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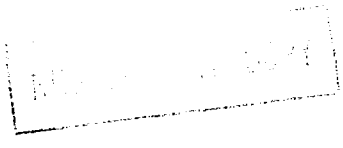

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ABSTRACT

The authors give a self-consistent description of experimental yields of the $^{90}Y^{m}(7^{+})$ isomeric level in (n,γ), (n,p) and (n,α) reactions using statistical and gamma-cascade models. On the basis of $^{175}Lu(n,\gamma)^{176}Lu^{m}$ and $^{179}Hf(n,2n)^{178}Hf^{m2}$ reactions, they show that statistical modelling of the branching ratios of γ transitions between discrete levels can be used to calculate the isomeric cross-sections of nuclei with unknown γ decay schemes.

INTRODUCTION

Theoretical studies of isomer formation cross-sections are of interest because they enable us to investigate the mechanism of formation and transfer of momenta in various nuclear reactions and the level density spin distribution for excited nuclei [1, 2]. In addition to investigation of basic aspects of nuclear reaction theory, there is also a practical need to be able to predict long-lived nuclide accumulation, both in operating nuclear reactors and in fusion devices which are being developed.

Over the past years the tendency has been to describe isomeric cross-sections by modelling low-lying level schemes and the γ transitions between them [3-5]. This type of modelling was necessary because, firstly, there were no experimental data on the branching ratios of discrete levels and, secondly, calculations give gross underestimates of isomer yield if the levels above them are represented as a continuum. A feature of Refs [3-5] is the construction of rotational bands and transition schemes between their levels which is equivalent to increasing the number of high-spin states and, hence, increasing the isomer yields.

Despite the fact that some success has been achieved in theoretical description of individual isomeric cross-sections [1-6], the situation as a whole is not quite clear. To date we do not have any reliable systematics based on physical principles to describe, with reasonable accuracy, the isomeric ratios even at individual energy points for which there is a large amount of experimental data. This is most likely due to the inability of the theory to predict isomeric cross-sections with sufficient reliability.

In the present study we show that in order to describe the excitation functions of the isomeric levels we can calculate the branching ratios for

γ transitions between the discrete levels, using the ordinary statistical correlations, in which the radiative strength functions for E1 transitions are calculated from the modified energy dependences given in Refs [7, 8], and the strength functions for M1 and E2 transitions from the Lorentz dependences. We can thus describe the experimental isomer yields in different reactions, using a single approach without any additional individual modelling of the rotational bands. The uncertainties of the statistical model perameters can be substantially compensated for by means of a self-consistent description of cross-sections leading to the same residual nucleus.

THEORETICAL MODEL

The excitation function of the isomeric levels are calculated with the use of the statistical model for nuclear reactions and the γ cascade evaporative model for decay of the excited nucleus. Since the relations of the statistical model are well known, we give only the basic relations of the cascade evaporative model [9].

Population of levels with quantum numbers $(E',J'^{\pi'})$ by γ transitions from levels (E,J^{π}) is determined by the branching ratio, i.e. by the ratio of the γ transition partial width $\Gamma_{\gamma}(E,J^{\pi};\ E',J'^{\pi'})$ to the full widths $\Gamma(E,J^{\pi})$. The level population $W(E',J'^{\pi'})$ after n γ transitions can be calculated as:

$$W(E',J'^{\pi'})\Delta E' = \sum_{\pi}\sum_{J_{\pi}} \int_{E'}^{E_m} dE\ W^{n-1}(E,J^{\pi}) \frac{\Gamma_{\gamma}(E,J^{\pi};E',J'^{\pi'})}{\Gamma(E,J^{\pi})} \rho_{\gamma}(E',J'^{\pi'})\Delta E' \qquad (1)$$

where E_m is the maximum excitation energy of the decaying nucleus and $\rho_{\gamma}(E',J')$ the density of the levels populated with γ transitions.
Integral equation (1) is solved numerically for a fixed energy E'.

The radiative width $\Gamma_\gamma(E,J^\pi)$ is calculated in terms of transmission T_γ as

$$\Gamma_\gamma(E,J^\pi)= \frac{1}{2\pi\rho(E,J)} \sum_{J'\pi'} \sum_{xL} \int d\varepsilon_\gamma T_{\gamma xL}(\varepsilon_\gamma)\rho(E-\varepsilon_\gamma,J'^{\pi'}) \qquad (2)$$

and the partial width of the γ transition between the separated states as

$$\Gamma_\gamma(E,J^\pi;E',J'^{\pi'})= \sum_{xL} T_{\gamma xL}(E-E') \qquad (3)$$

Summation in Eqs (1)-(3) over total spin J, parity π, type x and multipolarity L of radiative transition takes into account the laws of conservation of the total angular momentum and parity.

The radiative transmission is calculated by the formula

$$T_{\gamma xL}(\varepsilon_\gamma)= 2\pi\, f_{xL}(\varepsilon_\gamma)\, \varepsilon_\gamma^{(2L+1)} \qquad (4)$$

where f_{xL} is the radiative strength function characterizing the average electromagnetic properties of the excited nucleus and ε_γ the photon energy.

