

International Atomic Energy Agency

INDC(CCP)-354
Distr. G

INDC

INTERNATIONAL NUCLEAR DATA COMMITTEE

**EVALUATION OF EXCITATION FUNCTIONS FOR
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1991

IAEA NUCLEAR DATA SECTION, WAGRAMERSTRASSE 5, A-1400 VIENNA

Printed by the IAEA in Austria
July 1993

93-02786

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ABSTRACT

The authors consider the use of theoretical models to describe experimental excitation functions for isomeric levels in neutron reactions and to predict the cross-sections when no experimental data are available. It is shown that, in many cases, experimental data can be described quite satisfactorily by calculations without adjustment of parameters. For threshold reactions at a neutron energy of ~ 14 MeV the agreement between calculated and experimental isomeric ratios is $\sim 20\%$ and is determined mainly by errors in the experimental ratios. However, for some reactions there are considerable differences between experimental and calculated data, which are due, in the authors' opinion, to uncertainties in the schemes of the low-lying levels and of gamma transitions between levels and to the spin dependence of level density. The small isomeric ratio values $R < 0.1$ are described with the lowest accuracy. A formula is suggested for the energy dependence of the isomeric ratio in the (n,γ) reaction.

INTRODUCTION

The study of cross-sections for isomer formation is of interest from a theoretical standpoint because it offers a unique opportunity to study the mechanism of momentum formation and transfer in various nuclear reactions. Using a simplified statistical model, Huizenga and Vandenbosch [1] were able to describe to a high degree of accuracy the cross-sections for isomer formation in (n,γ) reactions for the thermal energy of neutrons. Vonach [2] carried out a detailed analysis of the excitation of isomeric levels in inelastic neutron scattering reactions and proposed a systematics for the cross-sections. Experimental data for the $(n,2n)$ and (n,n') reactions have been described successfully in Refs [3, 4, 14]. This incomplete list of publications demonstrates the persistent interest in the study of isomer formation cross-sections.

It is not only the basic aspects of the theory of nuclear reactions, but also practical requirements which are responsible for the interest in the problem. Knowledge of a large number of excitation functions for isomeric levels in (n,γ) , (n,n') , (n,p) , (n,d) , (n,t) , (n,α) and $(n,2n)$ reactions in the neutron energy range of up to 20 MeV is needed in order to predict the accumulation of long-lived reaction products in both operating reactors and planned fusion devices [5]. There are clearly insufficient experimental data to carry out the required evaluations. It is thus natural, for the purpose of evaluation, to resort to the use of theoretical models of the processes being investigated.

Despite some progress made in the theoretical description of individual isomer formation cross-sections, the situation as a whole is not so simple. Thus far, no systematics has been developed that can be used to describe with

reasonable accuracy the isomer formation cross-sections even at the individual energy points, thermal or 14 MeV, for which a large amount of experimental data has been accumulated; excitation cross-sections for states with the same spin for the same reactions and adjacent isotopes differ severalfold, which also does not have an unequivocal explanation; calculations using theoretical models are extremely laborious and do not guarantee the required accuracy.

In the present work we consider the applicability of theoretical models for calculation of isomer formation cross-sections in various reactions in a wide range of energies. We study the influence of parameters on the calculation results. We show that, owing to the uncertainties in the initial characteristics, it is advisable to evaluate isomer formation cross-sections by means of "splitting" a known reaction cross-section with the aid of the isomeric ratio.

THE THEORETICAL MODEL

The excitation functions for isomeric levels were calculated within the framework of the statistical model of nuclear reactions and the gamma-cascade evaporation model for the decay of an excited nucleus.

The calculations were made by the STAPRE code [6], which applies the Hauser-Feshbach formalism and the gamma-cascade evaporation model. Calculation of the probability of gamma transitions between low-lying levels was added to the existing capabilities of the code. Level density was calculated by a phenomenological variant of the unified superfluid model of the nucleus [7] with parameters from the systematics of Ref. [8]. At low excitation energies, instead of a model description with the help of level density, we used experimental schemes (energy, spin and parity) [9] of

low-lying discrete levels of nuclei after they had been analysed for level transmission, and the experimental schemes of gamma transitions between these levels (intensity and multipolarity of gamma rays). The transmission coefficients were calculated by the SCAT 2 code. The radiative strength functions were calculated from the photo-absorption cross-section in accordance with Brink's hypothesis [10], and the energy dependence of this cross-section was taken in the form of a Lorentz curve with parameters from the systematics of Ref. [11]. The calculated radiative widths were normalized to the experimental values of the average gamma widths of neutron s-resonances from Ref. [12].

The description of the experimental excitation functions for the isomeric levels in the theoretical model considered is given in Fig. 1 for $^{93}\text{Nb}(n,2n)$, $^{93}\text{Nb}(n,n')$ and $^{85}\text{Rb}(n,\gamma)$ reactions. In the calculations we used Arthur's neutron potential [13] and the experimental schemes of gamma transitions in residual nuclei [9]. It should be emphasized that good agreement with experimental data was achieved without adjustment of parameters. Evidently, the main reason for this is that the neutron optical potential [13] was specially selected for the group of nuclei with $85 < A < 95$ in a wide energy region, whereas the gamma transition schemes are fairly complete.

