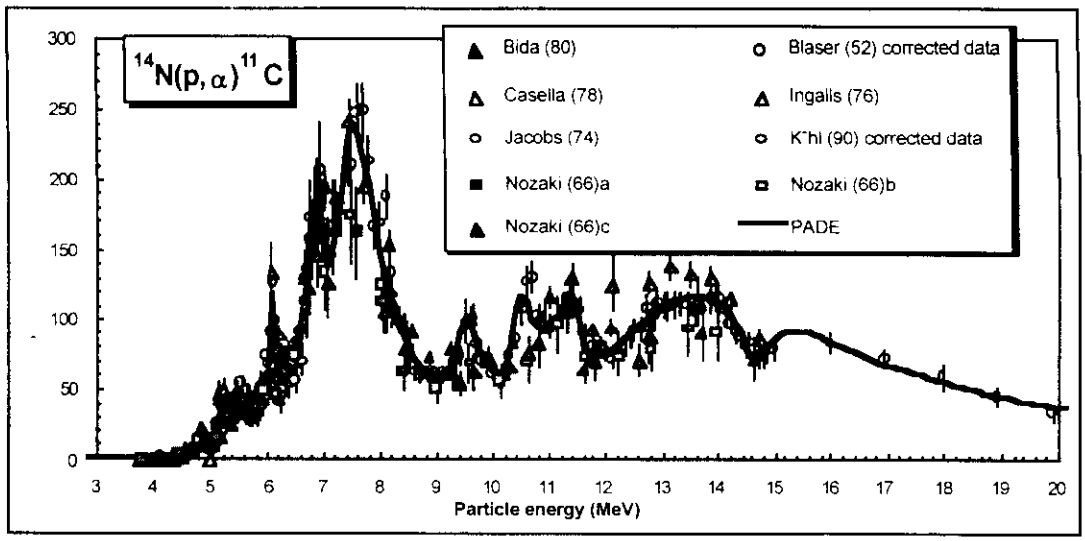

$^{nat}Kr(p,xn)^{81}Rb$
Kovacs et al. (91)
Steyn et al. (91) [I]
Steyn et al. (91) [II]
ALICE-IPPE
PADE-13
Particle energy (MeV)

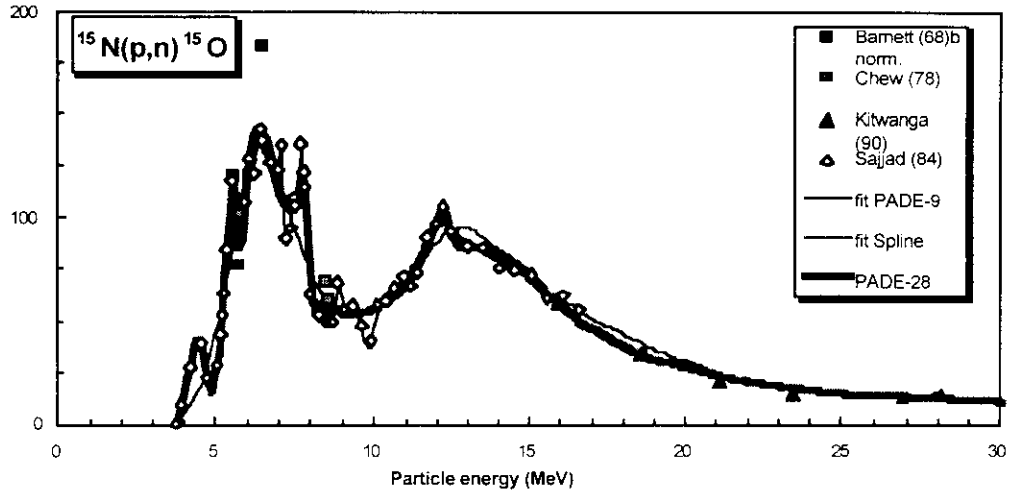

Cross sections of the $^{124}Xe(p,2n)^{123}Cs$ reaction
All literature data
Kurenkov et al. (1989)
Tárkányi et al. (1991)
PADE-10
ALICE-IPPE
Proton energy (MeV)