The most common method for calculating radiative strength functions is based on the Brink hypothesis [10-11], which treats photon emission rates in terms of photoabsorption cross-sections. In this approach the expression for the E1 strength function is written as

$$f_{E1}(\varepsilon_\gamma)= \text{Const}\ \frac{\sigma_0 \varepsilon_\gamma \Gamma^2}{(\varepsilon_\gamma^2 - E^2)^2 + \varepsilon_\gamma^2 \Gamma^2} \qquad (5)$$

where σ_0, Γ and E are the giant resonance parameters derived from experimental data on the photoabsorption cross-section. In the case of strongly deformed nuclei, where splitting of the cross-section curve is observed, a combination of two Lorentzian curves (5) with approximately selected paramenters is used. In addition to E1 radiation, this approach can also be applied successfully to M1 and E2 radiation. The theoretically more consistent model for describing E1 strength functions based on the Fermi liquid theory [7] yields an expression which differs slightly from Eq. (5)

$$f_{E1}(\varepsilon_\gamma,T)= \text{Const}\ \frac{\varepsilon_\gamma\Gamma(\varepsilon_\gamma)}{(\varepsilon_\gamma^2 - E^2) + \varepsilon_\gamma^2\Gamma(\varepsilon_\gamma)^2} + \frac{0.7\Gamma 4\pi^2T^2}{E^5})\sigma_o\Gamma \qquad (6)$$

where $\Gamma(\varepsilon_\gamma) = \Gamma\frac{\varepsilon_\gamma^2+4\pi^2T^2}{E^2}$ is the energy-dependent width and T the nuclear temperature.

A distinguishing feature of the strength function obtained is that the calculated $f_{E1}(\varepsilon_\gamma)$ has a value different from zero for $\varepsilon_\gamma = 0$. Henceforth expression (5) will be called the Lorentzian dependence and expression (6) the generalized Lorentzian dependence.

A detailed analysis of existing methods to describe radiative strength functions and their influence on the calculated values of observed photon spectra, reaction cross-sections and average radiative widths is given in Ref. [8], where on the basis of a comparison of experimental data and theoretical calculations it is concluded that use of the generalized Lorentzian dependence is preferable to describe the strength functions for E1-transitions.

RESULTS OF CALCULATIONS

Population of isomeric levels in the A(n,x)B reaction takes place both directly after x particle emission and through γ cascades from more highly excited levels. The γ cascade isomer population is often subdivided into two stages: γ decays of an excited nucleus from the continuum and γ transitions between discrete levels [6]. The idea behind this division is that γ transitions are calculated from relations (1)-(4) for the continuum, while for the discrete levels they are given by the experimental branching ratios.

Using the mechanism of isomeric level population, we can determine the model characterstics which influence the calculated cross-sections. They are the optical potential parameters of particles in the entrance and exit channels of reaction, the γ decay characteristics and the level density spin distribution for the residual nucleus. In an earlier paper [6] we examined in detail the extent and nature of the influence of these characteristics. Our analysis showed that the optical potential parameters had little influence on the calculated isomeric ratios, which were affected mainly by discrete transition schemes and by the level density spin distribution for the residual nucleus. We were able to obtain a satisfactory description of experimental data by varying parameter σ^2 for well-known γ decay schemes. One question remained unanswered, however, namely, how to calculate the isomeric ratios when experimental data for the branching ratios are lacking or incomplete.

The calculations were carried out by the STAPRE code [9] using the Hauser-Feshbach formalism and the γ cascade evaporative model. The level density was calculated by the phenomological variant of the generalized superfluid model [12] of nuclei with parameters taken from the systematics of Ref. [13]. At low excitation energies experimental schemes of low-lying

discrete levels of nuclei [14] were used instead of the model description of level density. The particle transmission coefficients were calculated by the SCAT2 program with different sets of optical model parameters, which were selected so as to describe the whole set of the corresponding experimental data for the given range of mass numbers. The radiative strength functions were calculated using the two approaches described earlier. The giant resonance parameters were taken from the systematics described in Ref. [8].

An extra feature added to the STAPRE code is that it can be used to calculate the branching ratios for γ transitions between discrete levels, as in the case of the above calculation procedure for γ transitions in the continuum.

The branching ratio BR_{ij} shows the probability of transition from a given initial level i to different levels j of residual nuclei, where $\sum_j BR_{ij}=1$. Calculations generally use experimental values of BR[14], but it often happens that such data are either lacking or incomplete. In this case, we used a relation which takes the form

$$BR_{ij} = \sum T_{\gamma \times L}(E_i - E_j) \qquad (7)$$

where transmissions T_γ are calculated from Eq. (4), and summation is performed with allowance for the conservation laws. After the branching ratios for the particular level i have been calculated the sum of the branching ratios for this level are normalized to unity. This method of calculating the branching ratios for discrete levels in the statistical approach does not, of course, claim to be a detailed description of particular transitions. This is, however, not required for the calculation of the

integral populations of isomeric levels as the sum of transitions between discrete levels. Furthermore, in calculating isomeric populations we are not interested in the absolute magnitude of the transition strength but in the relative contribution to this magnitude by photons of different multiplicities.