Such a situation is far from frequent, and it is therefore of interest to explain the sensitivity of the calculations to initial data:

- Choice of optical potential;
- Parameter of the spin dependence of level density σ^2 ;
- The inclusion of the low-lying levels of the residual nucleus in the calculation;
- Gamma-transition schemes and intensities.

Figures 2a,b show five variants of the model description of the excitation function for the isomeric level $J^P = 7/2^+$, $E_m = 39.8$ keV in the $^{103}\text{Rh}(n,n')$ reaction and the results of calculations of the excitation function for the isomer $^{58}\text{Co}^m$ (see Table 1) in the $^{58}\text{Ni}(n,p)^{58}\text{Co}^m$ reaction. The first variant of the calculation was performed with a set of initial data comprising the Becchetti-Greenlees neutron optical potential, 16 discrete levels and the experimental scheme of gamma transitions between them. In the second variant the neutron potential was replaced by the Willmore-Hodgson potential giving a 30% higher neutron absorption cross-section at $E_n < 5$ MeV. In the third, we used a calculated scheme of gamma transitions between the residual nucleus levels, the remaining data being the same as those in variant 1. In the fourth, the model description of level density began after the isomeric level, and in the fifth variant the parameter of the level density spin dependence was increased by a factor of 1.25, while the discrete levels specified were the same as in the fourth variant.

As can be seen in Fig. 2, all the above characteristics have an appreciable influence on the value of the isomer formation cross-section. Not only does the absolute value of the cross-section change, but so does the energy dependence.

The change in cross-section due to the influence of neutron optical potential can be explained by the change in neutron absorption cross-section, and consequently in the total reaction cross-section. Moreover, the momentum distribution in the input channel of the reaction changes. The effect of the characteristics of the residual nucleus on the excitation cross-section for the isomeric level leads mainly to a redistribution of the total cross-section between the isomeric and ground levels. Thus, an increase in the spin

dependence parameter leads to a growth in the density of high-spin levels and, consequently, to an increase in the population of the level of the high-spin isomeric pair (in this case, it is an isomer). As neutron energy rises, the influence of the change in σ^2 increases (compare curves 4 and 5). It should be borne in mind that the change in the value of σ^2 and the inclusion of different numbers of discrete levels in the calculation result in a change in the absolute value of level density and consequently in the total reaction cross-section.

Here we will not deal in detail with the description of cross-sections in the near-threshold region, where "joining" of the $\rho(U, J)$ value to discrete levels and adjustment of the optical potential parameters to the experimental strength functions have a noticeable effect. It is assumed that all these operations can be performed correctly.

We will consider the influence of the basic characteristics on the value of the isomeric ratio $R = \sigma_m / (\sigma_m + \sigma_g)$, where σ_m and σ_g are the excitation cross-sections for the isomeric and ground levels, respectively. Figure 3 shows the results of calculations of the isomeric ratio similar to those given in Fig. 2. It can be seen that, as before, the gamma transition schemes and the value of parameter σ^2 bring about considerable changes, while the choice of optical potential has less influence on the value of R . Therefore, it seems more advisable to evaluate the isomer excitation functions with the use of the isomeric ratio and the total reaction cross-section, shifting the problems of normalization of the isomeric cross-sections to the region of evaluation of the total reaction cross-sections. Such an approach is justified because the methods of reaction cross-section evaluation are fairly well developed (there is extensive experience of work, and the

systematics and large cross-section libraries have been developed. Consequently, in order to obtain the isomeric cross-section for a known isomeric ratio, we need to "split" the cross-sections of the corresponding $(\sigma_m + \sigma_g)$ reaction into σ_m and σ_g components. Thus, the problem reduces to studying and evaluating the isomeric ratios, since it is here that all the problems and difficulties of evaluation of isomeric cross-sections are concentrated.

In contrast to threshold reactions, which are characterized by fairly small changes in R as a function of energy, in the radiative capture process the isomeric ratio changes substantially when we go over from thermal energy to ~ 100 keV (Fig. 4). The reason for such behaviour appears to be an increase in the total momentum of the nucleus with an increase in the contribution of the p - and higher waves to the absorption cross-section.

In order to verify the applicability of the model described above for the evaluation of R in a wide range of mass numbers and to various reactions, we analyse in more detail the data for 14 MeV and the thermal point.

THE POSSIBILITY OF PREDICTING THE ISOMERIC RATIO FOR AN EXTENSIVE SET OF NUCLEI AND NUCLEAR REACTIONS

Table 1 gives the calculation results for nuclei with $50 < A < 150$ and for various reactions at a neutron energy of ~ 14 MeV. The value of R_1 is obtained with the help of the theoretical spin dependence of level density and parameter σ^2 (superfluid model, beyond the phase transition point - rigid-body evaluation), and R_2 with the use of $\sigma^2/2$. In the tables and further on in the figures $R = \sigma_{>} / (\sigma_m + \sigma_g)$, where $\sigma_{>}$ is the cross-section for population of the high-spin state.

