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# **Direct Radiative Capture: Test of the Lane-Lynn Model and Development of a Methodology for Calculations**

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DIRECT RADIATIVE CAPTURE: TEST OF THE LANE-LYNN MODEL  
AND DEVELOPMENT OF A METHODOLOGY  
FOR CALCULATIONS

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## Abstract

The Lane-Lynn model for direct radiative capture (DRC) is extended to isotopes where no experimental information on the low-lying levels (spectroscopic factors etc.) is available. To this end we assumed that all the partial transitions to the final levels are lumped in the  $S_{1/2 \rightarrow P_{3/2}}$ ,  $S_{1/2 \rightarrow P_{1/2}}$  transitions only (where the p-wave final states are single particle states with complete strength). Within these assumptions the direct capture cross sections for calcium isotopes between  $A = 40$  and  $A = 48$  as well as for  $^{136}\text{Xe}$  were calculated. We showed that the uncertainties of these calculations are  $\lesssim 30\%$  if we compare the results to the calculations with the Lane-Lynn model for  $^{42, 48}\text{Ca}$  and  $^{136}\text{Xe}$  where the experimental informations required are available. The new approach allows for an evaluation of thermal cross sections and, more important, for the calculation of DRC cross sections of extremely neutron rich nuclei which are significant for nucleosynthesis of the heavy elements in the rapid neutron capture process (r-process).

Direkter Strahlungseinfang: Test des Lane-Lynn-Modells und Entwicklung einer Methodologie für Rechnungen

## Zusammenfassung

Das Lane-Lynn-Modell für direkten Strahlungseinfang (DRC) wird auf Isotope ausgedehnt, für die keine experimentelle Information über niedrigliegende Zustände existiert (spektroskopische Faktoren etc.). Statt dessen wurde angenommen, daß alle partiellen Übergänge zu den Endzuständen ausschließlich in den  $S_{1/2 \rightarrow P_{3/2}}$ ,  $S_{1/2 \rightarrow P_{1/2}}$  Übergängen konzentriert sind (wobei die Endzustände mit  $l=1$  reine Einteilchenzustände sind). Mit diesen Annahmen wurden die Querschnitte für direkten Einfang für die Calciumisotope von  $A = 40$  bis  $A = 48$  und für  $^{136}\text{Xe}$  berechnet. Es wird gezeigt, daß die Unsicherheit der Rechnung  $\leq 30\%$  beträgt, wenn man mit Ergebnissen des Lane-Lynn-Modells für  $^{40, 48}\text{Ca}$  und  $^{136}\text{Xe}$  vergleicht, wo die benötigte experimentelle Information verfügbar ist. Der neue Ansatz ermöglicht die Evaluation thermischer Querschnitte und, was wichtiger ist, die Berechnung der DRC-Querschnitte für extrem neutronreiche Kerne, die für die Synthese der schweren Elemente im sogenannten r-Prozeß von Bedeutung sind.

## Introduction

The inclusion of the photon channel in the general dispersion formalism for the nuclear reactions was first pointed out by Lane and Lynn (1). A term in the collision matrix without resonance behaviour was recognized and referred as "HARD-SPHERE" capture. This is the most important contribution to what is called "POTENTIAL" or simply "DIRECT" capture, the remaining term being the contribution of distant levels.

In the past years the Lane-Lynn model has been used successfully to describe the interaction of thermal neutrons with nuclear matter (2).

Here, we first discuss briefly the expression for the direct radiative capture cross section (DRC) in this model and then from the test cases of several calcium isotopes and of  $^{136}\text{Xe}(n,\gamma)$  we discuss the reliability of the model in the vicinity of closed neutron shells. With some assumptions the DRC can be calculated even where no experimental informations are available for a direct use of the model. This possibility is important for the nuclear physics associated with the neutron radiative capture along the r-process path (rapid neutron capture nucleosynthesis of heavy elements by an intensive neutron burst), where the usual compound nuclear theory may not be sufficient for the calculation of  $(n,\gamma)$  reaction rates (3).