We demonstrate the efficiency of the statistical modelling of the branching ratios described above on the basis of two examples. The first example is the isomeric ratio $R = \sigma_m/(\sigma_m+\sigma_g)$ of the $^{59}Co(n,2n)^{58}Co^m(5^+)$ reaction. This reaction is characterized by a high threshold (10.46 MeV) and, consequently, in the neutron energy range up to 20 MeV discrete γ transition schemes have a decisive influence. The second reaction, $^{93}Nb(n,\alpha)^{90}Y^m(7^+)$, has a low energy threshold and consequently, apart from discrete γ transitions, the level density spin distribution influences the calculated isomeric ratio to an equal degree. The reactions result in population of isomeric levels of the ^{58}Co and ^{90}Y nuclei, respectively, for which there are experimental data on the branching ratios [14]. We used 20 discrete levels in the discrete level scheme of ^{58}Co and 12 in that of ^{90}Y. In Fig. 1 we compare the energy dependencies of the isomeric ratio calculated with the use of different approaches to determine γ transitions. Curves 1 and 3 show the isomeric ratios calculated from the experimental branching ratios but with different radiative strength functions for the continuum: 1 - E1 on the basis of the generalized Lorentzian dependence and M1, E2 on the basis of the Weisskopf theory; 3 - E1 on the basis of the generalized Lorentzian dependence and M1, E2 on the basis of the Lorentzian dependence. Comparison of curves 1 and 3 shows that γ transitions in the continuum have little

influence on the isomeric ratio. Curves 2 and 4 show the isomeric ratios calculated from the computed branching ratios with different radiative strength functions: 2 - E1 on the basis of the generalized Lorentzian dependence and M1, E2 on the basis of the Weisskopf theory; 4 - E1 on the basis of the generalized Lorentzian dependence and M1, E2 on the basis of the Lorentzian dependence. It can be seen from the figure that, even when the discrete γ transitions have a decisive influence on the magnitude of the isomeric ratio, statistical modelling of the branching ratios yields satisfactory results in the calculations of the isomeric ratio. Thus, without claiming to give a detailed description of the branching ratios, we can use statistical calculations of these values to calculate the isomer excitation cross-sections. Further development of this approach will evidently involve refining the radiative strength function ratios for different multiplicities of radiation, for example, M1/E1 and E2/E1.

DESCRIPTION OF $^{90}Y^{m}$ ISOMER YIELDS

For many nuclei and reactions good descriptions of isomeric cross-sections based on theoretical models can be found [1-6]. Sometimes good agreement is attained without any fitting or variation of the parameters; in other cases extremely painstaking work is required to construct schemes of discrete states and the γ transitions between them [3-5]. While in the latter case, experimental data can be described to the required level of accuracy, it remains unclear how strongly the parameters are distorted and how valid these constructions are. This can only be clarified through self-consistent description of the yields of the same isomer in different reactions in a wide neutron energy range.

A suitable candidate for testing the theoretical model is the

$^{90}Y^{m}(J^{\pi} = 7^{+})$ isomer. For this nucleus there are extensive experimental data [15-16] on total reaction cross-sections and isomer population cross-sections in $^{89}Y(n,\gamma)$, $^{90}Zr(n,p)$ and $^{93}Nb(n,\alpha)$ reactions, which result in the ^{90}Y residual nucleus. Thus, a self-consistent description of an entire set of heterogeneous data can be given.

The optical potential parameters used in the calculations were: Arthur's parameters for neutrons, Perry's for protons and McFadden's for α particles. The choice of potentials was based on numerous confirmations of their suitability for the given mass number range. The level density parameters for all the reaction channels are presented in Table 1. These parameters were not varied during the calculations since they are dependent on the description of the competing channels in all three reactions. In Fig. 2 we compare data for the $^{93}Nb(n,2n)$ reaction: reaction cross-sections (2a), excitation cross-section for the isomer $^{92}Nb^{m}$ (2b) and isomeric ratio (2c). The description of the observed cross-sections was obtained without any fitting of the parameters. Curve 2 shows the results of isomeric ratio calculations using the semirigid-body moment of inertia to determine the level density spin dependence parameter for the ^{92}Nb nucleus. For the latter nucleus this parameter obviously needs no correction.

The data for the investigated reactions which lead to the formation of the ^{90}Y nucleus are compared in Figs 3a, 4a and 5a. It can be seen that a good description of the experimental data has been achieved, indicating that the parameters in all the reaction channels are well balanced. We note that these cross-sections are not dependent on the differential characteristics of the γ transitions of the ^{90}Y nucleus since they are the sum of the population cross-sections for the initial and isomeric states.