It is difficult to find any correlation between R_{exp} and R_1 (Figs 5a, 6a, 7a) for all the reactions considered. A better agreement can be seen for the (n,2n) reaction. A typical feature of the data is the overestimation of R_1 , i.e. of the contribution of high-spin states. The situation improves considerably when σ^2 is reduced (Figs 5b, 6b, 7b). As can be seen from Fig. 8b, which shows values of $k_2 = R_{\text{exp}}/R_2$, there is good agreement with the experiment. The average value of k_2 and its standard deviation are equal to (0.95 ± 0.19) . No dependence on mass number and spin of the state is observed. The value of 19% can be regarded as the estimate of the accuracy of the theoretical predictions for threshold reactions. It includes both experimental errors and the errors of theoretical calculations. The experimental errors are 10-20%, which value is commensurate with the error mentioned above.

Table 2 shows $\langle k_1 \rangle$ and $\langle k_2 \rangle$ and their standard deviation separately for each reaction. The following characteristics should be noted. The quality of the theoretical predictions does not depend on the reaction. The lower sensitivity of the (n,2n) reaction to changes in spin dependence is most likely associated with the increase in the contribution of the population of the low-lying states immediately after emission of the second neutron.

Similar data for the (n, γ) reaction at the thermal point are given in Table 3 and in Fig. 9. In contrast to the threshold reactions, the (n, γ) reaction is characterized by a much larger spread of data (Fig. 9). A satisfactory agreement between R_{exp} and R_1 can be observed only in the case of the higher isomeric ratios $0.1 < R < 1$. No characteristic connected with high spin values was found. It is difficult to give a definite explanation for the large spread of data for small R. It may be associated with the higher sensitivity of the calculations to the level scheme for small R or with some purely calculation-related characteristics. However, given that the number of

isomers with small R is high ($\sim 50\%$), a solution to this problem is undoubtedly of great interest.

SPIN DEPENDENCE OF LEVEL DENSITY

The above-mentioned need to decrease the contribution of large momenta in threshold reactions is connected with the inaccuracy in the calculation of the contribution of large momenta in the input channel (optical potential), and also with the spin dependence of level density.

The need to reduce parameter σ^2 arises during the analysis of different experimental data. In Ref. [15], σ^2 was obtained from the angular distributions of neutrons in (p,n) reactions. In the $A < 100$ region, the spin dependence is close to the rigid-body evaluation, while for $A > 100$, it needs to be reduced substantially (by a factor of ~ 10). In Ref. [20], σ^2 was determined from the distribution of spins of the low-lying levels for $A > 230$. The experimental values are lower than the theoretical evaluations by several factors. The data analysed in the present work show a similar trend. However, there are clearly not sufficient grounds at the present time for a definitive conclusion. Although the data for the (n, γ) reaction have a large spread, they do not indicate any need for a change in spin dependence. Moreover, the isomer population process in neutron capture is free from the uncertainties associated with the influence of spin distribution in the input channel.

These results obviously cannot be used as a basis for changing the currently-used global dependences of parameter σ^2 on excitation energy and mass number. However, they do show the need for further refinement of this dependence with the use of all the available experimental data. Such an analysis must certainly include the excitation functions for isomeric levels.

SYSTEMATICS OF ISOMERIC RATIOS

The population of isomeric states is achieved in the $A(n,x)B$ reaction through the following processes:

- (a) Immediately after emission of particle x , the isomeric and other low-lying states are excited in residual nucleus B ;
- (b) The low-lying states, including the isomeric state, are excited as a result of a gamma ray cascade from the highly excited compound nucleus;
- (c) The isomer formation cross-section observed in the experiment results from the gamma transitions between the low-lying levels populated in processes (a) and (b). Smooth systematic dependences are typical for processes (a) and (b), but (c) has its own character, which varies from one nucleus to another. This seems to account for the failure of attempts to construct an acceptable systematics for the isomeric ratio as a function of the individual characteristics of the nucleus, as is demonstrated by the results given below.

A typical feature of the experimental data is the large spread of isomeric ratios R for the same values of J_m and J_g [16-19]. As the above analysis shows, specific level schemes and the schemes of gamma transition between levels have an appreciable influence on the value of the isomeric ratio. Figure 10 gives the experimental and calculated values of R for (n,p) reactions as a function of $(J_m + J_g)/2$. Theoretical calculation gives a spread of R close in scale to the spread of the experimental points. Figure 8(a) shows the values of k , when $R = 0.5$ is taken as the estimate of

the isomeric ratio. Such an assumption considerably reduces the quality of agreement of the description, but can be justified where no data are available on the scheme of the low-lying levels.

As noted above, the strong energy dependence of R for radiative capture may be associated with an increase in the contribution of l -waves to the neutron absorption cross-section. In this connection, the evaluation of the excitation functions for isomers in the (n,γ) reaction has its own peculiarities - we could use the partial isomeric ratios R_l for each neutron l -wave at the stage of determination of the detailed behaviour of the isomeric ratio (including the resonance region). However, this approach is highly laborious, and can be ineffective due to lack of information about R_l . In such a situation one can use the l -averaged isomeric ratio after assigning to it some energy dependence normalized to the available experimental data, for example

$$R(E) = R_0 + (R(E_1) - R_0) * v_l(E) / v_l(E_1), \quad (1)$$

where v_l is the penetration of the centrifugal barrier by p -neutrons, R_0 and $R(E_1)$ are experimental values of the isomeric ratio for thermal and E_1 neutrons, respectively. In Fig. 4 the curves show the results of calculation by formula (1), calculations by the STAPRE code, SINCROSACT calculations [5] and experimental data. It can be seen that a simple description with the use of expression (1) agrees satisfactorily with the experimental data and with the more rigorous theoretical calculations of the isomeric ratio.

