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Multilevel Resonance Analysis of the Total Neutron Cross Sections of ^{23}Na and Ca below 1 MeV

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Abstract

The total neutron cross sections of ^{23}Na and Ca measured with the time-of-flight facility at the Karlsruhe Isochronous Cyclotron have been analyzed below 1 MeV in order to provide neutron resonance parameters. The analysis uses the standard multilevel R-matrix formulae for a single open channel. A chi-squared fitting procedure is used for shape analysis. Resonance widths and energies have been assigned for ^{23}Na up to 900 keV. The values of l and J have been determined up to 432 keV; above this energy the assigned J values are only lower limits. In the case of Ca, the parameters of resonances between 0.5 and 1.2 MeV have been determined. In many cases we have used new differential data for Ca to verify the l value obtained by fitting the resonance. The channel radius and s and p-wave strength functions of this nucleus are also discussed.

Zusammenfassung

Die mit dem Flugzeitspektrometer am Karlsruher Isochron-Zyklotron gemessenen totalen Neutronenwirkungsquerschnitte für ^{23}Na und Ca wurden unterhalb 1 MeV zur Bestimmung von Resonanzparametern mit dem R-Matrix Formalismus analysiert. Zur Anpassung nach der Methode der kleinsten Fehlerquadrate wurde eine Ein-Kanal-Multiniveauformel verwendet. Resonanzenergien und Breiten wurden für ^{23}Na bis 900 keV zugeordnet. Spins und Paritäten (l-Werte) wurden bis 432 keV bestimmt; oberhalb dieser Energie gelten die zugeordneten J-Werte nur als untere Grenze. Für Ca wurden Resonanzparameter im Energiebereich von 0.5 bis 1.2 MeV bestimmt. Neue differentielle elastische Streuquerschnittsdaten für Ca wurden in vielen Fällen zur Bestätigung der l-Werte herangezogen. Der Kanalradius und die s- und p-Wellen-Stärkefunktionen werden für diesen Kern ebenfalls diskutiert.

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MULTILEVEL RESONANCE ANALYSIS OF THE TOTAL NEUTRON CROSS SECTION OF ^{23}Na AND Ca BELOW 1 MeV

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1. INTRODUCTION

The neutron total cross section of Na is of obvious importance for fast reactor calculations. In recent years, several new measurements have been performed [1 - 6]. In this work, these measurements are compared, and our results are analyzed by the multilevel one-channel R-matrix formalism. In spite of the wealth of data for Na, there appears to be a paucity of detailed analysis, the work of Stelson and Preston [7] and of Hibdon [8] being exceptions. At least for high neutron energies, ($E > 0.432$ MeV), this is due to the lack of a reliable two-channel multilevel fitting program. This work attempts an extension of the one-channel description to higher energies where it is clearly an incorrect description. The first excited state of the ^{23}Na nucleus occurs at 0.432 MeV, but the "elastic scattering only" description has been pushed to 1 MeV. It was hoped that the failure of the description could also provide some indication of the extent and influence of inelastic scattering in this region. In fact, it has been found that the elastic scattering picture does provide a fairly good phenomenological description up to 1 MeV. The interpreted J-values must be taken as lower limits and one must be very careful about reading too much physical meaning into the results above 0.5 MeV.

The ^{40}Ca results may be of interest because the l- and J-values reported were determined from our high resolution, differential elastic scattering cross section measurements. The assignments were accomplished by studying the resonance shapes as a function of the scattering angle. The formalism required has been highly developed by Blatt and Biedenharn [9]. This work is currently in press [23]. The results of a preliminary study [10] and some differential scattering measurements and analysis of ^{12}C [11] have already been published.

Calcium also provides an example of a clean nucleus for the single channel description. The inelastic channel is not open until 3.354 MeV and the ground state spin is zero, making the channel spin unique. Furthermore, a quick view of any high resolution data for calcium above a few hundred keV indicates that multilevel interference will be important. For these reasons, analysis of this neutron cross section is discussed here.