Figures 3b, 4b and 5b show data on excitation of the $^{90}Y^{m}$ isomeric level in (n,γ), (n,p) and (n,α) reactions. These cross-sections are determined by γ transition characteristics and by the level density spin distribution for the residual nucleus if the remaining model characteristics are fixed by the description of the total cross-sections. Curves 1 give the results of calculations using radiative transmissions, which were calculated in terms of strength functions based on the generalized Lorentzian dependence for E1 radiation and on the Lorentzian dependence for M1 and E2 radiation and with a rigid-body moment of inertia. Curves 2 show the results obtained with the same $f_{\gamma xL}$, but with a semirigid-body moment of inertia for the ^{90}Y nucleus. Evidently, a better description of the experimental data is obtained in the second case. Figures 3c, 4c and 5c give a similar comparison in the case of isomeric ratios. When a semirigid-body moment of inertia is used, there is good agreement between the isomeric ratios in (n,p) and (n,γ) reactions. Divergence between experimental and calculated data for the (n,α) reaction cannot be eliminated by changing the characteristics of the ^{90}Y nucleus (level density and γ transitions) and is most likely due to uncertainties in α particle distributions over orbital angular momenta in the exit channel of the reaction.

Thus, on the basis of $^{90}Y^{m}$ isomer yields in neutron reactions we have successfully demonstrated how the statistical theory of nuclear reactions and the γ cascade model of excited nucleus decay can self-consistently describe all the available experimental data if the model parameters are selected correctly.

PREDICTION OF ISOMER YIELDS

It would be interesting to check whether our method for calculating isomeric cross-sections can be used for other nuclei. It would be most

useful to do this in the case of cross-sections whose description has caused difficulties in the past. One such example is excitation of the $^{179}Hf^{m2}$ isomer with E = 2.446 MeV and spin $J^{\pi} = 16^{+}$ in the $^{179}Hf(n,2n)$ reaction. In order to describe the experimental isomeric cross-section, Chadwick and Young [5] modelled the rotational band constructed for the isomeric level. It was only after this procedure had been carried out that a calculated cross-section value of 2.9 mb was obtained. It is obvious, however, that modelling of the rotational band leads to an effective increase in the number of levels with high spins and, consequently, to an increase in the isomeric state population.

The $^{178}Hf^{m2}$ isomer is very specific since it is in fact located in the excitation level continuum and has sequence number 95, according to the ENSDF file data [14]. It is difficult to calculate the excitation cross-sections of this isomer since in the calculations it is necessary to give input data for all discrete levels and - what is especially difficult - also the scheme of γ transitions between them, which is unknown. The method of determining branching ratios from statistical correlations (2)-(5) can be used to calculate γ transition schemes and, consequently, to overcome this difficulty in preparing the initial data for the calculation.

Figure 6 compares experimental data [17, 18] for the excitation cross-section of the $^{178}Hf^{m2}$ isomer with the calculation results. Curve 1 on this figure shows the calculation results obtained with the modelled γ transition scheme with a rigid-body moment of inertia to determine σ^2 and curve 2 shows those obtained with a semirigid-body moment of inertia. It is evident that the calculated and experimental data show good agreement within the uncertainty of the spin dependence parameter. Unfortunately, there are no cross-section data for the $^{179}Hf(n,2n)$ reaction and self-consistent

calculations cannot be performed although the agreement obtained for the isomeric cross-section demonstrates the reliability of the method used to model γ transitions between discrete levels.

Another interesting case is the $^{175}Lu(n,\gamma)^{176}Lu^{m}$ reaction. Isomer yield data in this reaction are given in Fig. 7. The experimental cross-section ratio σ_m/σ_g [19, 20] lies in the range of 2-5 for a neutron energy of 25-30 keV (points on Fig. 7). In order to achieve agreement with experimental data Gardner and co-workers [4] modelled several rotational bands constructed for known discrete levels. Our calculations (curve 1) of the σ_m/σ_g ratio with radiative strength functions obtained from the Weisskopf correlations for M1 and E2 radiation agree approximately with the result of Ref. [4] without modelling of the rotational bands. When radiative strength functions based on the generalized Lorentzian dependence for E1 and on the Lorentzian dependence for M1 and E2 transitions are used in calculations of γ transition branching ratios, the calculation results (curve 2) are close to the experimental values. Curve 3 on Fig. 7 shows the results of calculations using a semirigid-body moment of inertia. It is clear that the difference between the calculated (curve 2) and experimental values of σ_m/σ_g is determined by the uncertainties of the level density spin dependence parameter.

The results of comparison of experimental and calculated data for isomer yields in $^{179}Hf(n,2n)^{178}Hf^{m2}$ and $^{175}Lu(n,\gamma)^{176}Lu^{m}$ reactions indicate that statistical modelling of the branching ratios of discrete γ transitions can be used to calculate the isomeric cross-sections of these reactions. This conclusion seems very promising since these reactions are very sensitive to the γ transition scheme.

CONCLUSION

In this study we investigated the possibility of using current theoretical models to describe isomer yields in neutron reactions. We obtained a self-consistent description of $^{90}Y^{m}(7^{+})$ isomer yields in (n,γ), (n,p) and (n,α) reactions. The level density spin dependence for the ^{90}Y nucleus needs to be refined in order to improve the description of experimental data. It has been shown that we can overcome the fundamental difficulty in calculating isomeric cross-sections - the lack of experimental γ transition branching ratios for discrete levels - if we employ the ordinary statistical relations with correctly chosen energy dependences of the radiative strength functions. There was no need to model or modify the discrete level schemes in order to describe the experimental isomer yields. Agreement with experimental data was attained after refining the relationships between the radiative strength functions of different multipolarities and their energy dependences.