CONCLUSION

Analysis of the calculated and experimental data for a large number of reactions leads to the following conclusions:

1. In the majority of cases the experimental data can be described with an accuracy not lower than 20% virtually without adjustment of the model parameters. However, for small values of R (mainly for radiative capture) the difference between theoretical predictions and experiment reaches several orders of magnitude. The reason for such behaviour is not clear and requires further study;
2. Experimental errors make an appreciable contribution to the spread of $k = R_{\text{exp}}/R_{\text{calc}}$. A characteristic as important as spin dependence of nuclear level density can be studied successfully only if the accuracy of the experimental data is improved substantially;
3. The considerable influence exerted on the isomeric ratio by a specific scheme of low-lying levels reduces the predictive character of systematics which are based on some smooth dependences. One can hardly expect a description of a quality better than that obtained on the assumption of $R = 0.5$ for $(J_m + J_g)/2 < 4$.
4. Different model assumptions change not only the value of R , but also its energy dependence. This peculiarity should be borne in mind during the evaluation of the energy dependence of the isomer formation cross-sections by normalizing the theoretical curves to experimental data at 14 MeV.

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Table 1. Isomeric ratios for threshold reactions at $E_n = \sim 14$ MeV

Isomer	J^P	E, keV	Reaction	R_{exp}	R_1	R_2
58mCo	5+	24.88	(n,2n)	0.60	0.67	0.67
			(n,p)	0.53	0.56	0.48
62mCo	5+	22.0	(n,p)	0.53	0.55	0.47
			(n,a)	0.58	0.59	0.50
69mZn	9/2+	140	(n,2n)	0.56	0.55	0.48
			(n,p)	0.41	0.62	0.45
			(n,a)	0.53	0.60	0.45
75mGe	7/2+	139.7	(n,2n)	0.60	0.81	0.79
			(n,p)	0.50	0.81	0.70
86mRb	6-	556.1	(n,2n)	0.38	0.36	0.32
			(n,p)	0.15	0.32	0.18
95mNb	1/2-	235.7	(n,p)	0.85	0.84	0.79
			(n,a)	0.27	0.18	0.20
106mAg	6+	90.0	(n,2n)	0.41	0.53	0.46
			(n,p)	0.42	0.55	0.45
115mCd	11/2-	180	(n,2n)	0.49	0.56	0.35
			(n,p)	0.45	0.69	0.43
			(n,a)	0.21	0.73	0.26
112mIn	4+	155.5	(n,2n)	0.80	0.86	0.85
			(n,p)	0.36	0.79	0.60
123mSn	3/2+	24.0	(n,2n)	0.62	0.91	0.75
			(n,p)	0.39	0.83	0.45
127mTe	11/2-	88.26	(n,2n)	0.55	0.66	0.63
			(n,p)	0.50	0.69	0.60
133mXe	11/2-	233.2	(n,2n)	0.45	0.65	0.57
			(n,p)	0.46	0.69	0.60
148mPm	6-	137	(n,p)	0.60	0.54	0.46
			(n,a)	0.52	0.72	0.53

Table 2. Average values of k_1 , k_2 and their standard deviation for various reactions

Reaction	$\langle k_1 \rangle \pm \Delta k_1$	$\langle k_2 \rangle \pm \Delta k_2$	$\langle k_2 \rangle / \langle k_1 \rangle$
(n,2n)	0.86 ± 0.21	0.98 ± 0.26	1.13
(n,p)	0.73 ± 0.21	0.93 ± 0.19	1.27
(n,alf)	0.78 ± 0.20	0.96 ± 0.19	1.23

Table 3. Isomeric ratios for (n, γ) reaction at thermal point

Nucleus	J_m	J_R	R_{exp}	R_1
60Co	2	5	0.451	0.44
69Zn	4.5	0.5	0.0672	0.089
81Se	3.5	0.5	0.131	0.25
86Rb	6	2	0.11	0.018
88Sr	0.5	4.5	0.31	0.37
90Y	7	2	0.78-3	0.14-4
95Nb	0.5	4.5	0.971	0.964
105Rh	6	1	0.313	0.26
111Cd	5.5	0.5	0.0127	0.0085
115Cd	5.5	0.5	0.107	0.0073
121Sn	5.5	1.5	0.0071	0.088
123Sn	1.5	5.5	0.006	0.02
125Sn	1.5	5.5	0.03	0.05
127Te	5.5	1.5	0.13	0.011
129Te	5.5	1.5	0.0698	0.022
125Xe	4.5	0.5	0.17	0.085
133Xe	5.5	1.5	0.111	0.15-3
135Xe	5.5	1.5	0.0113	0.84-4
148Pm	6	1	0.43	0.36
151Eu	0	3	0.641	0.78
151Eu	8	3	0.44-3	0.39-2

Fig. 1. Excitation functions for isomeric levels.