## The Model

The expression for the capture cross section of an s-wave neutron with energy  $E_n$  by a target nucleus  $^A_Z$  of spin  $I_\alpha$  in a final p-wave state with spin  $J_\mu$  and emission of a  $\gamma$ -ray with energy  $\epsilon_\gamma$  and multipolarity  $E1$  is (4):

$$\sigma_{\gamma\mu}^{\text{DRC}} = \frac{0.062}{R\sqrt{E_n}} \left(\frac{Z}{A}\right)^2 \delta \frac{2J_\mu+1}{6(2I_\alpha+1)} S_J \left(\frac{y+3}{y+1}\right)^2 y^2 \left(1 + \frac{R-R'}{R} \frac{y}{y+3}\right)^2 \quad 1.$$

where  $R \equiv 1.35 A^{1/3}$  is the nuclear interaction radius in fermis,  $E_n$  is the energy (in eV) of the incoming neutron,

$\gamma^2 = \frac{2 m \epsilon_\gamma}{\hbar^2} R^2$ ,  $S_J$  is the spectroscopic factor of the final state  $\mu$  and  $m$  is the reduced mass. The parameter  $\delta$  takes into account the incident channel spin multiplicity:

$$\delta \equiv \begin{cases} 1 & \text{for } J_\mu = I_\alpha \pm 3/2 \quad \text{and for } I_\alpha = 0 \\ 2 & \text{for } J_\mu = I_\alpha \pm 1/2 \end{cases}$$

In eq. 1,  $R'$  is the scattering radius. Of course we have that:

$$\sigma_{n,\gamma}^{\text{DRC}} = \sum_{\mu} \sigma_{\gamma\mu}^{\text{DRC}} \quad (\text{barn}). \quad 2.$$

Eq. 1 contains two terms: the "Hard-Sphere" term and the contribution from distant levels. Thus, what we calculate with equation 1 is the fraction of the capture cross section which does not exhibit a resonance behaviour. A contribution to the capture cross section coming from a compound state located in correspondence with the energy  $E_n$  should, in principle, be included to obtain the total capture cross section.

One expects that the DRC mechanism is dominant for thermal neutron capture:

- 1) where no positive and/or negative neutron energy resonances are located close to the thermal energy.
- 2) in the mass region of the minimum of  $R'$  (see fig. 1).

Experimental evidence for DRC are the observed correlations between the gamma ray intensities for the different transitions and the spectroscopic factors of the low-lying levels.

These correlations have been found by Mughabghab (4) for  $^{136}\text{Xe}$ . Moreover, one of the reasons for developing the DRC theory in the earlier work of Lane and Lynn (1) was just the anomalous behaviour of  $\gamma$ -ray spectra around  $A \simeq 50$  proving the role of this mechanism in this mass region. The analysis of the correlations between  $\gamma$ -ray intensities and spectroscopic

factors are shown for  $^{40}, ^{42}\text{Ca}$  in ref. 5 and 6 too.

In view of the importance of this capture mechanism it is desirable to generalize the Lane-Lynn model because the experimental information required by this model is not always available. Therefore, we investigated the possibility to replace the experimental information by two simple assumptions concerning the single particle characteristics of the low-lying levels and the systematics of the scattering radius. The capability of this approach is demonstrated for the DRC of  $^{42}, ^{48}\text{Ca}$  and  $^{136}\text{Xe}$ , and calculations are performed for all even-mass calcium isotopes from  $A = 40$  to  $A = 48$ .

Calculations for  $^{42}, ^{48}\text{Ca}$  and for  $^{136}\text{Xe}$

In appendix A the input for the calculations of  $\sigma_{n,\gamma}^{\text{DRC}}$  is given in detail for  $^{42}, ^{48}\text{Ca}$  as well as for  $^{136}\text{Xe}$ . Equations 1 and 2 yield for these isotopes:

Isotope	$\sigma_{n,\gamma}^{\text{DRC}}$ (mb)	$\sigma_{n,\gamma}^{\text{exp}}$ (mb)
$^{42}\text{Ca}$	568 $\pm$ 55	680 $\pm$ 70
$^{48}\text{Ca}$	868 $\pm$ 43	1090 $\pm$ 140
$^{136}\text{Xe}$	247	260 $\pm$ 20