It is suggested that the branching ratios of γ transitions between discrete levels should be calculated with the use of the ordinary formulae of the statistical model with radiative strength functions based on the generalized Lorentzian dependence for E1 and with those based on the ordinary Lorentzian dependence for M1 and E2 transitions. The method has been validated in the description of isomeric level excitation in cases where experimental branching ratios are available and in isomer yield calculations in $^{175}Lu(n,\gamma)^{176}Lu^{m}$ and $^{179}Hf(n,2n)^{178}Hf^{m2}$ reactions, where description has hitherto required modelling of both the discrete level schemes and the schemes of γ transitions between them. In our opinion, the proposed approach to calculating the isomeric level excitation functions in neutron reactions can be used successfully to determine the yields of long-lived isomers in a fusion reactor.

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Table 1.

Level density parameters used for self-consistent calculations of ^{90}Y isomer yields in neutron reactions. The second column gives the asymptotic level density parameters, the third column the corrections for even-odd differences, the fourth column the corrections to the mass formula for shell effects, the fifth column the energies of the first collective levels, and the sixth and seventh columns give $N_0(U_0)$ - the point above which the model representation of level density was used.

Nucleus	a, MeV^{-1}	δ, MeV	δW, MeV	ω_{2+}, MeV	N_0	U_0, MeV
^{94}Nb	9.15	2.86	-0.79	0.89		
^{93}Nb	8.55	2.11	-1.18	1.06	12	1.297
^{92}Nb	8.56	2.88	-2.32	1.22	11	1.310
^{91}Nb	8.97	2.29	-2.65	1.39	9	1.790
^{93}Zr	10.15	1.23	-1.21	0.92	9	1.464
^{92}Zr	7.84	0.48	-1.43	0.93	6	2.067
^{91}Zr	7.91	1.60	-2.57	1.56		
^{90}Zr	8.88	0.26	-2.94	2.16	10	3.589
^{90}Y	9.32	2.52	-2.73	1.51	11	1.417
^{89}Y	8.79	0.97	-3.24	1.47	12	3.068
^{88}Y	8.70	2.76	-1.55	1.45	8	0.715
^{89}Sr	7.16	1.21	-2.66	1.33	13	2.707
^{86}Rb	7.58	2.78	-1.51	1.32	12	1.122

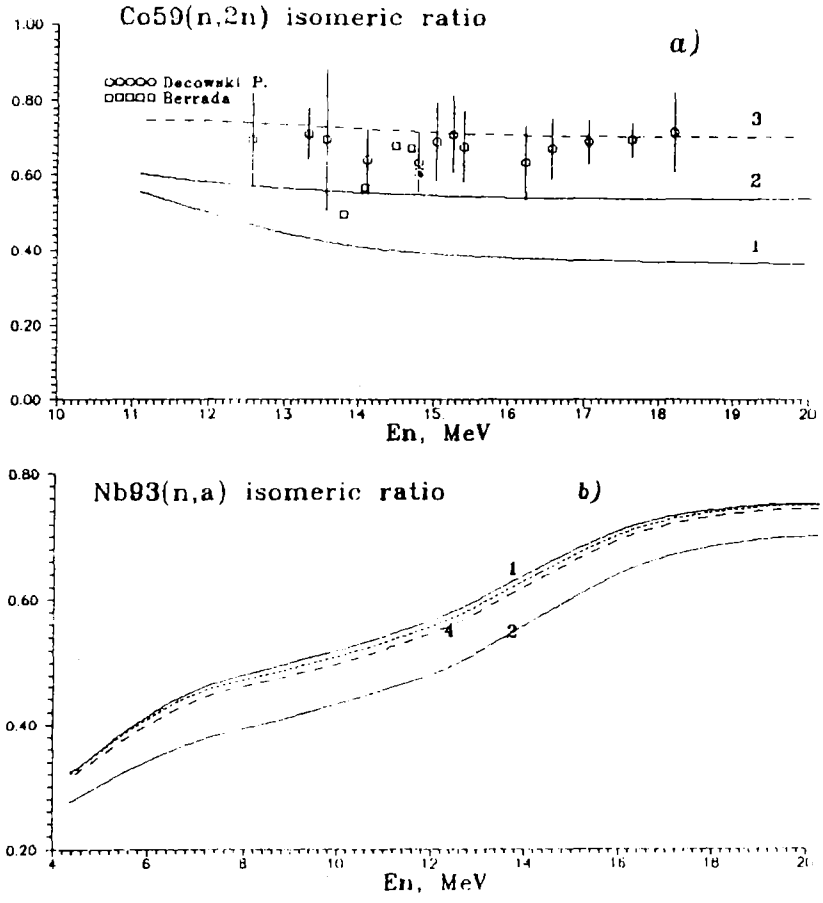

Fig. 1(a). Comparison of model calculations of the isomeric ratio for the $^{59}Co(n,2n)^{58}Co^{m}$ reaction. Curves 1 and 3 are the isomeric ratios obtained from experimental branching ratios and different radiative strength functions for the continuum:

1 - E1 on the basis of the generalized Lorentzian dependence and E2 on the basis of the Weisskopf theory; 2 - E1 on the basis of the generalized Lorentzian dependence and M1, E2 on the basis of the Lorentzian dependence. Curves 2 and 4 are the isomeric ratios obtained from calculated branching ratios with different radiative strength functions:

2 - E1 on the basis of the generalized Lorentzian dependence and M1, E2 on the basis of the Weisskopf theory;

4 - E1 on the basis of the generalized Lorentzian dependence and M1, E2 on the basis of the Lorentzian dependence.