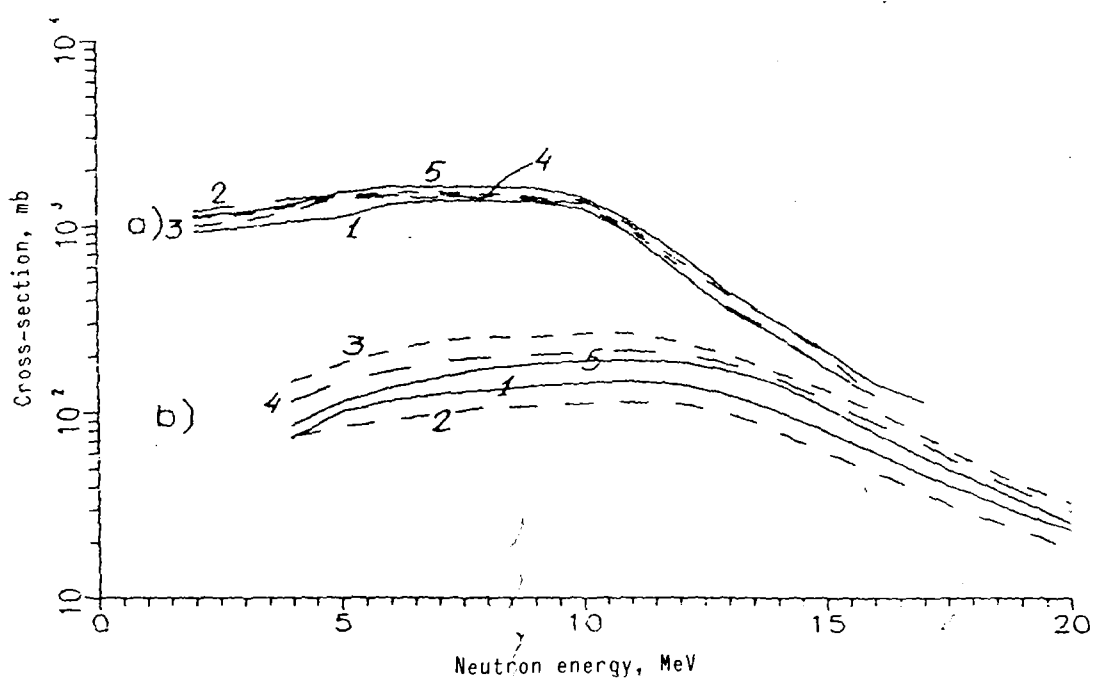
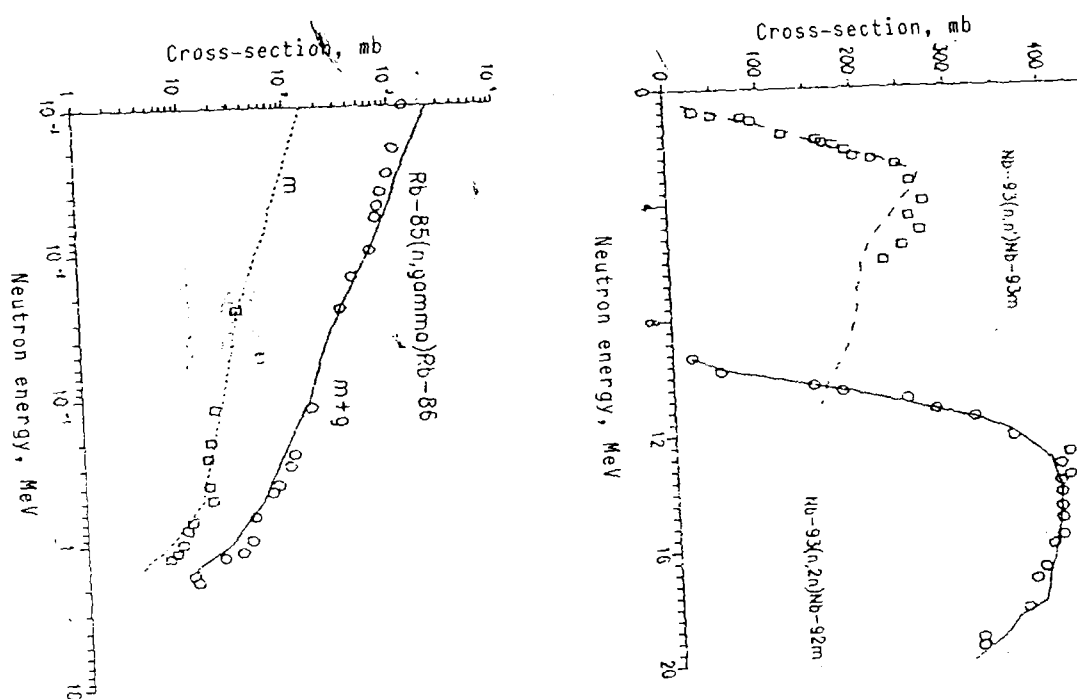


Fig. 2. (a) Influence of model parameters and residual nucleus characteristics on the results of calculation of the cross-section for ¹⁰³Rh(n, n')¹⁰³Rh^m reaction; (b) Influence of model parameters and residual nucleus characteristics on the results of calculation of the cross-section for ⁵⁸Ni(n, p)⁵⁸Co^m reaction.

