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FINAL REPORT ON RESEARCH CONTRACT 5472/RB

# ANALYSIS OF EXPERIMENTAL DATA ON NEUTRON-INDUCED REACTIONS AND DEVELOPMENT OF CODE PCROSS FOR THE CALCULATION OF DIFFERENTIAL PRE-EQUILIBRIUM EMISSION SPECTRA WITH MODELLING OF LEVEL DENSITY FUNCTION

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(Translated by the IAEA)

March 1991

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## Abstract

A new PC code PCROSS for neutron induced reaction calculations up to 25 MeV incident energy was developed, where the latest theoretical development in the preequilibrium model was employed.

For the proper description of the high energy tail of the emission spectra and excitation function calculations a combination of the Exciton model and direct reaction parametrization was used.

In the PCROSS code several models for level density calculations are available.

The code is user-friendly, as it included a subroutine to generate the input data.

In the present paper some calculation results for (n,n') and (n,p) emission spectra and for (n,p) and (n,2n) excitation functions up to 20 MEV have been shown. A good description of the experimental data was achieved.



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# ANALYSIS OF EXPERIMENTAL DATA ON NEUTRON-INDUCED REACTIONS AND DEVELOPMENT OF CODE PCROSS FOR THE CALCULATION OF DIFFERENTIAL PRE-EQUILIBRIUM EMISSION SPECTRA WITH MODELLING OF LEVEL DENSITY FUNCTION

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## I. INTRODUCTION

This report covers the period from 15.12.88 to 30.2.90, during which active work was carried out to fulfil the following objectives of the contract:

- Analysis of experimental data on excitation functions and particle and gamma-ray emission spectra for comparison with the theoretical results;
- Development of a code using the statistical pre-equilibrium model for calculation of cross-sections and emission spectra of particles and gamma-rays in neutron-induced reactions;
- Variation of the models used for level density and comparison with experiment;
- Calculations of emission spectra and excitation functions and comparison with experiment for fission and fusion reactor structural materials.

In Section II of the report we describe the theoretical formalism used in the code and in Section III we discuss the results obtained in describing emission spectra and excitation functions. Section IV contains the conclusions.

## II. DESCRIPTION OF THE WORK PERFORMED

1. We compiled experimental data on emission spectra [(n,n'), (n,p), (n,$\alpha$), (n,$\gamma$) and (p,n)] and excitation functions [(n,p), (n,$\alpha$), and (n,2n)] in nucleon-induced reactions using as the index for search the last

volume of CINDA [1], the "Handbook on Nuclear Activation Data" [2] and also the results of a compilation made by a Dresden Technical University team made available to us by Dr. H.H. Kalka [3]. It should be pointed out that we also used the EXFOR experimental data obtained by computerized search from magnetic tapes supplied by the IAEA. This enabled us to keep ourselves abreast of the latest data collected and validated by the Agency.

2. We developed a code which permits the use of the Weisskopf-Ewing evaporation model or the exciton model to calculate the (n,n'), (n,p), (n,$\alpha$) and (n,$\gamma$) emission spectra and the (n,p), (n,$\alpha$) and (n,2n) excitation functions in reactions induced by neutrons of up to 25 MeV. The code also included consideration of the direct excitation of low excitation energy levels in the calculation of (n,n') inelastic scattering spectra. Below we describe the theoretical formalism employed.

2.1. The Exciton Model

The PCROSS code uses a unified model based on the solution of the master equation [4] in the form proposed by Cline [5] and Ribansky [6]. Integrating the master equation over time, we can write:

$$-q(n,t=0) = \lambda^{+}(E,n+2)\tau(n+2) + \lambda^{-}(E,n-2)\tau(n-2) - [\lambda^{+}(E,n) + \lambda^{-}(E,n) + W_{t}(E,n)]\,\tau(n) \qquad (1)$$

where the usual notations are employed, q(n,t=0) is the initial condition of the process and E the excitation energy of the compound nucleus.

In order to solve the system of algebraic equations (1), we use the algorithm proposed by Akkermans, Gruppelaar and Reffo [7], which gives an accurate result for any initial condition of the problem. The use of master equation (1), which includes both the probabilities of transition to equilibrium $\lambda^{+}(E,n)$ and the probabilities of return to less complex states $\lambda^{-}(E,n)$, enables us to calculate in a unified manner the pre-equilibrium and equilibrium emission spectrum in accordance with:

$$\frac{d\sigma_{ab}}{d\epsilon_{b}}(\epsilon_{b}) = \sigma^{r}_{ab}(E_{inc})\; D_{ab}(E_{inc}) \sum_{n} W_{b}(E,n,\epsilon_{b})\,\tau(n) \qquad (2)$$

where $\sigma^{r}_{ab}(E_{inc})$ is the cross-section of reaction (a,b);

$W_b(E,n,\varepsilon_b)$ is the probability of emission of a particle of type b with energy $\varepsilon_b$ from a state with n excitons and excitation energy E of the compound nucleus;

$\tau(n)$ is the solution of the master equation which represents the time during which the system remains in a state characterized by n excitons; and

$D_{ab}(E_{inc})$ is a coefficient which takes into account the decrease in the available cross-section due to particle emission by direct interactions with low excitation energy levels of the target nucleus; $D_{ab}(E_{inc}) = 1 - \sigma^{dir}_{ab}/\sigma^{r}_{ab}$, $\sigma^{dir}_{ab}$ being the cross-section of direct interaction of the incident particle with the target nucleus (see 2.2).

### 2.1.1. Particle-hole state densities

The equidistant spacing model has been used extensively to derive formulae for partial state densities employed in the pre-equilibrium models. Several authors have obtained formulae in which the Pauli principle is either not considered [8, 9] or considered in an approximate manner by means of statistical methods [10] or the theory of numbers [11]. The PCROSS code at present uses the Williams formula [10], where the Pauli correction is calculated in accordance with Kalbach [12]. Moreover, the pairing corrections of Fu [13] or Kalbach [14] may be used optionally. In its simplest form, the partial state density can be written as

$$\omega(p,h,E)=g\,\frac{[g(E-D)-A_{ph}]^{p+h-1}}{p!\,h!\,(p+h-1)!} \qquad (3)$$

where g is the single-particle level density parameter, D the pairing parameter and Pauli correction $A_{ph}$ [12] is equal to

$$A_{ph}= 1/4\ [p(p-1) + h(h-1)] \qquad (4)$$

Under this research contract we carried out a more detailed study of the formulations of particle-hole densities which are used in calculations by pre-equilibrium models. Recently Zhang [15] proposed a new formulation for $\omega(p,h,E)$ in the equidistant spacing model and obtained new values of the Pauli correction. Applying the Darwin-Fowler method, our team derived an accurate formula for particle-hole densities and for correction for the Pauli principle.[*] On the basis of the results of Ref. [16] we can write the particle-hole state density in the form:

$$\omega(p,h,E)= \sum_{k=0}^{n-1} \binom{n-1}{k} G_{p,h}(k) \left[E-E_{Pauli}(p,h)\right]^{n-k-1} \qquad (5)$$

where coefficients $G_{p,h}(k)$ are tabulated in Ref. [16] and the Pauli energy is defined as: $E_{Pauli}(p,h) = (p^2+h^2)/2$ A method was proposed for consideration in this new formulation of the pairing correction in the form suggested by Kalbach [14]. It was also demonstrated that our results were more accurate than those obtained by Zhang [15] since the latter following approximation was used in the latter paper for calculation of the track in the exciton model

$$Tr\{\exp(-J\beta\mu/g)\}=\frac{1}{2 \times sh[\beta J/(2g)]} \approx \frac{g}{\beta J} \qquad (6)$$

At present we are working on implementation of the accurate formulation obtained in PCROSS since we have only the analytical partial densities for $p,h \leq 5$. One of the immediate tasks of our team is to study the impact of this new formulation on nuclear data calculations.

For calculation of the partial state densities it is necessary to know parameters g and D, which are obtained from the description of the existing level density data with a formula given by the total state density. The literature contains several compilations of these parameters [17-19]. We

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[*] It has been published in Zeitschrift für Physik A - Atomic Nuclei 334 (1989) 397-402.

recommend that preferably the set of parameters obtained in Ref. [19] be used since it guarantees consistency between the equilibrium and pre-equilibrium calculations, which is given by the following condition

$$\sum_{p} \omega(p,h,E) = \frac{1}{\sqrt{48}} \frac{\exp[2\sqrt{a(E-D)}]}{E - D} \qquad (7)$$

It should be pointed out that by using parameters g and D from Ref. [19] we can avoid renormalization of particle-hole densities suggested by Akkermans and Gruppelaar [20] and thus simplify the calculation algorithm. However, the accuracy of the systematization obtained in Ref. [19] for the values of the pairing parameter is not good so that in some cases it is unavoidable to re-adjust the value of D for an appropriate description of the experimental data on emission spectra and excitation functions.