(b). Same as in Fig. 1(a) but for the $^{93}Nb(n,\alpha)^{90}Y^{m}$ reaction.

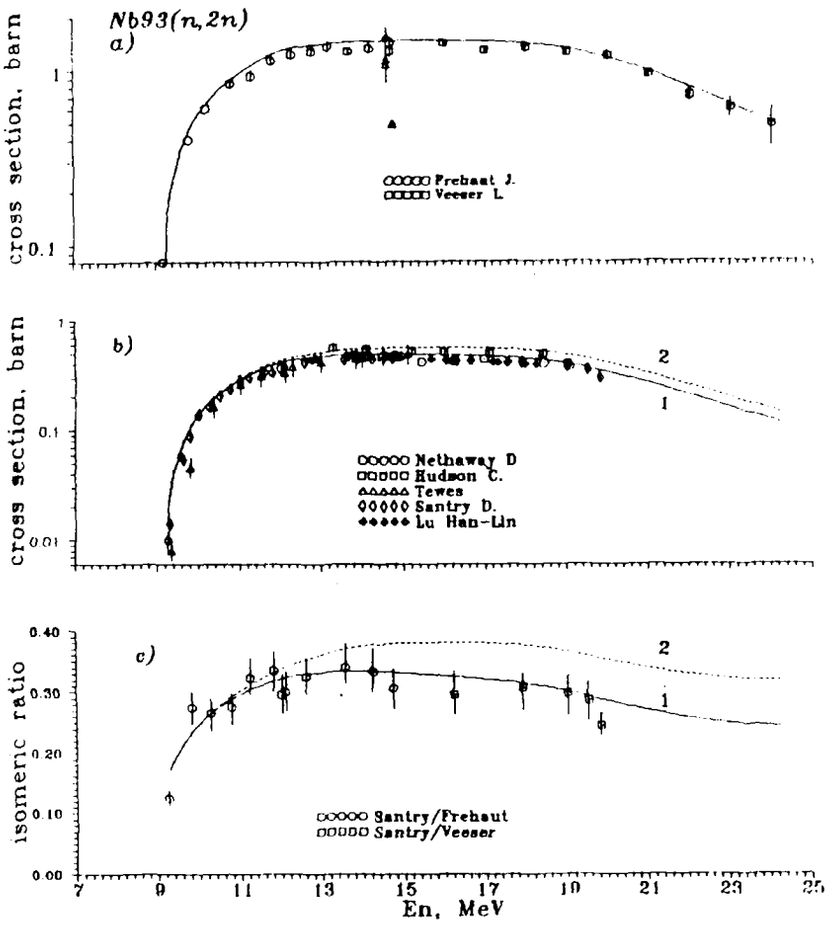

Fig. 2. Data on the excitation function for the ^{93}Nb(n,2n) reaction. Experimental data taken from the handbook [15] are shown as points and the curves represent the results of STAPRE code calculation: (a) reaction cross-section, (b) isomer excitation cross-section, (c) isomeric ratio $\sigma_m/(\sigma_m + \sigma_g)$. Curves 1 are calculated with a rigid-body moment of inertia and curves 2 with a semirigid-body moment of inertia.