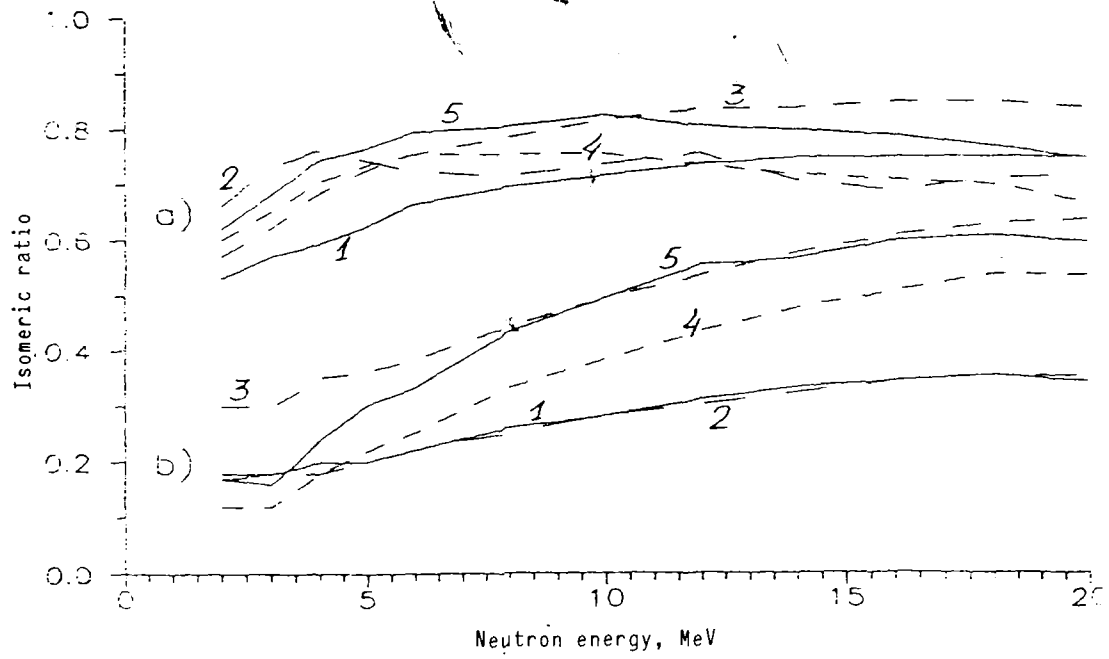


Fig. 3. Same as Fig. 2, but for isomeric ratio.

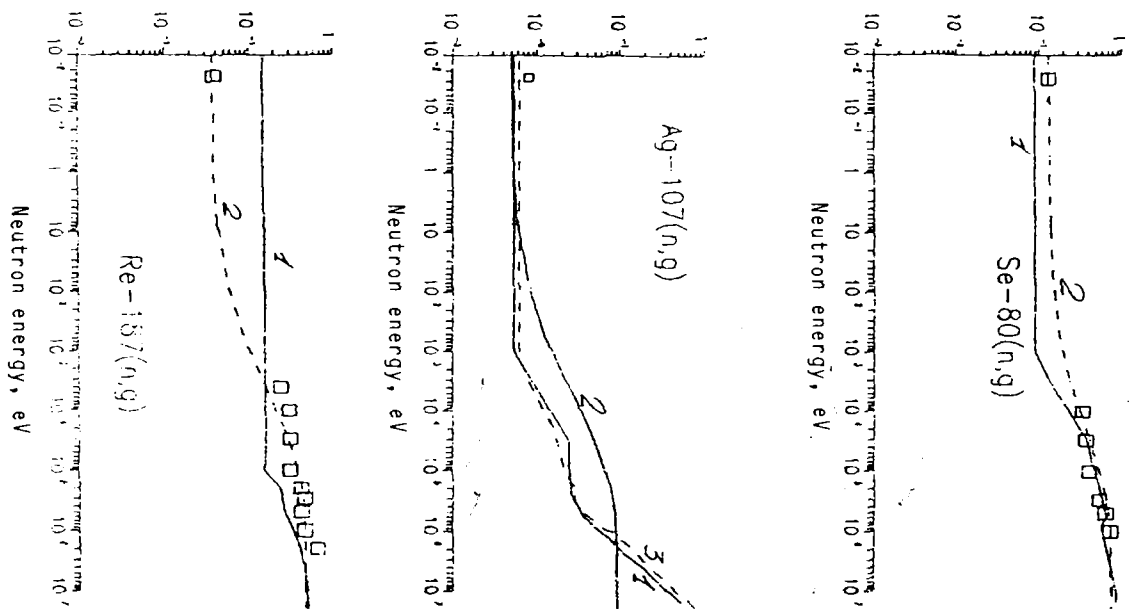


Fig. 4. Isomeric ratio data for $^{80}\text{Se}(n,\gamma)$, $^{107}\text{Ag}(n,\gamma)$ and $^{187}\text{Re}(n,\gamma)$ reactions. Experimental data are indicated by points and the curves show results of calculations: (1) calculation using STAPRE code; (2) calculation using formula (1). For $^{107}\text{Ag}(n,\gamma)$ reaction, curve 3 shows SINCROSACT library calculation data.