For incident energies above 30 MeV it is necessary in the particle-hole density calculation to consider corrections for the depth of potential well $V_R$, as was pointed out in Ref. [21]. In the PCROSS code one can use the corrections for potential well depth formulated by Betak and Dobes [22] or else the simplified expression obtained by Kalbach [12, 23]. In the latter case, the particle-hole density can be written in the following form:

$$\omega(p,h,E,V)=\omega(p,h,E)f(p) \qquad (8)$$

$$f(p) = \sum_{j=0}^{h} (-1)^j \binom{h}{j} \left(\frac{E - jV}{E}\right) \theta(E - jV)$$

2.1.2. Internal transition rates

As has been shown in numerous papers (for example, [24]), there is a strong dependence of the calculated emission spectra on the parameter of matrix element K if the parametrizations proposed by Kalbach [25, 26] are used in the calculations of internal transition rates $\lambda^i (i = +,-)$ and it is sought to achieve a good ajustment of the theoretical calculations to the experimental spectra. In order to avoid such a strong dependence, we preferred to use the parametrization of transition rate proposed by

Blann [27], which is based on existing experimental data on nucleon scattering and considers the Pauli principle in an approximate way. Using this parametrization and considering the particle-hole state densities from the Williams formula [10], we can obtain for internal transition rates the expressions found by Machner [28]:

$$\lambda^{+}(E,n)=\frac{1}{k_{mfp}}\left(1.4\times10^{21}\ E'-\frac{2}{n+1}\ 6\times10^{18}\ E'^{2}\right)$$
$$\lambda^{-}(E,n)=\frac{1}{k_{mfp}}\frac{(n-1)(n-2)ph}{(gE')^{2}}\left(1.4\times10^{21}E'-\frac{2}{n-1}6\times10^{18}E'^{2}\right) \qquad (9)$$

The PCROSS code takes into account an additional factor 3/8 multiplying the right-hand side of (9), which was introduced by Gupta [29] in deriving the expressions for calculation by the exciton model from its bicomponent formulation, and includes approximate consideration of the Pauli principle by replacing E' by E-[p(p+1) + h(h+1)]/4 in $\lambda^{+}$ and by E-[p(p-1) + h(h-1)]4 in $\lambda^{-}$ [15].

If in deriving the internal transition rates $\lambda^{+}(E,n)$, $\lambda^{-}(E,n)$ the Williams formula [10] is replaced by the accurate formulation for the particle-hole state densities [16] (see formula (5)), the following expressions [30] can be obtained

$$\lambda^{+}(E,n)=\frac{1}{k_{mfp}}\frac{1.4\times10^{21}}{\omega(p,h,E)}\sum_{k=0}^{n-1}\binom{n-2}{k}G_{p-1,h}(k)\left\{\frac{[E-E_{p}(p-1,h)]}{(n-k-1)\ (n-k)}-\right.$$
$$\left.-\frac{[-E_{p}(p-1,h)]^{n-k-1}}{(n-k-1)}\times\left[-\frac{E_{p}(p-1,h)}{(n-k)}+E\right]\right\}+\left\{\begin{array}{c}\text{interchange term}\\ p\Leftrightarrow h\end{array}\right\} \qquad (10)$$

$$\lambda^{-}(E,n)=\frac{1}{k_{mfp}}\frac{1.4\times10^{21}}{\omega(p,h,E)}\sum_{k=0}^{n-4}\binom{n-4}{k}G_{p-2,h-1}(k)\left\{\frac{[E-E_{p}(p-2,h-1)]}{(n-k-3)\ (n-k-2)}-\right.$$
$$\left.-\frac{[-E_{p}(p-2,h-1)]^{n-k-2}}{(n-k-3)}\times\left[-\frac{E_{p}(p-2,h-1)}{(n-k-2)}+E\right]\right\}+\left\{\begin{array}{c}\text{interchange term}\\ p\Leftrightarrow h\end{array}\right\} \qquad (11)$$

With these expressions it is sufficient to calculate the Pauli energy and to replace coefficients $G_{p,h}(k)$ by their numerical values [16] in order

to obtain the values of internal transition rates. It should be noted that the use of Blann's parametrization [27] for internal transition rate calculation involves the introduction of the parameter of mean free path $k_{mfp}$ so called because its value determines the mean free path of the nucleon in the nuclear matter. As was pointed out by Blann [27], this parameter allows an increase in m.f.p, with simulation of effects which are not considered in the calculations, such as conservation of parity and angular momentum in intranuclear transitions. As the direct excitations of levels of a collective nature are considered in the present version of PCROSS, the hard part of the emission spectrum can be described satisfactorily with a global value of $k_{mfp} = 1.3$, which is smaller than that reported earlier [31]. This value corresponds to that expected for the mean free path of nucleons in nuclear matter from independent experimental data and indicates a solution to the extensively discussed problem of mean free path in the exciton model. This value cannot be obtained for $k_{mfp}$ if, firstly, the direct interaction is not considered and, secondly, no consistency is achieved between the equilibrium and pre-equilibrium calculations. Both conditions are guaranteed in the present work.

2.1.3. Probabilities of nucleon emission

For the probability of nucleon emission the method used is that of Kalbach and Cline [4, 5, 23], who obtained the expressions for emission probability applying the principle of detailed balance in a way similar to that in the evaporation model. The probability of emission $W_b(E,n,\varepsilon_b)$ of a nucleon b with energy $\varepsilon_b$ from a state with n excitons is given by:

$$W_b(E,n,\varepsilon_b)=\frac{2s_b+1}{\pi^2\hbar^3}\,\mu_b\varepsilon_b\sigma_b^{inv}(\varepsilon_b)\,\frac{\omega(p-b,h,U)}{\omega(p,h,E)}\,Q_b(p,h) \qquad (12)$$

where E is the energy of excitation of the compound nucleus, U that of the residual nucleus and $\sigma_b^{inv}(\varepsilon_b)$ the inverse channel reaction cross-section.

Factor $Q_b(p,h)$ which takes into account the difference between neutrons and protons can be used in the Kalbach form [23] or as proposed by Gupta [29]. In both cases it is guaranteed that if $n > n_{eq}$ then $Q_b(p,h) \equiv 1$. Moreover, both factors are equal if the quantity of neutrons in the compound nucleus is equal to that of protons. The results obtained show that the relative importance of using factor Q increases with the mass number and that it is decisive in the case of medium and heavy nuclei, where the neutron-proton difference is appreciable.

2.1.4. Probability of alpha particle emission

For consideration of alpha emission within the framework of the exciton model there are two possibilties:

(a) To use formula (12), taking into account $Q_b(p,h) = 1$ and multiplying the right-hand part of this formula by an empirical factor $\gamma_\alpha$. It is purely a method of adjustment and only permits consideration of the competition of alpha emission in a rough form.

(b) To use the method proposed by Iwamoto and Harada [32], subsequently parametrized and improved in Refs [33-35]. In accordance with it, the probability of alpha particle emission can be expressed as:

$$W_\alpha(E,n,\varepsilon)=\frac{2s+1}{\pi^2\hbar^3}\,\mu\,\varepsilon\,\sigma_\alpha^{inv}(\varepsilon)\,\frac{\sum_{m+l=4} F_{lm}^\alpha(\varepsilon)Q_{lm}^\alpha(p,h)\omega(p-l,h,E)}{\omega(p,h,E)} \qquad (13)$$

where factor $Q_{lm}^\alpha(p,h)$ is a generalization of factor $Q_b(p,h)$ which takes into account the probabilities of the outgoing particle being formed with l particles situated above and m below the Fermi surface [35] and factor $F_{lm}^\alpha(\varepsilon)$ gives the probability of formation of the alpha particle as a function of its energy. The last factor is calculated in PCROSS in accordance with the parametrization obtained by S. Iijima and used in Ref. [36] for calculations by the modified TNG code.

The latest calculations by the IH method show encouraging results although no systematic study has been made of the joint description of the

emission spectra of nucleons and alpha particles. Nor has the influence of factor $Q^{\alpha}_{lm}(p,h)$ on emission spectra been investigated. Studies are in progress to make an exhaustive comparison of calculation with the experimental results on alpha emission for nucleon-induced reactions.

2.1.5. Probability of gamma emission

The probability of emission of gamma radiation is derived in a way similar to $W_b(E,n,\varepsilon_b)$ with the use of the principle of detailed balance [27-39] and can be expressed as:

$$W_\gamma(E,n,\varepsilon) = \frac{1}{\pi^2\hbar^3c^2}\,\varepsilon^2\,\sigma_\gamma^{inv}(\varepsilon)\,\frac{\sum_k b(k\to n,\varepsilon)\omega(p,h,U)}{\omega(p,h,E)} \qquad (14)$$

Coefficients $b(k \to n,\varepsilon)$ are the branching ratios and their expressions were obtained from the paper of Akkermans and Gruppelaar [37], with guaranteed consistency between the equilibrium and the pre-equilibrium gamma emission. The inverse cross-section of reaction $\sigma_\gamma^{inv}(\varepsilon)$ in the gamma channel is calculated with consideration of only the contribution of the giant dipolar resonance (GDR) by the model which assumes an energy dependence of the GDR shape. This model was developed by Gardner and co-workers [40-43] and modified in Ref. [44] to achieve a better description of the experimental data on radiative strength functions for nuclei with mass number A between 50 and 90.