The experimental values of the third column are from ref. 2. The error given for the calculated cross sections corresponds to the error introduced by the experimental uncertainties of the scattering radius as taken from ref. 2. In the  $^{136}\text{Xe}$  ( $n,\gamma$ ) calculations a scattering radius of 4.8 fermis was taken from the systematics of fig. 1. The agreement between calculation and experiment is quite good. It should be noted that no parameter adjustment was performed for these calculations. In the light of these results and together with the analysis of the correlations in  $^{42}\text{Ca}$  and  $^{136}\text{Xe}$  of ref. 5, we conclude that the Lane-Lynn model, as expressed in eq. 1, is

able to describe the neutron capture mechanism at thermal energy in the mass regions  $A \sim 40$ ,  $A \sim 140$ .

### Assumptions for the DRC calculations

The calculation of  $\sigma_{n,\gamma}^{\text{DRC}}$  using eq. 1 is straight forward when the experimental information concerning the low-lying levels (spin, energy, spectroscopic factor) is known. The additional knowledge of the scattering radius is also necessary for the use of eq. 1. Where these informations are not available, one has to introduce reasonable assumptions.

One may notice that, because of the almost linear dependence of  $\sigma_{\gamma\mu}^{\text{DRC}}$  on the  $\gamma$ -energy  $\epsilon_\gamma$  (through the factor  $y^2$ ), one can replace the final state levels by:

$$\bar{E}_J = \frac{\sum_{\alpha} E_{J\alpha} S_{J\alpha}}{\sum_{\alpha} S_{J\alpha}} \quad \text{and} \quad S_J = \sum_{\alpha} S_{J\alpha}$$

where  $E_{J\alpha}$  is the energy of the level with spin  $J$  and spectroscopic factor  $S_{J\alpha}$ .

The natural assumption that follows this consideration is:

- i) the low-lying final states are replaced by single particle states (p-wave) with  $S_J \equiv 1$ . The energies  $\bar{E}_J$  are simply the centroid energies of the p-wave states of some single particle model (e.g. shell model).

This means that for each nucleus, we assume that all transitions to the low-lying levels are lumped in only two transitions:

$$s_{1/2} \longrightarrow p_{3/2} \quad \text{and} \quad s_{1/2} \longrightarrow p_{1/2}$$

### Estimated uncertainties of the model

As a test of this statement we repeated the calculations for the above isotopes which were performed using the information of experimental levels. Moreover, we calculated the DRC cross section for all the even mass calcium isotopes in  $40 \leq A \leq 48$ . The results are summarized in table I and plotted in graphic form in Fig. 2.

By comparison of the results obtained with the experimental centroid energies and strengths ( $S_J$  from (d,p) measurement) and those with the calculated centroid energies and  $S_J = 1$  (table I), we estimate a 20 % the uncertainty introduced by statement i).

The scattering radius  $R'$  that represents the second term in eq. 1 for  $\sigma_{n,\gamma}^{\text{DRC}}$  can be determined either from:

- 1) experiments
- 2) the systematics of fig. 1, or
- 3) by calculation through the relation:  $\sigma_{\text{SE}} = 4\pi(R')^2$   
where  $\sigma_{\text{SE}}$  is the shape elastic scattering cross section.

In the last case one has to perform an optical model calculation (e.g. using the Hauser-Feshbach formalism), as it is shown in Fig. 1 in comparison to experimental values. From this figure, it is found that the optical model calculations of  $R'$  fit the experimental data quite good. A maximum deviation of  $\sim 20\%$  is observed around  $A \sim 80$ . The influence of  $R'$  on the DRC calculation is illustrated in table I where the calculated cross sections are given with the error that corresponds to the experimental uncertainty in the scattering radius. One finds that an average uncertainty of 8 % in the scattering radius causes an average uncertainty of 10 % in the calculated cross section. We also notice that in the  $A \sim 40$  mass region, the scattering radius plays a fundamental role in the calculation of the DRC cross section. In fact, in this mass range the term containing  $R'$  in eq. 1 is about two times bigger than the Hard-Sphere contribution. In the mass region around  $A = 140$ , the systematics as well as the optical model calculations of the scattering radius are better defined. Thus, we can infer that an uncertainty of 10 % in the model calculations due to  $R'$  could be taken as an upper limit.