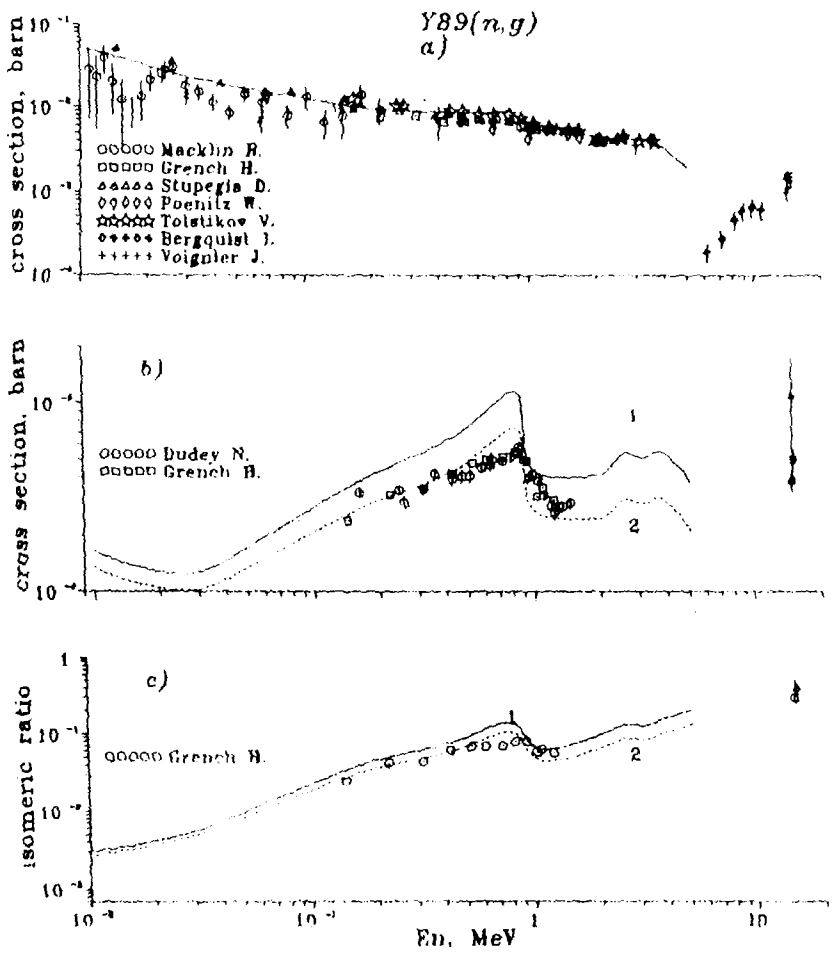

Fig. 3. Same as in Fig. 2 but for the $^{89}Y(n,\gamma)$ reaction. Experimental data taken from Ref. [16].

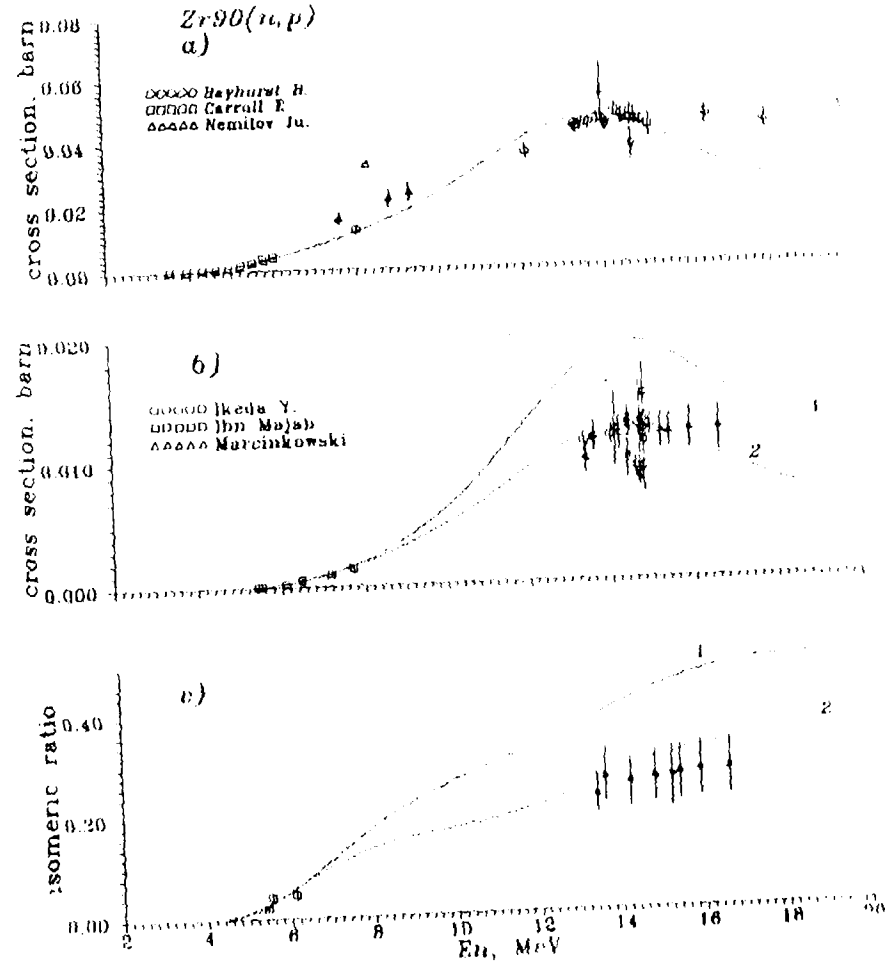

Fig. 4. Same as in Fig. 2 but for the $^{90}Zr(n,p)$ reaction.