2.1.6. Initial and equilibrium number of excitons

Calculations by the exciton model use $n_o = 1$, thus taking into account the direct gamma emission. $n_{eq}$ is taken equal to $\sqrt{1.4}\,gE$, as was suggested in Ref. [15], after the Pauli correction is modified.

2.2. Consideration of the direct reaction mechanism

It is well known that during nucleon scattering in vibrational nuclei there occur processes of direct excitation of low excitation energy levels of the collective type. At the latest specialists' meetings on nuclear data calculation it was pointed out that a correct description of the high-energy

emission spectrum in neutron-induced reactions could be obtained only if the direct processes were taken into account. The experimental evidence in support of this type of mechanism has been confirmed by the latest experiments with the (n,n') reactions with a very good energy resolution [45-47]. In the experimental spectra we can clearly see a structure of peaks corresponding to excitations of the direct type. The parametrization proposed by Kalka, Seeliger and Zhiropistsev [48] was adopted in PCROSS to describe this phenomenon. In accordance with this parametrization, the differential cross-section of neutron emission in the (n,n') reaction by direct interaction can be written as

$$\frac{d\sigma_{ab}^{dir}}{d\varepsilon_b}(\varepsilon_b) = \delta_{ab}\left[\frac{2\mu}{\hbar^2}\right]^2 \frac{\nu}{(k_a R)^2} \frac{k_b}{k_a} P_a(\varepsilon_a)\, P_b(\varepsilon_b)\, V_R^2 \sum_{\lambda=2}^{3} \frac{\beta_\lambda^2}{(2\lambda+1)}\, \delta(U-\omega_\lambda) \qquad (15)$$

where $\nu = \frac{4\pi}{3} R^3$ is the volume of the nucleus, $R = r_o A^{1/3}$; $V_R$ is the potential well depth taken to be equal to 48 MeV; $P_a(\varepsilon_a) = 4k_a K_a/(k_a + K_a)$ is the coefficient of penetrability, $k_a$ and $K_a$ being particle pulses inside and outside the nucleus; $\beta_\lambda, \omega_\lambda$ are the deformation and energy parameters corresponding to target nucleus levels of the collective type. Only the octupolar and quadrupolar oscillations are considered, the values of $\omega_2, \beta_2$ for even nuclei being taken from Ref. [49]. In the case of odd nuclei, on the assumption of a weak bond, the values corresponding to the neighbouring even nucleus are used. The values of $\omega_3$ were taken from Ref. [50], except in some cases where the experimental values were taken directly from Ref. [51]. The octupolar deformation parameters were calculated from

$$\beta_3^2 = (2\lambda + 1)\, \omega_3[\mathrm{MeV}]/1000$$

In order to perform the calculations, we replace function $\delta(U - \omega_\lambda)$, which relates the excitation energy of the residual nucleus to the energy of

the collective state and to emission energy, by a Gaussian whose semi-width is chosen taking into account the experimental energy resolution. As can be seen in (15), the parametrization used assumes the superficial nature of the direct interaction, which is reflected in the factor CUT IN

After calculation of the emission spectrum by the direct mechanism, we calculate the total interaction cross-section $\sigma_{ab}^{dir}(E_{inc})$ and thus we can obtain the attenuation factor $D_{ab}$ needed for the calculation of the emission spectra.

It is interesting to note that, in spite of the highly approximate nature of parametrization (15), the results obtained in the description of the emission spectra are very good, considering that no free parameters but only spectroscopic data are used.

## 2.3. Weisskopf-Ewing evaporation model

In the PCROSS code the evaporation model can be used for comparison or other purposes. All the input parameters in this case are the same as those used for calculations by the exciton model, including binding energies, inverse reaction cross-sections and the pairing and level-density parameters. The reaction cross-sections for channel b can be written as:

$$\sigma_{ab}^{WE} = \sigma_{ab}(E_{inc}) \frac{\Gamma_b}{\sum_{b'} \Gamma_{b'}} \qquad (16)$$

where

$$\Gamma_b = \frac{2s_b + 1}{\pi^2 \hbar^2} \mu_b \int d\varepsilon \, \sigma_b^{inv}(\varepsilon) \, \varepsilon \frac{\omega_1(U)}{\omega_1(E)} \qquad (17)$$

and the total single-particle level density is taken which is equal to

$$\omega_1(E) = \frac{1}{\sqrt{48}} \frac{\exp[2\sqrt{a(E-D)}]}{E - D}; \quad a = \frac{6}{\pi^2} g \qquad (18)$$

## 2.4. Reaction cross-sections

Reaction cross-sections obtained independently by the optical model can be used in the calculations in the PCROSS code. These cross-sections are read from a data file (channels n,p,α). The energy grid used in the calculations

may be irregular so that a small step is recommended to ensure a correct description of the evaporation maximum at low emission energies. If the reaction cross-sections are not introduced, the parametrization of Chatterjee and co-workers [52] are used to calculate the reaction cross-sections for channels n,p,α.

## 2.5. Multiple emission

In accordance with the studies of Akkermans and Gruppelaar [53, 54], up to energies of 50 MeV the pre-equilibrium emission subsequent to the primary emission can be neglected. For this reason, in PCROSS the secondary emission is calculated by the Weisskopf-Ewing evaporation model in all cases.

## 2.6. Input data

An auxiliary program called PDAT was developed in order to generate the input data files needed for PCROSS in an interactive way and with the essential minimum of information on the part of the user who in principle only needs to specify the incident particle, its energy, the target nucleus and the calculation method selected [W.E. or exciton model]. With the use of this program it is also possible to change the different options of calculation of PCROSS code such as:

- Method of calculation of inverse reaction cross-sections: Normally PCROSS uses the parametrization of Chatterjee [52] for inverse cross-section calculations. With PDAT the user can select the option of introducing the reaction cross-sections for channels n,p and α calculated by the optical model through a file;
- Method of calculation of binding energy: PCROSS normally uses the experimental binding energies from Refs [55, 56], which are tabulated in PDAT;
- Methods of calculation of state densities, well correction, pairing correction, parameters g and D used in the calculations, etc.

The annex contains a specimen of PCROSS input data file generated by PDAT and a brief description of the generated file (so that some parameters can be changed directly in the input data file without the need to re-run the PDAT program). At present the input data relating to the parametrization of the direct mechanism are not included in PDAT and should be added subsequently to the file which is being generated.

## III. RESULTS

The PCROSS code was used to study the influence of the different parametrizations of the state density on emission spectra and excitation functions. The best description was obtained with the parameters from Ref. [19] although it is necessary to adjust the value of pairing parameters D which are employed in order to obtain a good description of the experimental results.

The (n,p), (n,2n) excitation functions are especially sensitive to the value of the pairing parameter. After the value of D is adjusted, an appropriate description of the corresponding emission spectra is obtained, demonstrating the consistency of the method.

The adjustment of parameter D is necessary for three reasons:

- PDAT uses a systematization for calculation of D which may have deviations of up to 50% [19];
- The values of D reported in Ref. [19] were obtained by adjusting the total single-particle level density to the experimental data; however, the greatest deviations between experimental data and calculations occurred precisely at low excitation energies where the value of parameter D is of greater importance;
- The exciton model uses the partial state densities so that it would be necessary to obtain the values of D directly by using the sum of the partial densities and not the total level densities (see formula (7)), a point which no one has realized so far.

Bearing the above in mind, we performed calculations of the (n,p) and (n,2n) excitation functions in the $^{56}Fe$, $^{59}Co$, $^{54}Fe$ and $^{115}In$ nuclei, adjusting the pairing parameters of the corresponding residual nuclei. Thereafter we calculated the (n,n'), (n,p), (n,$\alpha$) and (n,$\gamma$) emission spectra for the above nuclei with the parameters obtained for incident neutron energies between 5 and 25 MeV. Calculations were also made for Ni, Cu and Cr isotopes. We compared the calculations with the experimental results on nucleon emission. The results obtained are very good for the description of the (n,n') spectra. In the case of the (n,p) spectra the description is acceptable although for heavier nuclei it can be improved. The (n,$\alpha$) and (n,$\gamma$) spectra were not compared with experimental measurements.

## CONCLUSIONS

We compared different sets of level density parameters reported in the literature, and found that a better description of experimental data was achieved with g and D taken from Ref. [19]. We generated a small experimental database which can be used for checking the calculation code developed.

The (n,p) and (n,2n) excitation functions were calculated for an energy range of up to 25 MeV, and a satisfactory description of experimental data was obtained with the simultaneous use of the exciton model and a parametrization of the direct reactions, a slight adjustment being made of pairing parameters D of the corresponding residual nuclei.

The (n,n'), (n,p), (n,$\alpha$) and (n,$\gamma$) emission spectra were also calculated. These were compared with the experimental data for the nucleon emission channels, and a good description was obtained. It is important to take the direct contribution into account for a correct description of the (n,n') channel for high emission energies.

We hope to continue the work so as to include in the code the accurate formulation of the particle-hole state densities and internal transition rates. Moreover, we have to make a systematic study of alpha emission,

comparing it with the existing experimental data [57-62], and also calculate the (n,α) excitation function. Lastly, it is necessary to include the pre-equilibrium effects in the secondary emission in order to be able to make reliable caclulations up to 100 MeV incident energy, and to compare them with the experimental results on emission spectra for charged-particle-induced reactions, of which a large number of measurements have been made recently [63-67].