In the following sections, the Karlsruhe experimental setup is reviewed and the R-matrix formulae used in this work are summarized. Both the experimental details [12] and the theory [13 - 15] are covered in much more detail elsewhere. Resonance parameters are given for Na and Ca. In the case of sodium some previous assignments are corrected. The calcium results considerably extend previous analysis.

2. EXPERIMENTAL DESCRIPTION

The total neutron cross sections of sodium and calcium were measured with the neutron time-of-flight facility at the Karlsruhe Isochronous Cyclotron and were previously published [5, 6]. The detailed description of the spectrometer has been given elsewhere [12] and hence only features pertinent to these measurements will be described here. These data were obtained for the energy range from 290 keV (500 keV Ca) to 40 MeV by transmission measurements with good geometry. Neutrons were produced in bursts of $\approx$ 1 nsec duration by bombarding a uranium target with deuterons of the internal cyclotron beam at a repetition rate of 19.13 kHz. Standard time-of-flight techniques were used for data collection. A liquid scintillator (NE-213), 9 cm in diameter by 1 cm thick, mounted on a XP-1040 photomultiplier was used for neutron detection. The incident neutron beam was monitored by a γ pulse-shape discriminating detector placed at 6° to the beam at a distance of 11 m from the source. About 8200 time channels were analyzed by a Laben UC-KB and recorded in a CDC on-line computer.

With a flight path of about 57 m, an overall resolution of better than 0.05 nsec/m was achieved. This corresponds to an energy resolution of 0.22 keV at 300 keV and 2.5 keV at 1.5 MeV. The scattering sample for sodium was a high purity (99.998 %) metal slab[1], 0.2323 atoms/barn, sealed in an aluminum can. The calcium sample had a thickness of 0.2133 atoms/barn and consisted of granulated metal enclosed in a cylindrical aluminum container with thin end windows. In both cases an identical empty can was put into the open beam position for background compensation. Spectra were measured with the sample in place and with sample removed in a typical cycle time of 20 min. Uncertainties in the calcium cross section due to counting statistics varied from 5 % at 800 keV to 3 % at 1.5 MeV. The sodium data have a statistical uncertainty of less than 0.3 % between 600 and 900 keV and smaller than 1 % between 420 and 600 keV. Corrections for background and dead time effects were applied. The combined corrections were typically a few percent of the open beam counting rate and did not exceed 20 % below 1 MeV. Corrections for in-scattering were less than 0.01 % and were not performed.

3. SINGLE CHANNEL MULTILEVEL DESCRIPTION

Since resonance widths are approaching the level spacings for Na and Ca in the energy region investigated, the usual Breit-Wigner single level formulae are not applicable. An appropriate formalism

[1]The machining and canning of this sample was performed by the CBNM, Geel.

is the multilevel R-matrix description with a single open channel for elastic scattering. This description will be exact for Ca and Na below the thresholds for inelastic scattering, assuming γ-ray channels to be negligible.

Of course much has been written about the R-matrix formalism [13 - 16]. The following is intended only to summarize the formulae used in this analysis. According to Lane and Thomas [13], the R-function can be divided into an explicit multilevel sum R'_{lJs} and a background term R^o_{lJs},

$$R_{lJs} = R^o_{lJs} + \sum_\lambda \frac{\gamma^2_{\lambda lJs}}{E_\lambda - E} \quad ,$$

where the sum is over λ levels of total angular momentum J, orbital momentum l and channel spin s. The quantities E_λ are the eigenvalues of the internal nuclear region and the reduced widths $\gamma_{\lambda lJs}$ are given by the projection of the internal wave functions onto the channel surface.