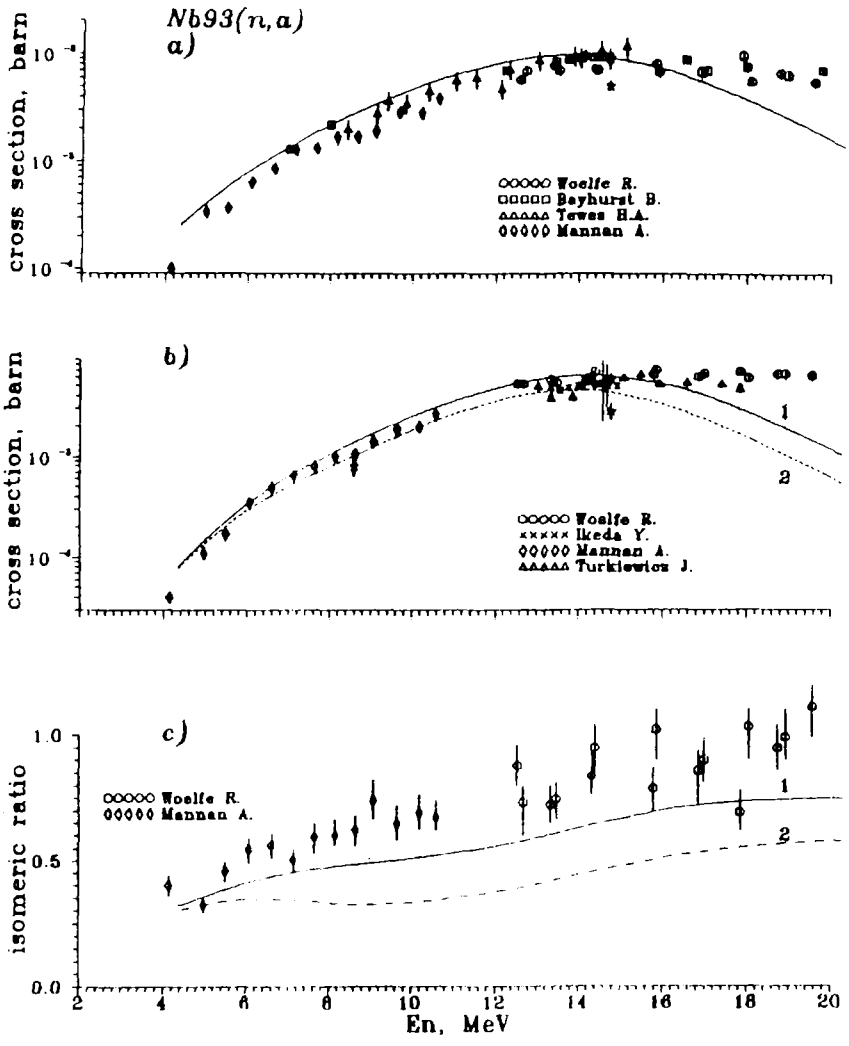

Fig. 5. Same as in Fig. 2 but for the $^{93}Nb(n,\alpha)$ reaction.

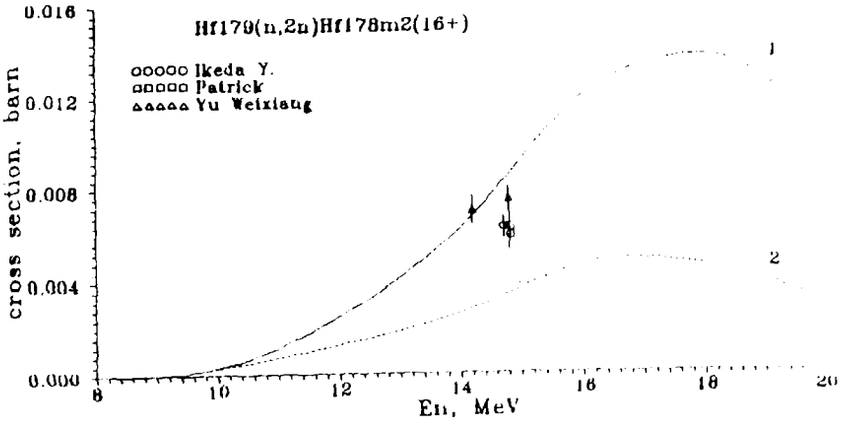

Fig. 6. Data on $^{179}Hf(n,2n)^{178}Hf^{m2}$ reaction cross-section. Experimental data taken from Refs [17, 18]. The curves represent the results of calculations with modelled γ transition schemes: 1 - with a rigid-body moment of inertia, 2 - with a semirigid-body moment of inertia.

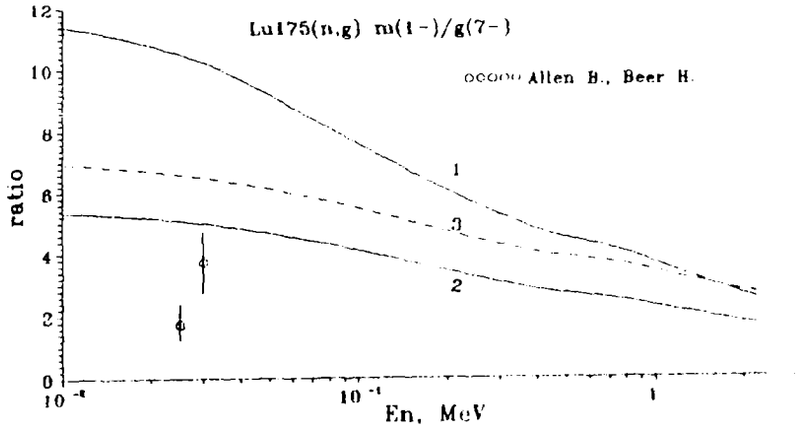

Fig. 7. Data on isomer yield in the $^{175}Lu(n,\gamma)^{176}Lu^{m}$ reaction. Experimental cross-section ratios $\sigma_m(1^-)/\sigma_g(7^-)$ taken from Refs [19, 20]. The curves represent the results of calculation with modelled γ transition schemes: 1 - with a rigid-body moment of inertia, 2 - with a semirigid-body moment of inertia.