ACKNOWLEDGMENT

The development of the PCROSS code was begun on the basis PREEQ of Betak [68] and PREANG of Gruppelaar and Akkermans [69].

## FIGURES

Fig. 1. The (n,n') emission spectra in cobalt. The experimental data were taken from Ref. [70].

Fig. 2. The (n,n') and (n,p) emission spectra in chromium. The experimental data were taken from Refs [71, 72] for the neutron channel and from Ref. [58] for the proton channel. In the neutron channel the contribution of the odd isotopes of chromium was taken into account.

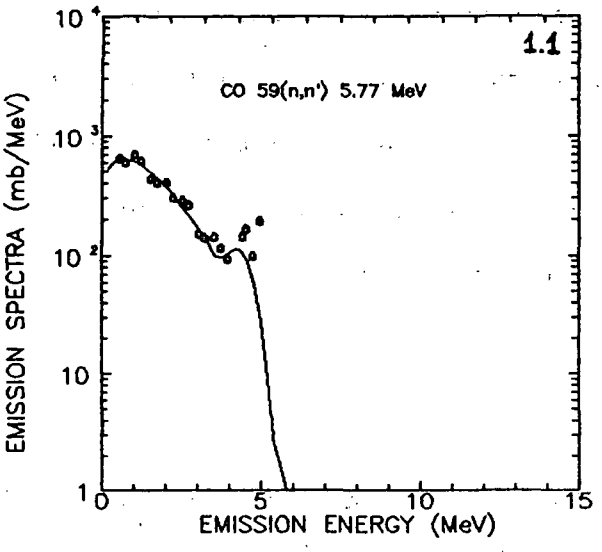
Fig. 3. The (n,n') and (n,p) emission spectra in copper. The experimental data were taken from Refs [71, 72] for the neutron channel and from Ref. [62] for the proton channel. In the neutron channel the contribution of the $^{63}Cu$ and $^{65}Cu$ nuclei was taken into account.

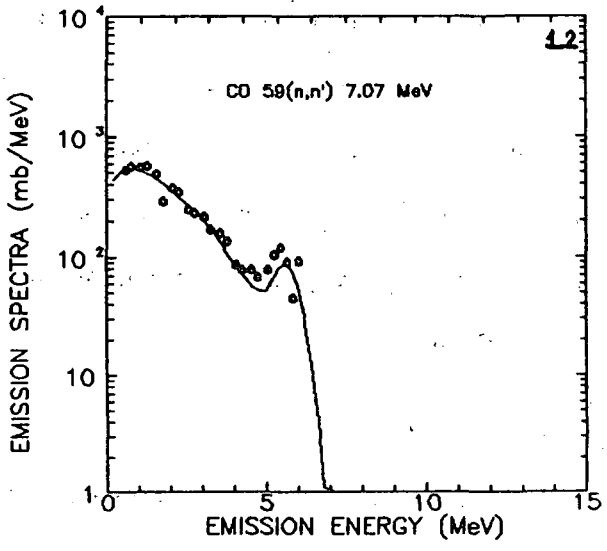
Fig. 4. The (n,n') and (n,p) emission spectra in iron. The experimental data were taken from Refs [71-73] for the neutron channel and from Ref. [58] for the proton channel.

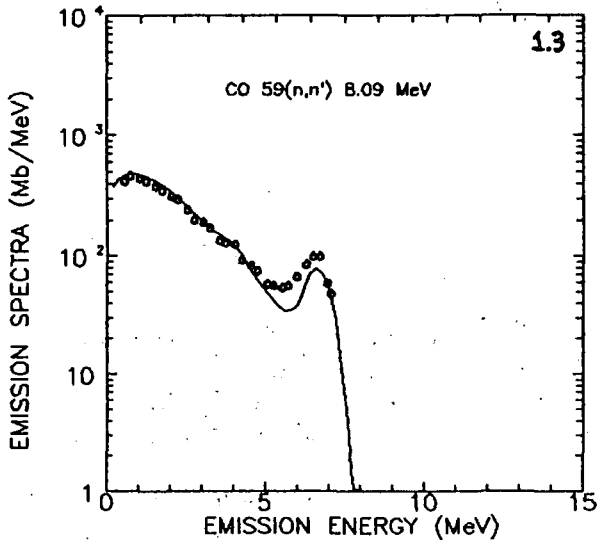
Fig. 5. The (n,n') and (n,p) emission spectra for indium. The experimental data were taken from Refs [70, 74] for the neutron channel and from Ref. [75] for the proton channel. In Fig. 5.4 the dotted line shows the contribution of the direct cross-section to the emission spectrum for 14 MeV incident neutron energy.

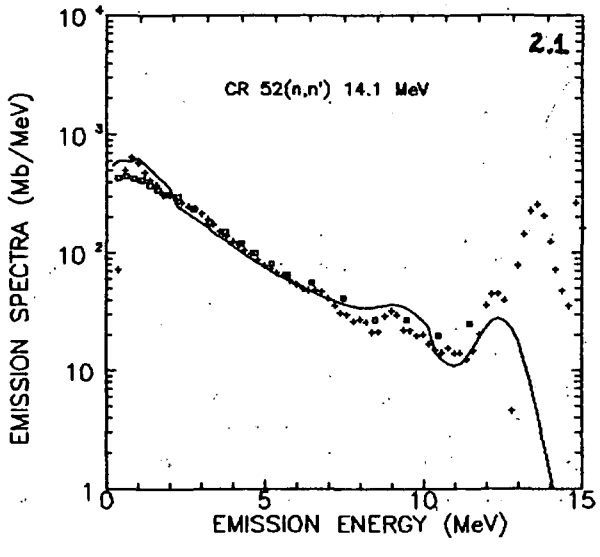
Fig. 6. The (n,n') and (n,p) emission spectra in niobium. The experimental data were taken from Refs [72, 76, 77] for the neutron channel and from Ref. [78] for the proton channel. Figure 6.5 shows the contribution of the direct cross-section to the emission spectrum for 25.7 MeV incident neutron energy.

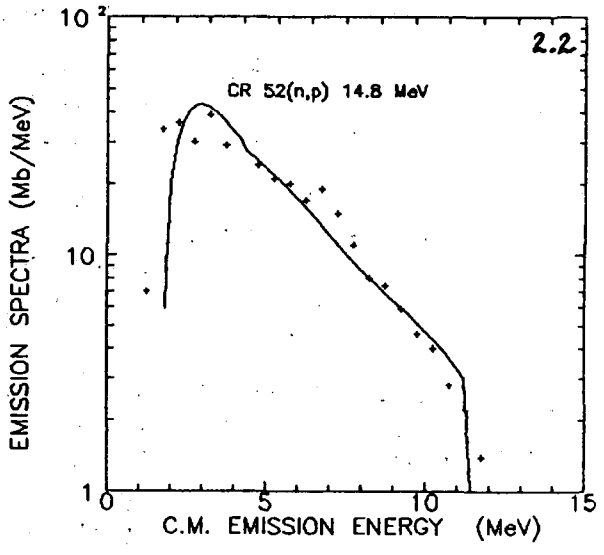
Fig. 7. The (n,p) and (n,2n) excitation functions calculated from the threshold to 20 MeV for the $^{54}Fe$, $^{56}Fe$ and $^{59}Co$ nuclei. The experimental data were taken from Refs [79-83] for the (n,p) reaction and from Refs [2, 84-86] for the (n,2n) reaction.