Methodology of calculation and further remarks

As mentioned in the introduction, our aim was neither a perfect calculation of the thermal cross sections nor a simple application of the DRC model. We intended to investigate the reliability of the model under assumptions that can provide the possibility to calculate the radiative capture cross section, even if no experimental informations are available for the nuclide in question. Indeed, we have shown that we can calculate the DRC cross sections having on hand nothing else but a good set of single particle potentials and the scattering radius  $R'$ .

In the calculation of the single particle eigenstates we have used a global set of potential parameters like those of Bear and Hodgson (see ref. 7) which also include a neutron asymmetry term. The single particle potential used was of the form:

$$V(r) = -V_0 f(r) - 2V_{so} \left\{ \frac{\hbar}{m c} \right\}^2 \frac{1}{r} \frac{df}{dr} \vec{l} \cdot \vec{s}$$

where:

$$f(r) = \frac{1}{1 + e^{\frac{r-R}{d}}}, \quad \begin{aligned} R &= 1.236 A^{1/3} \\ d &= 0.62 \text{ fm} \\ V_{so} &= 7.0 \text{ MeV} \\ V_0 &= 55.7 - 39.3 \left( \frac{N-Z}{A} \right) \text{ MeV.} \end{aligned}$$

$l$  is the orbital angular momentum of the single particle state ( $l = 1$  in our case) and  $s = 1/2$  is the neutron spin. This set of parameters was not primarily chosen to reproduce the experimental values of the thermal cross sections but because it provides a good fit to the systematics of bound single particle states for a broad range of nuclei ( $12 \leq A \leq 208$ ). This means that, most probably, the calculations can be further improved by a more careful choice of the potential parameters especially if one is only interested in limited mass regions.

The calculations performed with  $S_J \equiv 1$  and the calculated centroid energies

- 1) yield higher cross sections than if the experimental energies and strength were used.
- 2) This agree better with the experimental cross sections.

Point 1. could be explained, for instance considering that the total Hamiltonian of a given nucleus can be expressed as:

$$H_T = H_{sp} + V_{res}$$

where  $H_{sp}$  is a single particle Hamiltonian and  $V_{res}$  is the residual interaction responsible for the "sharing" of nuclear states. Part of the strength of the nuclear levels is within the continuum part of the spectra of  $H_T$  and thus, in a (d,p) experiment one cannot resolve the levels above a certain excitation energy. This, in other words, means always that  $S_J^{exp} \leq 1$ .

Indeed, part of our assumption is that all the strength of the final p-wave states is held by the levels themselves. This can only increase the calculations of the DRC cross section as

$$\sigma_{\gamma\mu}^{DRC} \propto S_J.$$

This effect is partially compensated by the position of the single particle level. The  $\sigma_{\gamma\mu}^{DRC}$  being sensitive to the energy of the emitted gamma-ray a depression of the calculated level produces an increase of the cross section and vice versa.

This also means that our calculations are model-dependent in the sense that the single particle potential has an influence on the calculations.

About point 2., one should first notice that the theory gives us only a lower limit for the capture cross section because the compound term needs also to be included. From the comment on point 1. one can conclude that the fictitious assumption of complete spectroscopic strength ( $S_J = 1$  for the final states)

is "responsible" for the improved results of the calculations.

Anyhow, looking at the plotted values in fig. 2 we conclude that the DIRECT mechanism gives a satisfactory explanation for thermal neutron capture in the mass region around  $A = 45$ .