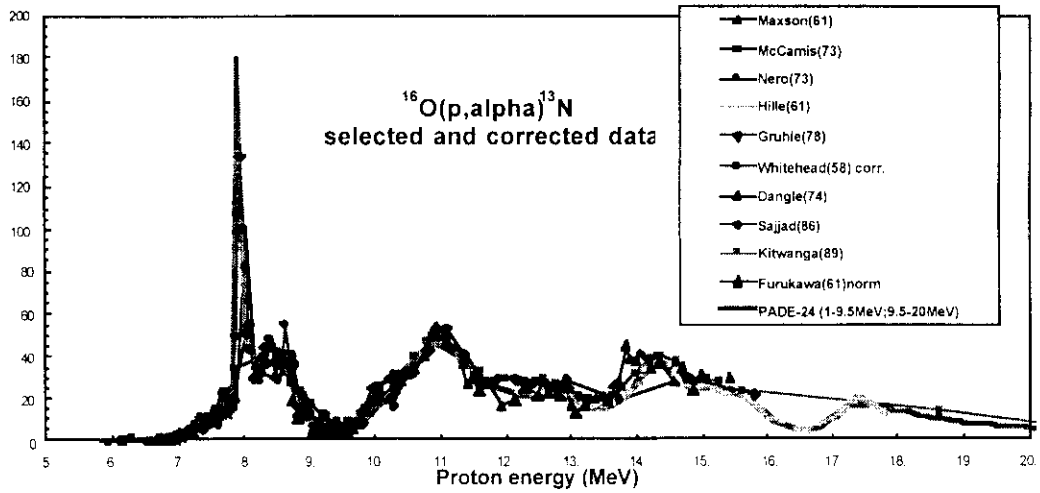

Cross sections of the $^{124}Xe(p,pn)^{123}Xe$ reaction
All literature data
Kurenkov et al. (1989)
Tárkányi et al. (1991)
PADE-10-Kurenkov
PADE-10-Tárkányi
ALICE-IPPE
Proton energy (MeV)

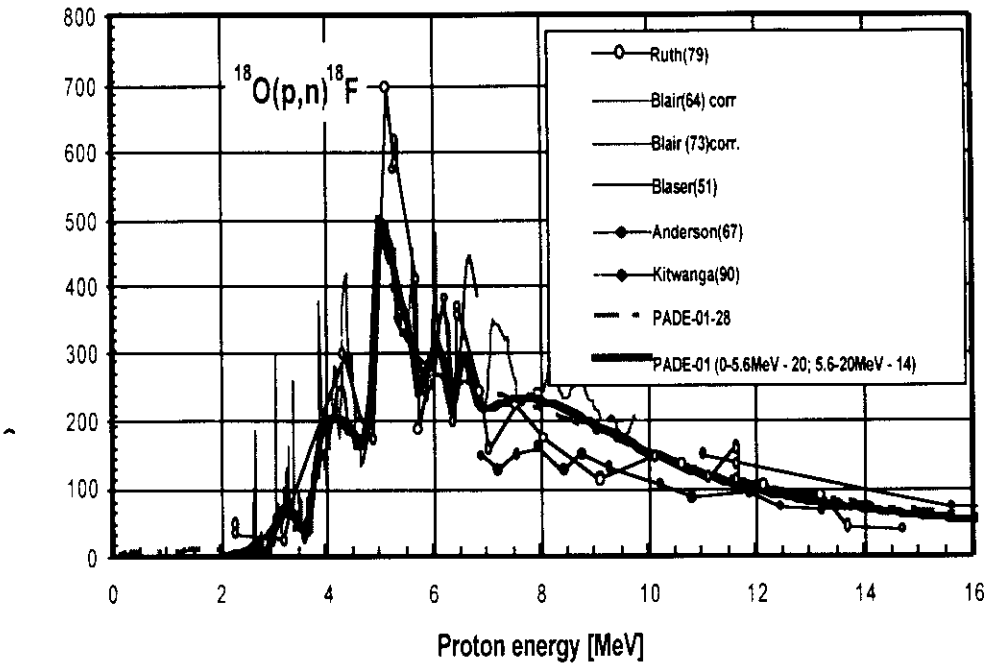

^{67}Zn(p,n) ^{67}Ga
Blaser et al. (51)
Bonardi and Birattari (83)
Hermanne (94)
Johnson et al. (60)
Kopecky (90)
Nortier et al. (91)
Szelecsényi et al. (98)
Tárkányi et al. (90)
ALICE-IPPE
PADE-8-01
Particle energy (MeV)


^{14}N(d,n)^{15}O
Sajjad (85)
Vera Ruiz (77)
Szucs (98)
K˙hl (90)
Nonaka (57)
Pade-10
Deuteron energy (MeV)


$^{14}N(p,\alpha)^{11}C$
Bida (80)
Blaser (52) corrected data
Casella (78)
Ingalis (76)
Jacobs (74)
K˜hl (90) corrected data
Nozaki (66)a
Nozaki (66)b
Nozaki (66)c
PADE
Particle energy (MeV)


$^{15}N(p,n)^{15}O$
Barnett (68)b norm.
Chew (78)
Kitwanga (90)
Sajjad (84)
fit PADE-9
fit Spline
PADE-28
Particle energy (MeV)


$^{16}O(p,alpha)^{13}N$
selected and corrected data
Maxson(61)
McCamis(73)
Nero(73)
Hille(61)
Gruhle(78)
Whitehead(58) corr.
Dangle(74)
Sajjad(86)
Kitwanga(89)
Furukawa(61)norm
PADE-24 (1-9.5MeV;9.5-20MeV)
Proton energy (MeV)


$^{18}O(p,n)^{18}F$
Ruth(79)
Blair(64) corr
Blair (73)corr.
Blaser(51)
Anderson(67)
Kitwanga(90)
PADE-01-28
PADE-01 (0-5.6MeV - 20; 5.6-20MeV - 14)
800
700
600
500
400
300
200
100
0
0
2
4
6
8
10
12
14
16
Proton energy [MeV]