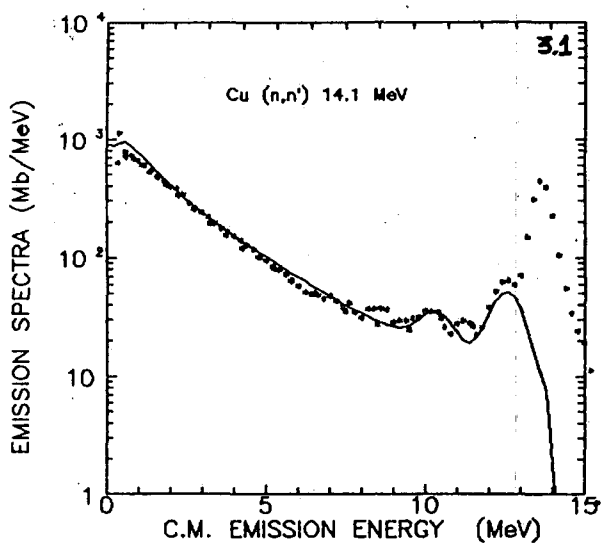

1.1
CO 59(n,n') 5.77 MeV
EMISSION SPECTRA (mb/MeV)
EMISSION ENERGY (MeV)

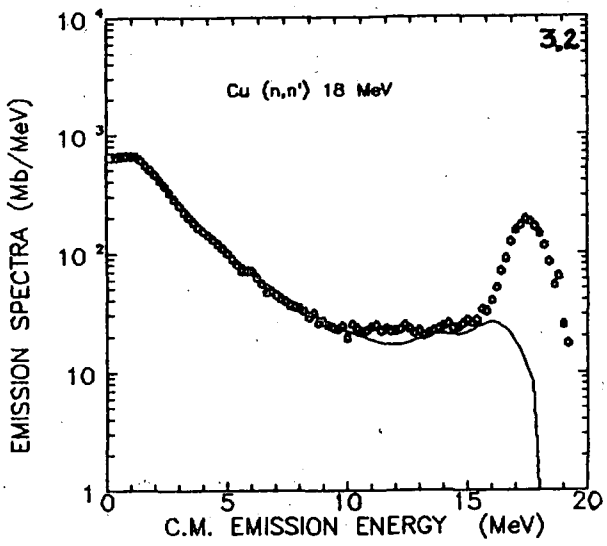

1.2
CO 59(n,n') 7.07 MeV
EMISSION SPECTRA (mb/MeV)
EMISSION ENERGY (MeV)

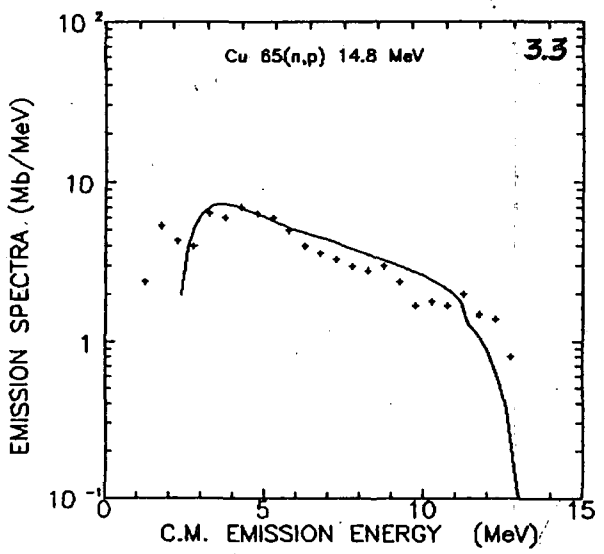

1.3
CO 59(n,n') 8.09 MeV
EMISSION SPECTRA (Mb/MeV)
EMISSION ENERGY (MeV)

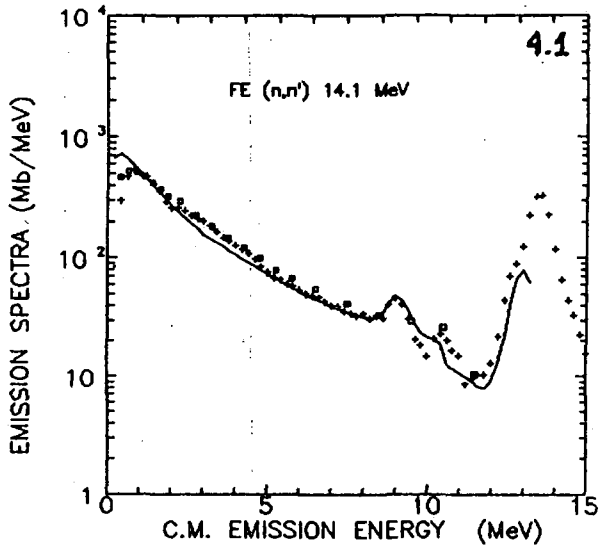

2.1
CR 52(n,n') 14.1 MeV
EMISSION SPECTRA (Mb/MeV)
EMISSION ENERGY (MeV)

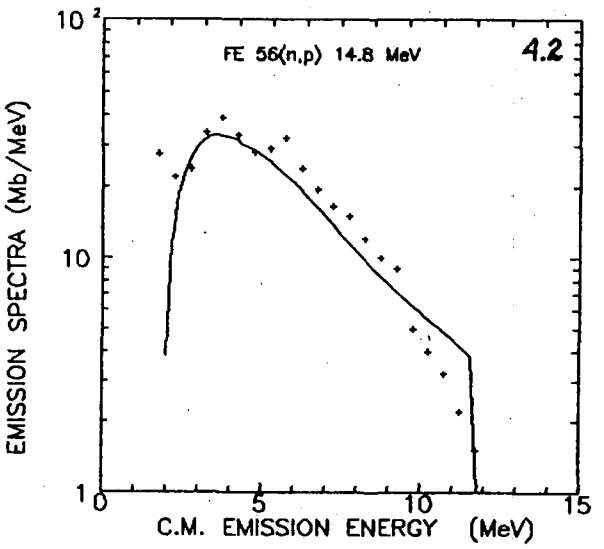

2.2
CR 52(n,p) 14.8 MeV
EMISSION SPECTRA (Mb/MeV)
C.M. EMISSION ENERGY (MeV)

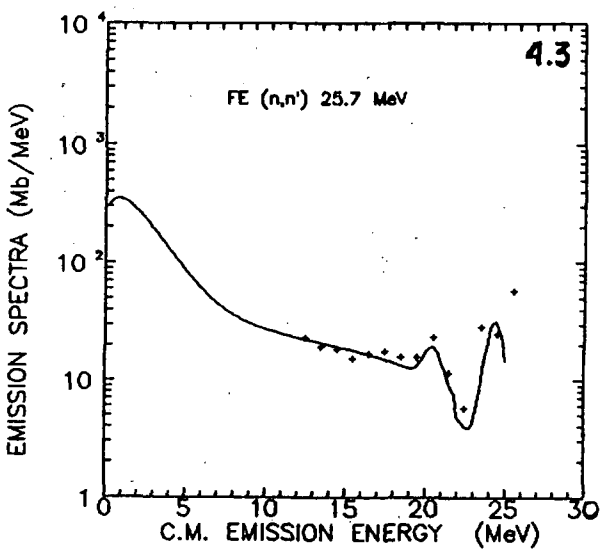

3.1
Cu (n,n') 14.1 MeV
EMISSION SPECTRA (Mb/MeV)
C.M. EMISSION ENERGY (MeV)

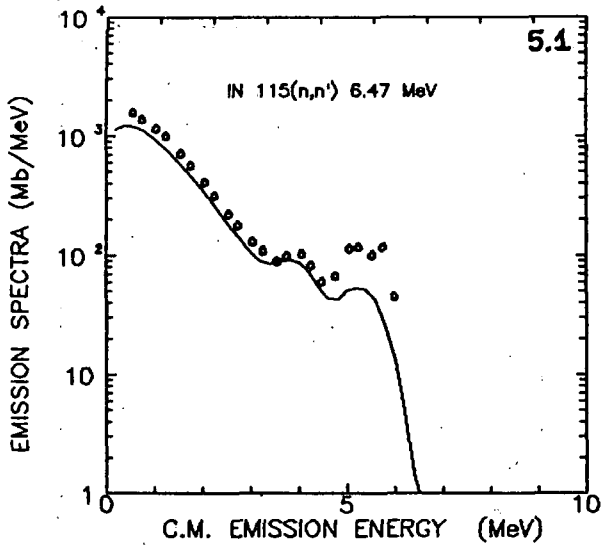

3.2
Cu (n,n') 18 MeV
EMISSION SPECTRA (Mb/MeV)
C.M. EMISSION ENERGY (MeV)

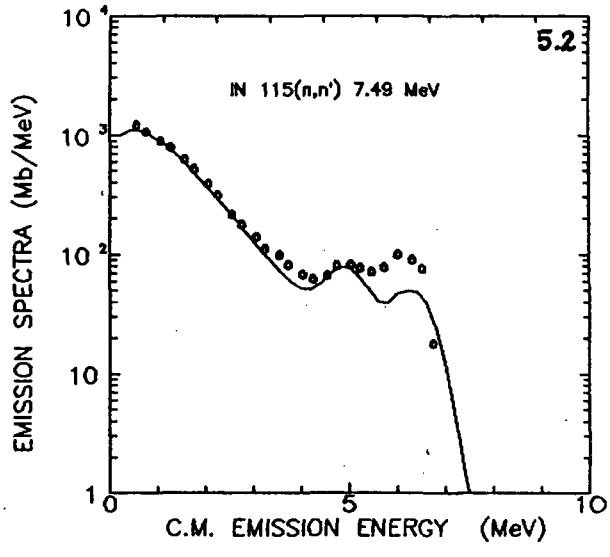

3.3
Cu 65(n,p) 14.8 MeV
EMISSION SPECTRA (Mb/MeV)
C.M. EMISSION ENERGY (MeV)

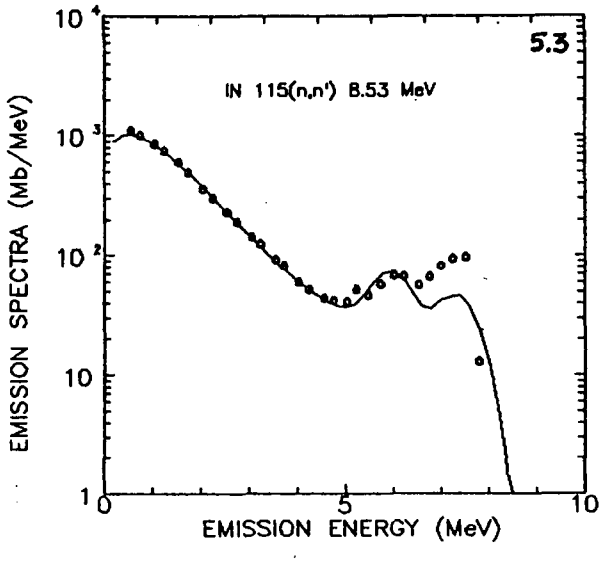

4.1
FE (n,n') 14.1 MeV
EMISSION SPECTRA (Mb/MeV)
C.M. EMISSION ENERGY (MeV)

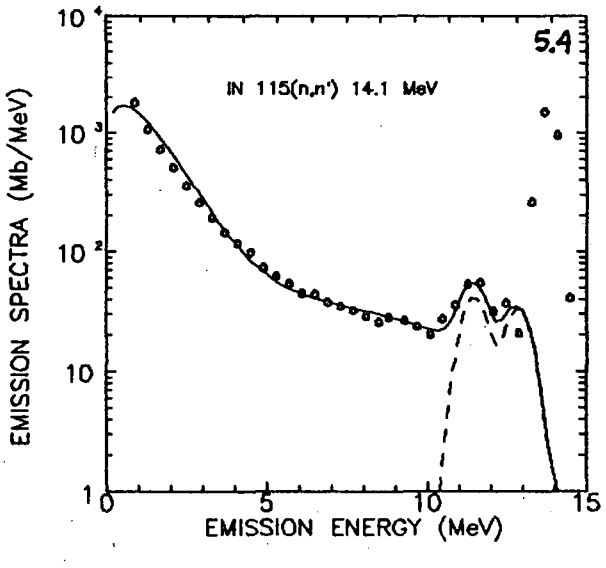

4.2
FE 56(n,p) 14.8 MeV
EMISSION SPECTRA (Mb/MeV)
C.M. EMISSION ENERGY (MeV)

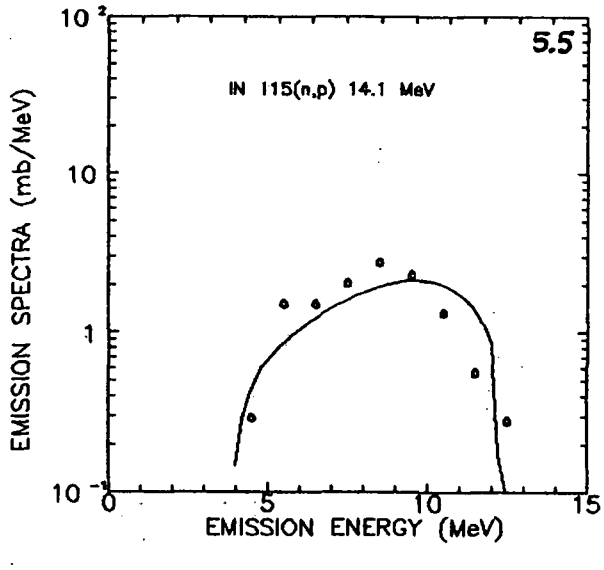

4.3
FE (n,n') 25.7 MeV
EMISSION SPECTRA (Mb/MeV)
C.M. EMISSION ENERGY (MeV)

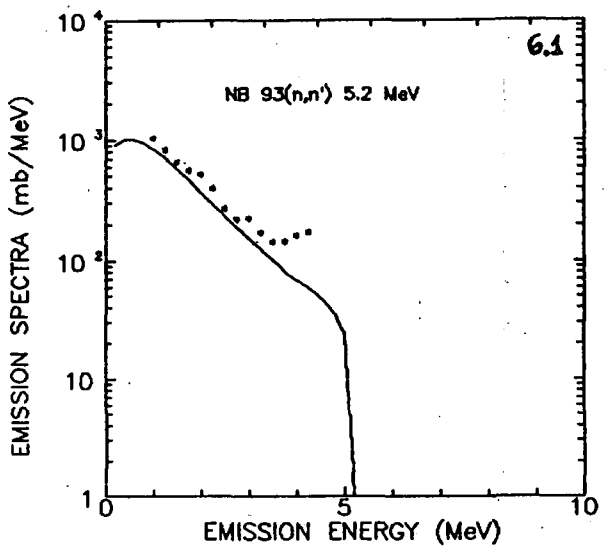

5.1
IN 115(n,n') 6.47 MeV
EMISSION SPECTRA (Mb/MeV)
C.M. EMISSION ENERGY (MeV)

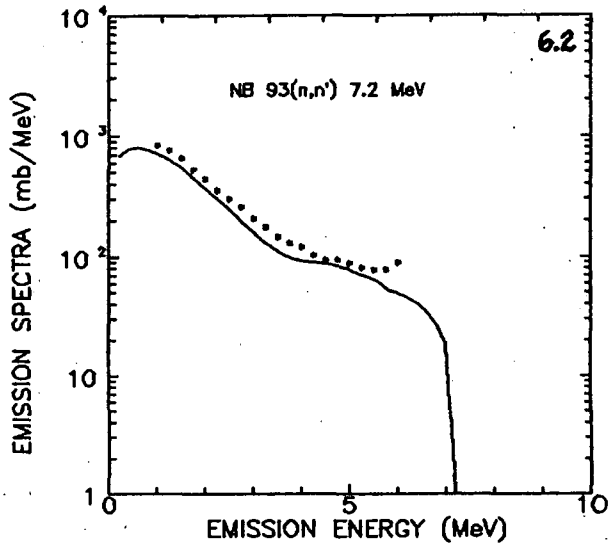

5.2
IN 115(n,n') 7.49 MeV
EMISSION SPECTRA (Mb/MeV)
C.M. EMISSION ENERGY (MeV)

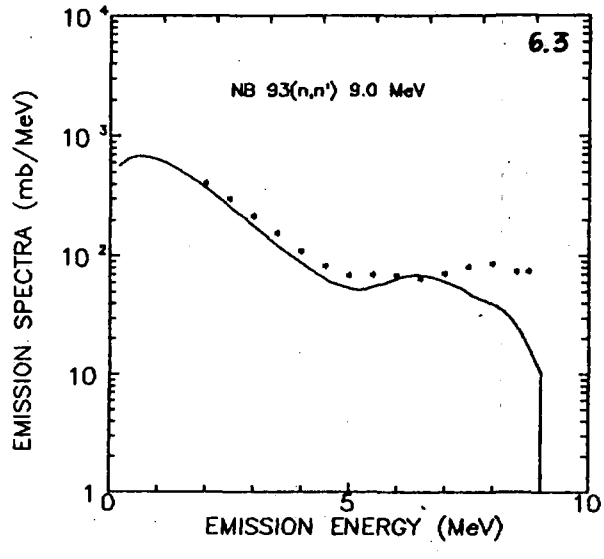

5.3
IN 115(n,n') 8.53 MeV
EMISSION SPECTRA (Mb/MeV)
EMISSION ENERGY (MeV)

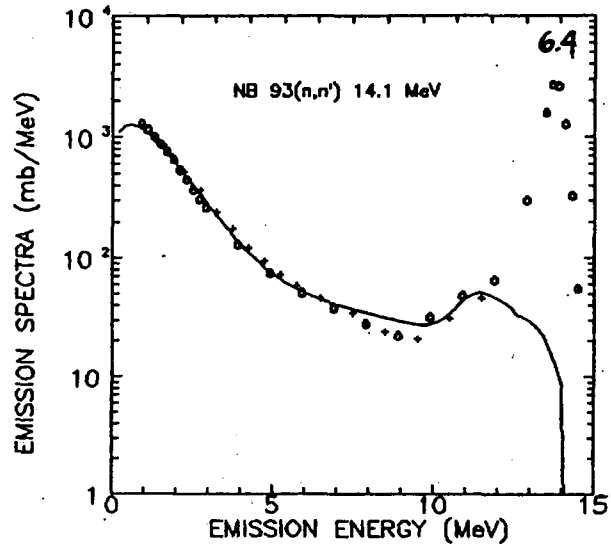

5.4
IN 115(n,n') 14.1 MeV
EMISSION SPECTRA (Mb/MeV)
EMISSION ENERGY (MeV)

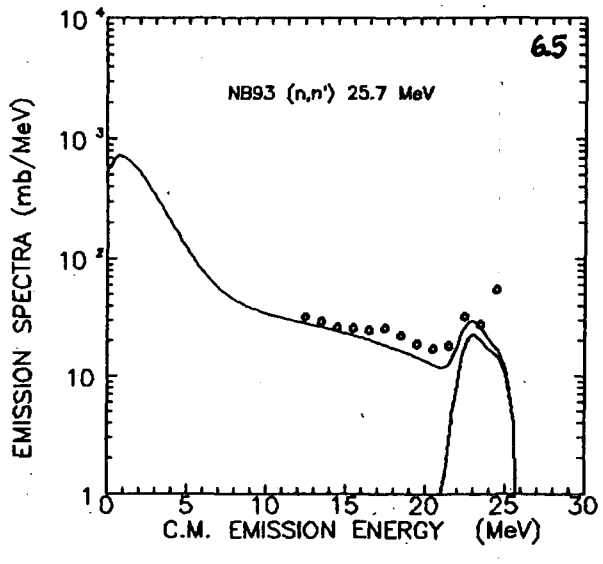

5.5
IN 115(n,p) 14.1 MeV
EMISSION SPECTRA (mb/MeV)
EMISSION ENERGY (MeV)

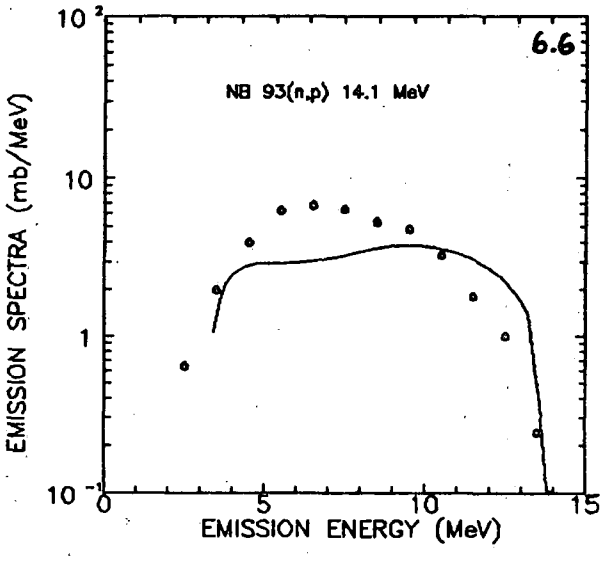

6.1
NB 93(n,n') 5.2 MeV
EMISSION SPECTRA (mb/MeV)
EMISSION ENERGY (MeV)

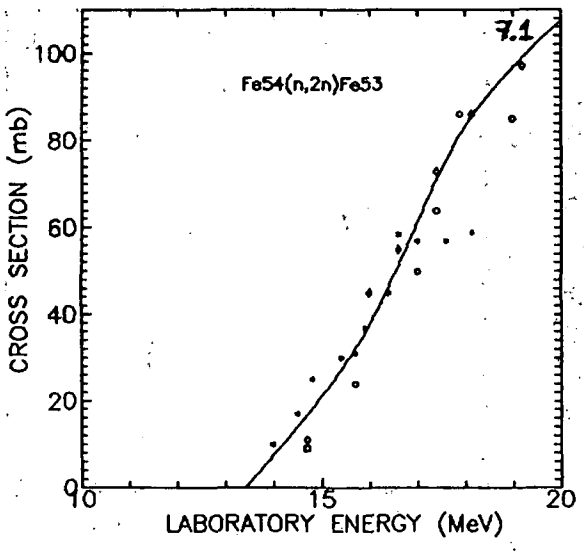

6.2
NB 93(n,n') 7.2 MeV
EMISSION SPECTRA (mb/MeV)
EMISSION ENERGY (MeV)

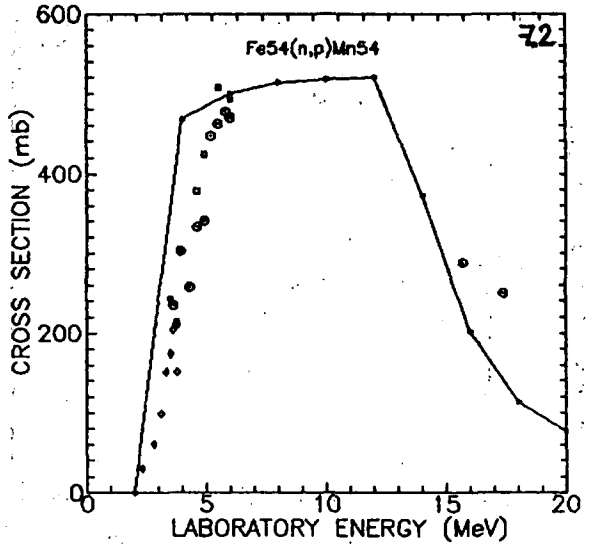

6.3
NB 93(n,n') 9.0 MeV
EMISSION SPECTRA (mb/MeV)
EMISSION ENERGY (MeV)

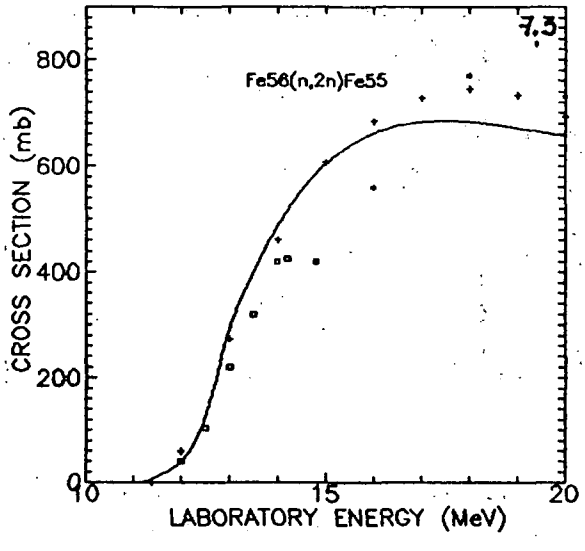

6.4
NB 93(n,n') 14.1 MeV
EMISSION SPECTRA (mb/MeV)
EMISSION ENERGY (MeV)

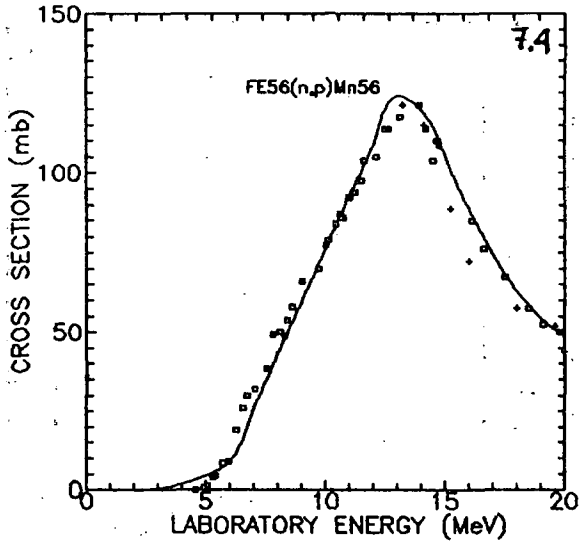

6.5
NB93 (n,n') 25.7 MeV
EMISSION SPECTRA (mb/MeV)
C.M. EMISSION ENERGY (MeV)

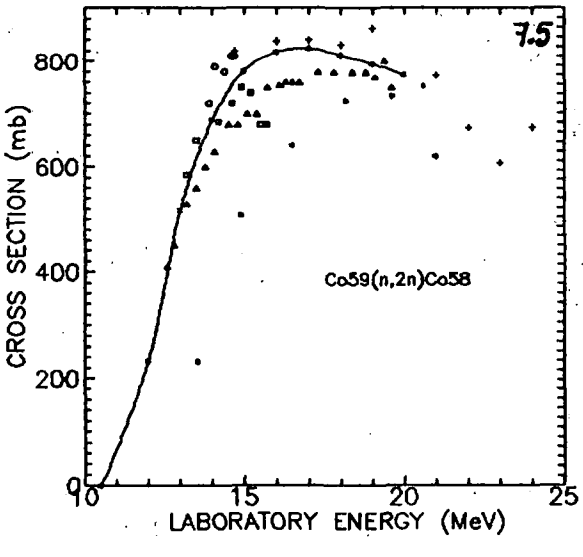

6.6
NB 93(n,p) 14.1 MeV
EMISSION SPECTRA (mb/MeV)
EMISSION ENERGY (MeV)

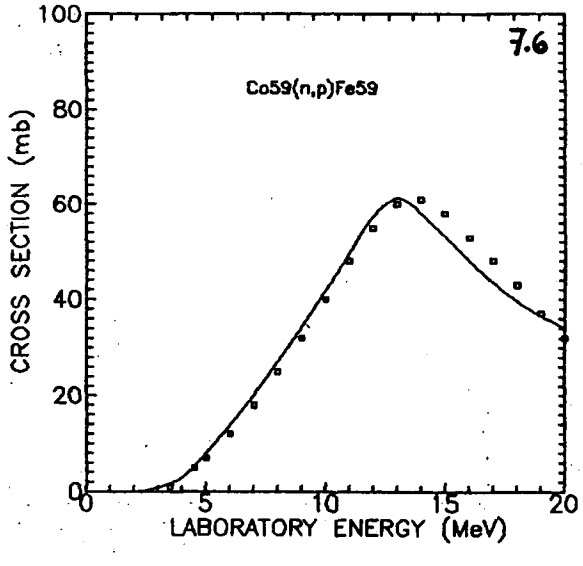

7.1
Fe54(n,2n)Fe53
CROSS SECTION (mb)
LABORATORY ENERGY (MeV)


7.2
Fe54(n,p)Mn54
CROSS SECTION (mb)
LABORATORY ENERGY (MeV)


7.3
Fe56(n,2n)Fe55
CROSS SECTION (mb)
LABORATORY ENERGY (MeV)


7.4
FE56(n,p)Mn56
CROSS SECTION (mb)
LABORATORY ENERGY (MeV)


7.5
Co59(n,2n)Co58
CROSS SECTION (mb)