Having established the "degree of confidence" of eq. 1 for the calculation of the DRC cross section with our assumptions, we give here the typical scheme of the input-output for the code "TOAST" developed for DRC calculations. As the most important subroutine the code includes the program for the calculation of the single particle energy levels (and wave functions if necessary) in a Saxon-Wood potential well (ref. 8):

INPUT:

- Mass and atomic number of the target nucleus
- Target spin  $I_{\alpha}$

Calculation with  
experimental levels

- Neutron separation energy for the  $n +$  target system
- Energy, Spin and spectroscopic factor of the final states

Calculation with  
single particle levels

- Potential parameters for the Saxon Wood well

OUTPUT:

- 1) Hard-sphere component of the DRC cross section (if the scattering radius  $R'$  is put equal to 0)
- 2) DRC cross section (eq. 1)

TOAST is running under TSO on the IBM 370/168 computer at KfK (Karlsruhe).

DRC at higher energies for very neutron rich nuclei

All the above considerations referred to thermal energies ( $E_n = 0.0253$  eV). Since  $\sigma_{n,\gamma}^{\text{DRC}}$  depends on the incident energy by  $1/\sqrt{E_n}$  (this holds at least for  $E_n \ll Q_s$ , where  $Q_s$  is the binding energy of the final state), the DRC cross section decreases drastically at higher energies. In fact, in the keV range  $\sigma_{n,\gamma}^{\text{DRC}}$  is of the order of several hundred micro barns and therefore this contribution can be neglected in comparison with the compound nucleus contribution (statistical model). This has been shown by Longo et al. (6) who compared the relative contributions of direct, statistical and valence capture for  $^{40}\text{Ca}(n,\gamma)$  from thermal energies up to 2 MeV. However, this situation is very different for extremely neutron rich nuclei where the neutron binding energies are significantly smaller (2 MeV or even less). In these cases the compound nucleus contribution to radiative capture is strongly reduced because of the low level densities and might even be smaller than the DRC as has recently been demonstrated (3) for the Cd isotopes at neutron energies around 100 keV.

We have to emphasize again that the DRC model, as formulated here, provides always a lower limit for the  $(n,\gamma)$  cross section particularly at high neutron energies. This is because:

- 1) the probability for compound states (resonances) becomes higher as the energy rises from thermal to the keV region and
- 2) contributions from direct capture of p-wave neutrons has to be taken into account, too.

This last point can be solved, in principle. In fact, the problem is the generalization of eq. 1 for higher angular momenta of the incoming particles as well as the calculations of s and d-wave final single particle states.

## Conclusions

In summary we can briefly conclude that:

- 1) The Lane-Lynn model gives a correct value for the capture cross section at thermal energies in the mass region  $A \approx 40$  and  $A \approx 140$ .
- 2) Adopting the calculated values for the centroid energies of the single particle p-wave states populated by direct capture of the incoming neutrons, we introduce an uncertainty of  $\lesssim 20$  %.
- 3) In addition a uncertainty of  $\approx 10$  % in the calculations has to be admitted due to the uncertainty of the scattering radius which accounts for the effect of distant levels in the DRC model. This uncertainty is smaller in those mass regions where the Hard-Sphere term becomes dominant.
- 4) The described model gives only a lower limit for the thermal cross section. In fact, a contribution from compound states located close to the thermal energy could be present.
- 5) At higher neutron energies a contribution from p-wave neutrons should be included in the DRC model.

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TABLE I

Isotope	R'	$\sigma_{n,\gamma}^{\text{DRC}^{\text{a)}}$ (mb)	$V_0$ (MeV)	$\sigma_{n,\gamma}^{\text{DRC}^{\text{b)}}$ (mb)	$\sigma_{n,\gamma}^{\text{exp}^{\text{c)}}$ (mb)
$^{40}\text{Ca}$	3.6 $\pm$ .3		55.7	574 $\pm$ 100*	410 $\pm$ 20
$^{42}\text{Ca}$	3.08 $\pm$ .2	568 $\pm$ 55*	53.8	693 $\pm$ 70 *	680 $\pm$ 70
$^{44}\text{Ca}$	1.79 $\pm$ .09		52.1	1088 $\pm$ 36*	880 $\pm$ 50
$^{46}\text{Ca}$	2.52 $\pm$ .25		50.6	747 $\pm$ 79*	740 $\pm$ 70
$^{48}\text{Ca}$	1.5 $\pm$ .15	868 $\pm$ 43*	49.2	1000 $\pm$ 51*	1090 $\pm$ 140
$^{136}\text{Xe}$	4.8	247	47.6	281	260 $\pm$ 20

a) DRC cross sections calculated with experimental centroid energies (see Appendix A)

b) DRC cross sections calculated with single particle p-wave states in a Saxon-Wood potential well (see text for explanations)

c) Experimental thermal capture cross sections from ref. 2.