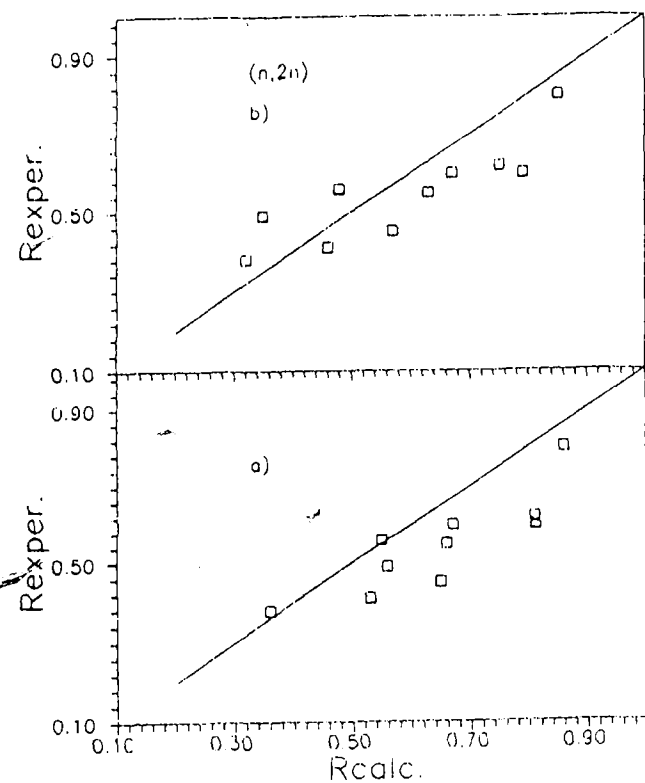


Fig. 5. Correlation between experimental and calculated isomeric ratios for (n,2n) reaction: (a) $R_{\text{calc}} = R_1$; (b) $R_{\text{calc}} = R_2$.

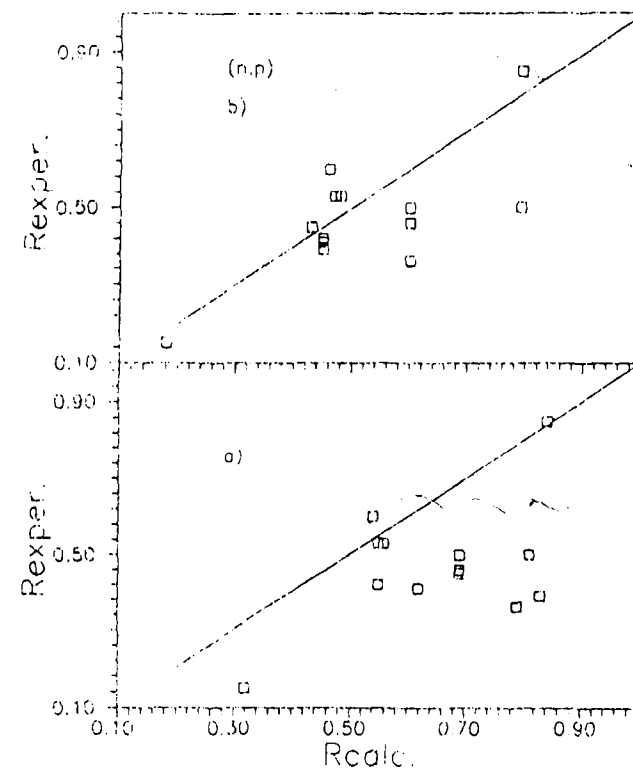


Fig. 6. Same as Fig. 5, but for (n,p) reaction.

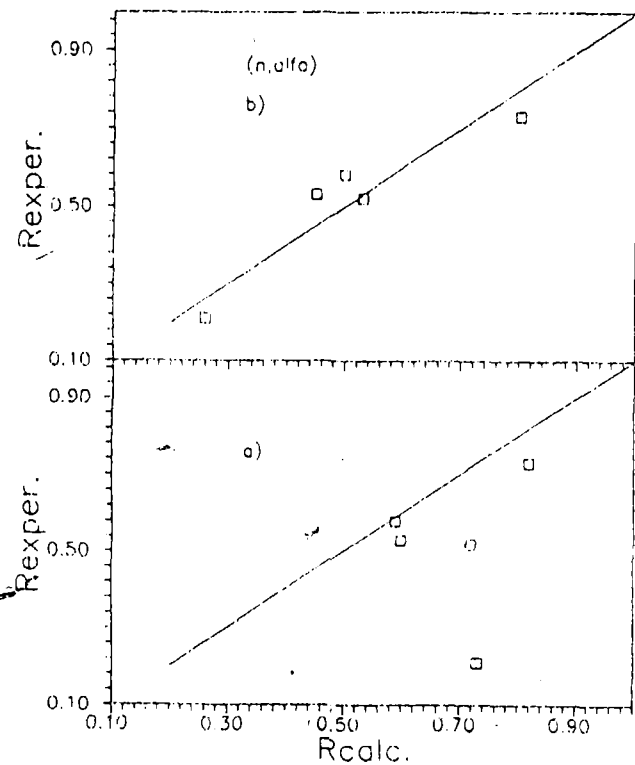


Fig. 7. Same as Fig. 5, but for (n,alpha) reaction.