LABORATORY ENERGY (MeV)


7.6
Co59(n,p)Fe59
CROSS SECTION (mb)
LABORATORY ENERGY (MeV)

ANEXO: Fichero de datos de entrada al PCROSS elaborado por el PDAT

```
N° Línea
1               INPUT FILE TO  P C R O S S
2               CONTROL PARAMETERS:
3
4       KA = MULTIPARTICLE EMISSION     IDENS = STATE DENSITY FORM.
5       IPOZO = DEPTH CORRECTION        IQ = Q-FACTOR (IQ=2 => Q=1)
6       IGR = GRAPHICAL OUTPUT          IALFA = METHOD FOR α CALC.
7       INCAL = REACTION MODEL          IFE = SPECTRA or EXCIT.FUNC
8       ICR = INPUT INV.CROSS SECTIONS OR INTERNAL CALCULATION
9       IENE = IRREGULAR or REGULAR ENERGY GRID
10      IPRINT = 0 => MINIMUM OUTPUT    IPOT = OPTICAL POTENTIAL
11      ILDM = 1 => LIQUID DROP BINDING ENERGY
12
13  FE56 Cross Section & Spectra Calculations (IAEA 5472)(.3-14.1,.7-18)
14   A    Z  INC    W2     B2      W3      B3    WDD     VR
15   56   26  1    .85    .24     4.80    .16    .5      48.
16  KA,IDENS,IPOZO,IQ,IGR,IALFA,INCAL,IFE,ICR,IENE,IPRINT,ILDM,IPOT
17  2     1     0   0  1    1     1     0   0    0     1     0    2
18  INCIDENT ENERGY(LAB)[MeV] , SIGR or ESTEP
19     25.7  -1.
20      BINDING ENERGIES  [MeV]
21      7.64
22      7.64     11.20     7.27      7.94      .00
23     10.56     10.19     9.08     11.14      .00
24      7.32      7.62     7.90     99.00      .00
25       .00       .00      .00       .00      .00
26      9.30      9.21    10.22
27      LEVEL DENSITY PARAMETER g [1/MeV]
28      3.45
29      3.20      3.23     3.29      3.08     3.20
30      3.54      3.29     3.15      3.47     3.54
31      3.06      3.08     3.47       .00     3.06
32      3.45      3.20     3.54      3.06     3.45
33      3.15      3.47     3.47
34      PAIRING ENERGIES [MeV]
35      -.84
36       .58       .26      .2       .69      .58
37     -2.91       .2      -.93    -1.38    -2.91
38      -.55       .69    -1.38      .00     -.55
39      -.84       .58    -2.91     -.55     -.84
40      1.40     -1.39    -1.39
41   CHANNEL COMPETITION { N,P,ALPHA,GAMMA }
42     1    1    1    1
43   FORMATION FACTORS { N,P,ALPHA,GAMMA }
44     1    1    10.    1
45   MEAN FREE PATH PARAMETER
46      1.30
47   SPECTRA OUTPUT OPTIONS { N,P,ALPHA,GAMMA }
48    1.0       1.0       1.0       1.0
49  2
```

## ANNEX: INPUT DATA FILE FOR PCROSS GENERATED BY PDAT

[See original.]

### DESCRIPTION OF INPUT DATA FILE

Lines 1-12: Comments with a brief description of input data to PCROSS.

Line 13: Title of data file.

Line 14: Comment

Line 15:

A: Target nucleus mass number.

Z: Target nucleus atomic number.

INC: Type of incident particle 1 - n; 2 - p; 3 - $\alpha$; 4 - $\gamma$.

W2,B2,W3,B3: Energies and deformation of vibrational levels of the collective type for target nucleus.

WDD: Parameter simulating the experimental energy resolution, takes values between 0.3 and 0.7.

VR: Depth of interaction potential = 48 MeV.

Line 16: Comment

Line 17:

KA = 2 Multiple emission is considered.
1 Only primary emission spectrum is calculated.

IDENS: Method of calculation of particle-hole state density.

= 0 Williams formula [10] without pairing.
1 Williams formula [10] with pairing by Fu [13].
2 Williams formula [10] with pairing by Kalbach [14].
3 Accurate formulation in equidistant model [16] - FUTURE.

IPOZO: Method of consideration of potential well depth.

= 0 No correction is made.
1 - FOR FUTURE USE
2 Betak and Dobes correction [22].
3 Kalbach correction [26].

IQ: Method of calculation of factor $Q_b(p,h)$.

= 0 Factor proposed by Kalbach [26].
1 Factor proposed by Gupta [29].
2 This factor is not considered (always equal to 1).

IGR = 1 - In this case, when the program is executed, it generates sequential files where the emission spectra corresponding to particles with output keys greater than zero are recorded (see line #48 of data file). The names of the files generated are:

| Spectrum | Name |
|---|---|
| (n,n') | SP - N.dat |
| (n,p) | SP - P.dat |
| (n,$\alpha$) | SP - A.dat |
| (n,$\gamma$) | SP - G.dat |

If excitation functions are being calculated, the same are recorded by the following names:

| Excitation function | Name |
|---|---|
| (n,p) | FE - P.dat |
| (n,α) | FE - A.dat |
| (n,2n) | FE - 2N.dat |

These files have the necessary format for producing graphics of the results with the GRAPHER. Thus the graphics accompanying this work were generated.

= 0 - Sequential files are not generated.

IALFA: Method of calculation of alpha emission spectrum.
= 0 A preformation parameter (Formation factor) is used.
1 Iwamoto-Harada method [32-36] is used.

INCAL: Theoretical model used.
= 0 Unified exciton model (Master equation).
1 Weisskopf-Ewing model (Evaporation).

IFE: Calculation of spectra or excitation functions.
= 0 Emission spectra of specified particles and cross-sections for the incident energy introduced into data (INCIDENT ENERGY) are calculated.
= 1 Excitation functions are calculated to a maximum given energy (INCIDENT ENERGY) with a given step (ESTEP).

ICR: = 0 - Inverse reaction cross-sections are calculated internally with use of Chatterjee's parametrization [52].
= 1 - Inverse reaction cross-sections in (n,p,α) channels are obtained from a file whose name is specified in the line following the incident energy. In the case of ICR = 0 the file name cannot be put in that position since this would cause error in data read out.

IENE: = 0 - For calculation of spectra an irregular grid is used which reduces its step at smaller energies in order to obtain an appropriate description of the evaporation peak.
= 1 - A step of 1 MeV is used for all energies. This option is quicker but the cross-section values obtained are not very accurate since the integration step is too large.

IPRINT: = 0 A minimum of information is printed at output.
= 1 Results are printed out fully, except multiple emission spectra, the printing of which is regulated by output options of spectra (see line 48 of data file).