\* The uncertainties given for the calculated cross sections correspond to the uncertainties in the R' values.

APPENDIX A : Details of the calculations for  $^{42,48}\text{Ca}$  and  $^{136}\text{Xe}$

1.  $^{42}\text{Ca}(n,\gamma)$   $E_n = \text{thermal}$

Target spin and parity  $I_\alpha^\pi = 0^+$

Neutron binding energy  $S_n = 7.933 \text{ MeV}$  (Ref.2)

Scattering radius derived (according to ref. 2) by

$$R' \approx \frac{b_{\text{coh}} - Z (-1.38 \times 10^{10-3})}{\left(\frac{A+1}{A}\right)} = 3.08 \pm 0.20 \text{ fm}$$

Low-lying p-wave levels:

The experimental centroid energy is defined by:

$$\bar{E}_J \equiv \frac{\sum_\alpha E_{J\alpha} S_{J\alpha}}{\sum_\alpha S_{J\alpha}} \quad \text{and} \quad \epsilon_\gamma \equiv S_n + E_n - \bar{E}_J.$$

(n l j)	$S_J$	$\epsilon_\gamma$ (MeV)	
2 p 3/2	0.876	5.775	(Ref.9)
2 p 1/2	0.645	4.243	

The calculated levels are:

2 p 3/2	1.0	5.877	Bear-Hodgson potential
2 p 1/2	1.0	3.950	parameters (7)

The DRC calculations yield:  $\sigma_{n,\gamma}^{\text{DRC}}$  (exp. levels) = 568 mb

$\sigma_{n,\gamma}^{\text{DRC}}$  (calculated levels) = 693 mb

2.  $^{48}\text{Ca} (n, \gamma)$   $E_n = \text{thermal}$   
Target spin and parity  $I_{\alpha}^{\pi} = 0^{+}$   
Neutron binding energy  $S_n = 5.142 \text{ MeV}$  (Ref. 2)  
 $R' \approx a_{\text{coh}} = 1.50 \pm 0.15 \text{ fm}$  (see above)

Low-lying p-wave levels:

(n l j)	$S_J$	$\epsilon_{\gamma}$ (MeV)	
2 p 3/2	0.953	5.044	(Ref.10)
2 p 1/2	0.980	3.114	

The calculated levels are:

2 p 3/2	1.0	5.348	Bear-Hodgson potential
2 p 1/2	1.0	3.552	parameters (7)

The DRC calculations yield:

$$\sigma_{n, \gamma}^{\text{DRC}} (\text{exp. levels}) = 868 \text{ mb}$$

$$\sigma_{n, \gamma}^{\text{DRC}} (\text{calc. levels}) = 1000 \text{ mb}$$

3.  $^{136}\text{Xe}(n,\gamma)$   $E_n = \text{thermal}$

Target spin and parity  $I_{\alpha}^{\pi} = 0^{+}$

Neutron binding energy  $S_n = 4.025$  (Ref. 5)

The scattering radius is taken from systematics of fig. 1 (see text):  $R' = 4.8$  fm

Low-lying p-wave levels

Cn l j)	$S_J$	$\epsilon_{\gamma}$ (MeV)	
3 p 3/2	0.49	3.475	(Ref. 2)
3 p 1/2	0.95	2.179	

The calculated levels are:

3 p 3/2	1.0	2.462	Baer-Hodgson potential
3 p 1/2	1.0	1.603	parameters (7)

The DRC calculations yield:  $\sigma_{n,\gamma}^{\text{DRC}}$  (exp. levels) = 247 mb

$\sigma_{n,\gamma}^{\text{DRC}}$  (calc. levels) = 281 mb

Figure captions

Fig. 1 The variation of  $R'$  with mass number  $A$  (ref. 2)  
The solid curve is based on deformed optical model calculations with the parameters  $V_0 = 43.5$  MeV,  $r_0 = 1.35$  fm,  $V_{s0} = 8$  MeV and a surface absorption  $W_D = 5.4$  MeV. The dotted curve describing the trend at low mass number is based on spherical optical model calculations using the same parameters.