The R-function is related to the collision function, U_{lJs}, by

$$U_{lJs} = \exp(-2i\phi'_l)\ (1 + 2i\ P'_l \frac{R'_{lJs}}{1-L'_l\ R'_{lJs}}) \quad ,$$

where the newly introduced quantities contain the background term R^o_{lJs}. These are defined as,

$$L'_l = S'_l + i\ P'_l$$

$$S'_l = [S_l(1 - R^o_{lJs}\ S_l) - R^o_{lJs}\ P_l^{\ 2}]\ /d$$

$$P'_l = P_l/d, \qquad d = (1 - R^o_{lJs}\ S_l)^2 + (R^o_{lJs}\ P_l)^2$$

$$\phi'_l = \phi_l - \arctan[R^o_{lJs}\ P_l/(1 - R^o_{lJs}\ S_l)]$$

$$S_l = S^o_l - B_l \quad ,$$

where S^o_l, P_l and ϕ_l are the usual shift factor, penetration factor and potential scattering phase shift.

The total neutron cross section is given by

$$\sigma_t = \frac{2\pi}{k^2} \sum_{lJs} g_J \, (1 - \mathrm{Re}\, U_{lJs}) \quad ,$$

where g_J is the spin weight factor.

Since the R-matrix formulation does not directly specify the eigenvalues E_λ and internal eigenfunctions, the boundary condition B_l is arbitrary. The total cross section is independent of the choice of this quantity. It is convenient to choose B_l in such a way that the level shift factor vanishes. Then, without strong resonance-potential interference, the physical resonance peaks occur at the energies E_λ. The level shift factor can be made zero by choosing $B_l = S_l(E)$, but the price of this energy dependent boundary condition is that the parameters E_λ and $\gamma_{\lambda lJs}$ are no longer simply related to the eigenvalues of the internal region and the projection of the eigenfunctions on the channel surface. The level shift is identically zero for s-wave neutrons and there is no change in interpretation from the usual energy independent boundary condition B = 0. It can also be shown that for higher l-values the energy dependence introduced into E_λ and $\gamma_{\lambda lJs}$ is small /14/.

Another important quantity to be considered in practical application of the R-matrix formulae is the channel radius which is closely related to the treatment of resonances outside the region of analysis. Detailed parameters can only be obtained for an energy range which includes a restricted number of local levels. Nevertheless, the influence of levels outside this range is not negligible. This may be accounted for by an expansion of the R^o_{lJs} background term about the median energy E_m of the region of analysis /17/,

$$R^o_{lJs} = A_{lJs} + B_{lJs}\,(E - E_m) + C_{lJs}\,(E - E_m)^2 + \ldots .$$

The coefficients A, B and C may be l and J dependent and represent parameters to be determined as well as the resonance energies and widths. Their influence and interpretation depend strongly on the nucleus and energy region.

The constant term A_{lJs} may be understood as a representation of the effect of very far away resonances in the energy region of interest. Such would be the case, for example, for a far removed "giant resonance" containing many individual levels. At low energies, it can be interpreted as a channel radius correction which makes the total cross section independent of the assumed channel radius. The effect is seen mainly in the potential scattering cross section. The coefficient B_{lJs} has been shown to be directly related to the corresponding strength function [17]. In particular it contains that fraction of the total strength not arising from the local levels which have been explicitly included in the level sum.

The above formulation has been programmed [18]. The code operates by a χ^2 minimization, given a particular input set of resonance assignments (l- and J-values). The results obtained are the E_λ, Γ_λ, A, B and C parameters for all possible l and J values. The experimental resolution function can also be folded with the theoretical cross section to better represent the experimental data.

4. CROSS SECTIONS AND RESONANCE PARAMETERS

Cross section data and resonance parameters are given here for sodium and calcium. The total neutron cross section for Na from 0.28 to 1.02 MeV is shown in Figure 1. The solid curve was calculated using the parameters listed in Table I. The first four columns of the table give the analyzed resonance energy, the fitted neutron width and the l and J values. These parameters are based on a one-channel description. Column 5 gives the observed total width which is different from the fitted neutron width only for the five cross section fluctuations observed above 500 keV. The A and B parameters discussed previously are shown at the bottom of the table. Several smaller resonances are also identified in the table; owing to their size and narrowness, no attempt has been made to analyze these levels. The assignments and parameters are discussed later.