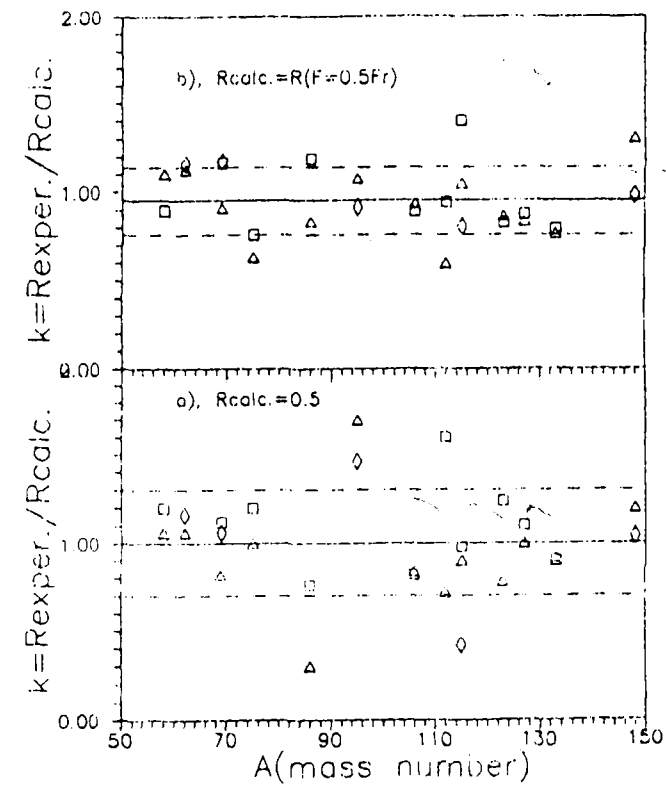


Fig. 8. Dependence of ratio k on mass number. Broken lines show the standard deviation.
 \square (n,2n), \triangle (n,p), \diamond (n,alpha)

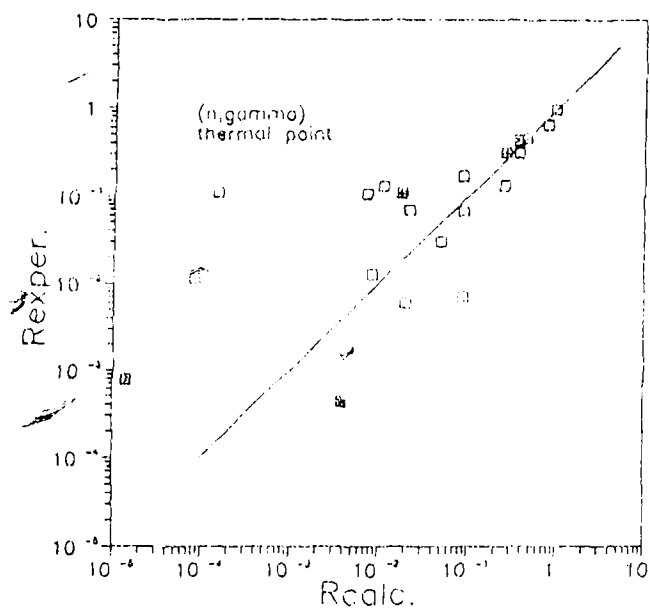


Fig. 9. Same as Fig. 5, but for (n,γ) reaction.
 $R_{\text{calc}} = R_1$. Asterisks denote data
 for $J > 6$.

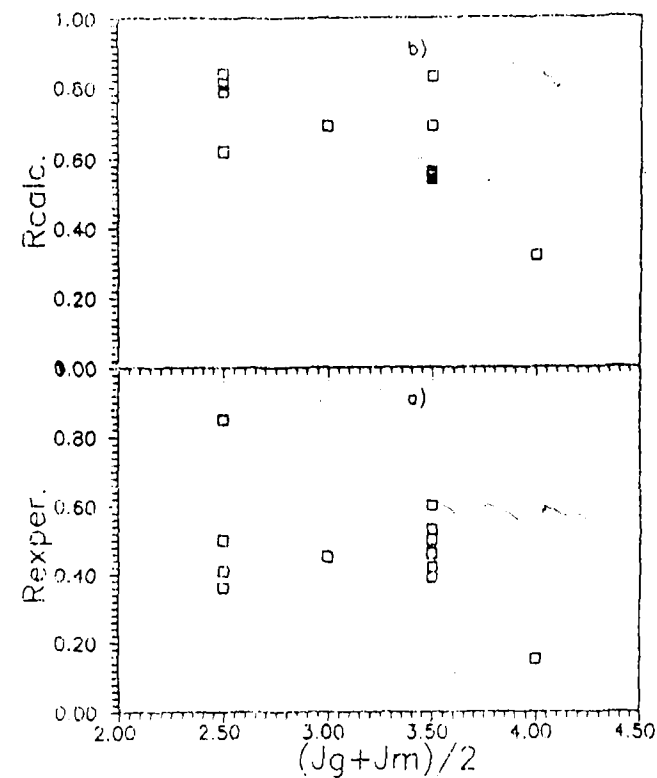


Fig. 10. Dependence of the experimental (a) and the
 theoretical (b) isomeric ratio for
 (n,p) reaction.