Fig. 2 Comparison of calculated DRC cross sections with experimental results from ref. (2) for even-mass calcium isotopes at thermal energy. The calculated values  $\sigma_{n,\gamma}^{DRC}$  (see Tab. I) are derived under the assumptions given in the text. The spread of the calculated values corresponds to the uncertainties of the scattering radius  $R'^{exp}$ .

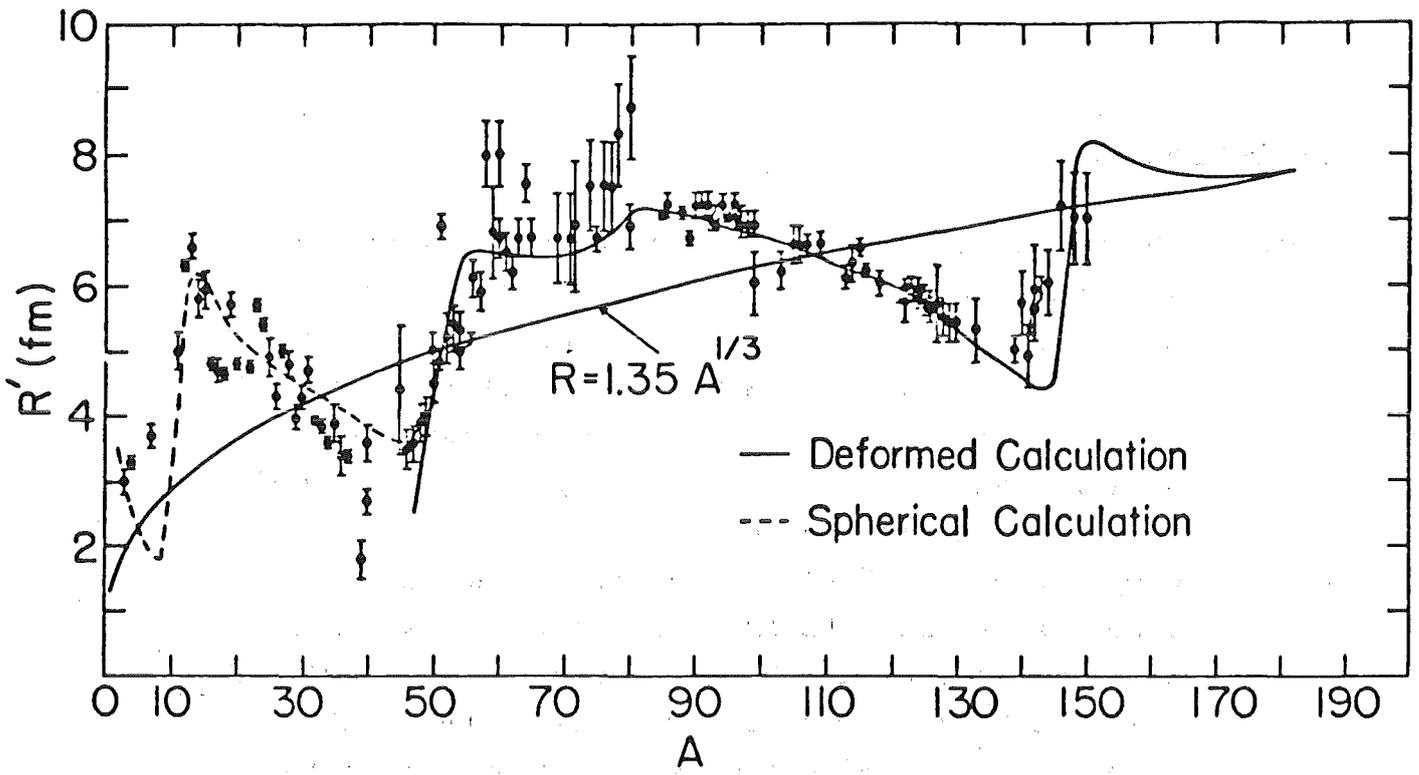


Fig. 1

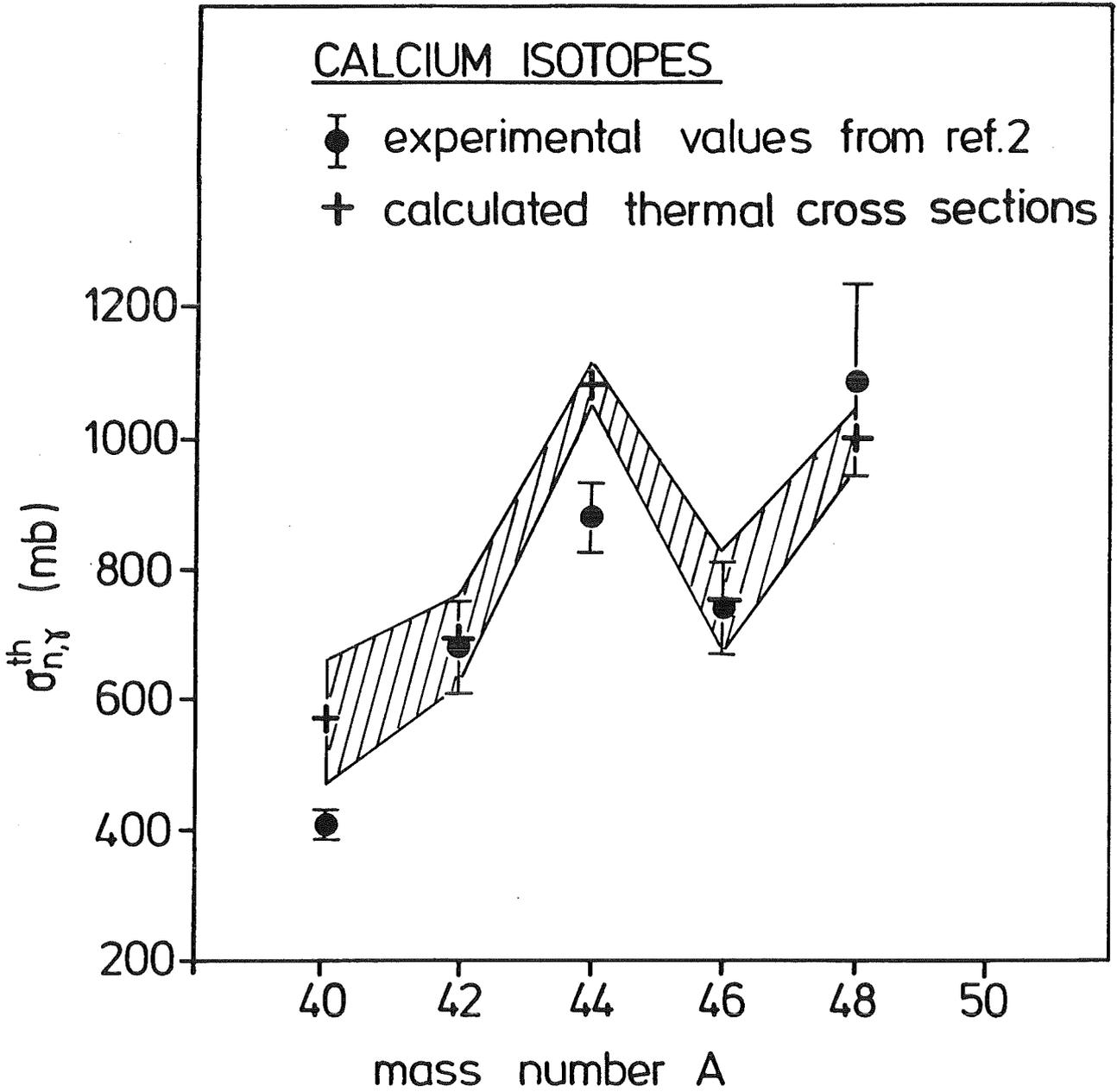


Fig. 2