Figure 2 compares these data with other total cross section data available from CCDN. Nearly all data lie in a band which is approximately 15% of the cross section value. The data of Hibdon [8] and Whalen et al. [4] demonstrate a significant shift of resonance peaks to higher energies. This is clearly seen for the 300 keV resonance. In general we agree best with the Langsford data [2], but neglecting the energy shift there is also excellent agreement in the regions between resonances with the Whalen data. Considering the point scatter of some of the earlier measurements the overall agreement is very satisfactory.

The total neutron cross section for calcium from 0.56 to 1.26 MeV is shown in Figures 3 and 4. The solid curve again illustrates the calculation. Only those resonances sufficiently resolved for analysis were included in the calculation. In this energy range, this unfortunately eliminates many narrow resonances. The ^{40}Ca resonance parameters are listed in Table II. In nearly all cases the l and J values were obtained by analysis of our differential scattering cross section data. The total cross section alone does not permit a clear separation of p- and d-wave resonances or of the appropriate J-values for narrow resonances.

The calcium resonance parameters have been further analyzed for the level spacing and s-wave strength function. An s-wave spacing of (38.6 ± 7.6) keV and a strength function of $(2.8 \pm 1.0) \times 10^{-4}$ are found. These values are in good agreement with other results [19, 20].

5. DISCUSSION

5.1 Analysis of Na Resonances

The resonance parameters obtained for ^{23}Na have been given in Table I. In this section, the analysis is discussed in further detail. The inelastic scattering cross section is not very large below 1 MeV. Recommended values for $\sigma_{n,n'}$ indicate about 300 mb [21]. Since a satisfactory two channel fitting procedure has not been available we decided to try to extend the elastic scattering formulae. However, above 500 keV, the reported J-values must be understood as lower limits. The true total cross section is reduced from that given by the one-channel formalism by approximately a factor $\Gamma_n/(\Gamma_n + \Gamma_{n'})$ due to inelastic scattering.

298 keV: Because of a pronounced interference shape, this level is assigned to s-wave neutrons. The J-value of 2 is also clear. This analysis yields a neutron width of 1.9 keV rather than 4 keV as reported previously [7]. It seems that just this problem of experimental resolution is the cause of the previous assignment to J=1. No evidence was seen for the J dependence of the s-wave potential scattering reported by Stelson and Preston.

394 keV: The parameters obtained for this level agree with those previously reported. Only slight changes in the resonance energy and neutron width have resulted from this analysis.

431 keV: This small level is assigned to p-wave neutrons with J=0; it had not been seen in previous cross section measurements. The J-value is certain for this 8 keV resonance width since the narrow 1.9 keV level at 298 keV was fully resolved in our data.

449 keV: This resonance is assigned to p- or d-wave neutrons and is well fitted by J=2. We find a width of 5.8 keV rather than the previously reported value of 9 keV for J=1. This again seems to be explainable by the experimental resolution. A value of $l=2$ is favoured by the differential data obtained by Chien [22].

537 keV: Because of the interference pattern, this level is certainly due to s-wave formation. The value of J=1 gives an excellent description. In principle, the J-value could be higher since inelastic scattering can occur. However, this is extremely unlikely since the inelastic neutron would have only about 100 keV and a small penetrability in comparison with a 537 keV s-wave neutron. The first excited level of ^{23}Na has been assigned $5/2^+$; thus the inelastically scattered neutron must have an orbital momentum $l \geq 2$ and a low penetrability.

597 keV: The cross section at this resonance agrees well with $l \geq 1$, J=1. Again the inelastic scattering width must be very large in order to permit an assignment J=2. However, this argument is less convincing for this $l \geq 1$ resonance than for the previous s-wave level.