ILDM: = 1 The binding energies of the liquid drop model are used, as suggested in Ref. [50].
= 0 Experimental binding energies are used [55, 56].

IPOT: Used only if ICR = 0, for optical potentials see Ref. [52].
0 Wilmore-Hodgson (n), Becchetti-Greenless (p), Huizenza-Igo (α).
= 1 Wilmore-Hodgson (n), Perey (p), Huizenza-Igo (α).
2 Becchetti-Greenless (n), Becchetti-Greenless (p), Huizenza-Igo (α).

Line 18: Comment

Line 19:

14.600 – It can be the incident particle energy (IFE = 0) or the maximum energy for which the excitation function (IFE = 1) is to be calculated.

1342.8 – If IFE = 0 (calculation of spectra), the reaction cross-section $\sigma_r$ for the given incident energy is specified here. If a number < 0 is specified, the reaction cross-section is calculated by Chatterjee's parametrization [52].

If IFE = 0 (calculation of excitation functions), here is specified the energy step for calculation of the excitation function from 1 MeV to the given maximum energy (ESTEP).

Line 20: Comment

Lines 21-26: Experimental binding energies of emitted particles and incident particle for the corresponding nuclei are specified.
To see the order of nuclei, print out the final table of results of PDAT and compare it with input data file.

Line 27: Comment

Lines 28-33: Level density-parameters are specified. To see the order of nuclei, print out the final table of results of PDAT and compare it with input data file.

Line 34: Comment

Lines 35-40: Pairing parameters D are specified. To see the order of nuclei, print out the final table of results of PDAT and compare it with input data file.

Line 41: Comment

Line 42: Channels which are taken into account in calculating emission rates (competition) are specified. If some channel is indicated as 0, it is not considered in the calculation.

Line 43: Comment

Line 44: Preformation factor of $\alpha$ particle. It is a parameter that makes up for deficiencies of the model used to treat emission of clusters. Used only if IALFA = 0.

Line 45: Comment

Line 46: Mean free path parameter. Its value fluctuates very little as a function of mass number. It should always have a value between 1 and 3. A value of 1.3 is recommended.

Line 47: Comment

Line 48: This line determines the results to be printed from each reaction channel (assuming that in line 42, all are = 1).

If 0 is specified for a channel, nothing is printed for this channel. If 1 is specified, primary and total emission spectra are printed. If 2 is specified, besides the primary and total emission spectra, the secondary emission spectra are printed.

Line 49: Should always be 2, indicating the end of program.for this channel. If 1 is specified, primary and total emission spectra are printed. If 2 is specified, besides the primary and total, the from

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