710 keV and 780 keV: The J-values assumed for these levels are only lower limits. Comparing the elastic scattering cross section based on these J-values with the measured total cross section, appreciable inelastic scattering is indicated. The situation is further complicated by the fact that the lower resonance is almost certainly a superposition of two non-interfering levels. We have assumed $l \geq 1$, $J=3$ at 697 keV and $l=2$, $J=4$ at 727 keV. These assignments give a reasonably good fit in a one-channel description. Such "assignments" have usefulness only for an empirical description and should not be taken as a correct physical interpretation. However, such parameters may be useful for reactor calculations. In this case, it is also unlikely that a two channel description would yield unique parameters.

911 keV and 985 keV: These two levels are reasonably fitted by $l=2$, $J=3$ and $l=2$, $J=1$ respectively. Since the calculated elastic cross section peak is lower than the total cross section a larger J-value is indicated. A J-value larger than 4 cannot be caused by d-wave neutrons. If the $J=4$ assignment is correct, an inelastic reaction width of about 10 keV is indicated for the 910 keV level. For increasingly higher J-values the inelastic width will increase accordingly.

5.2 Analysis of Ca Resonances

A superficial examination of the Ca cross section reveals regions of slowly varying cross section at the low energy side and an increasing density of resonances at higher energy. Many of the resonances appear to be broad and overlapping. Nearly 60 resolved resonances were analyzed between .56 and 1.26 MeV. For analysis, the entire region was subdivided into four intervals. No attempt was made to fit the structure above 1.26 MeV. Good agreement is obtained for nearly all analyzed resonances. In between the resonances the calculation is not satisfactory. This is due in part to the presence of unresolved resonance structure. Definite assignments and parameters for these levels are impossible though their existence is regarded as certain.

At the beginning of this analysis several difficulties were encountered. The high background cross section value in the minima of broad resonances suggested unusually large p-wave scattering. Shortcomings in the experimental data could be excluded by careful examination of our cross section data and detailed comparison with recent high resolution results from other laboratories. In some cases, the resonances seemed to be better described by assuming p-wave formation, leaving the background for s-wave potential scattering. This assumption yields an unreasonable high density of p-wave levels and p-wave strength. Furthermore all of the broad resonances have been assigned to J=1/2. The assignment of these resonances to s-wave formation has been confirmed by recent differential scattering measurements /23/.

The A and B coefficients obtained for p-waves indicate a large p-wave strength in this region. Only a small fraction of this strength can be accounted for by resonances resolved, assigned and explicitly included in the multilevel sum. Undoubtedly, some of the residual strength comes from unresolved local levels. In addition, otpical model calculations predict a peak in the p-wave strength function near 3 MeV. A giant resonance trend is evident in the calcium data reported in ref. /5/. The implication and interpretation of this structure are under investigation /24/.

In view of the limited success in representing the non-resonant part of the cross section, this analysis provides detailed information of the calcium structure, but a full description of the cross section requires further investigation.

6. SUMMARY

New assignments of Na resonances based on high resolution total neutron cross section data are given for the energy range between 280 keV and 1 MeV. A satisfactory phenomenological description of the data is presented using a one channel description even above the inelastic scattering threshold. However, the uncertainty in the

J-values emphasizes the need for measurements of the differential elastic scattering and a suitable two-channel multilevel code. For calcium a resonance parameter analysis was performed using highly resolved total neutron cross sections. Level assignments were mostly obtained from differential scattering cross section data. Evidence is found for a large p-wave strength in the energy region investigated.

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TABLE I

RESONANCE PARAMETERS[a)] FOR THE ^{23}Na TOTAL NEUTRON CROSS SECTION

E_R(keV)	$\Gamma_n(E_R)$ (keV)	l	J	Γ_{obs}(keV)
298.4	1.9	0	2	
393.8	25.8	1	1	
431.2	7.8	1	0	
448.4	5.7	2	2	
508.8				
536.6	35.3	0	1	
564.1				
597.8	25.8	(1)	1	21
599.8				
627.0				
683.4				
697.2	60.	(2)	(4)	} 72
726.6	45.	(1)	(3)	
748.3				
766.4				
780.5	43.6	(2)	(4)	38
911.2	40.1	(2)	(3)	32
968.0				
985.1	27.2	(2)	(1)	16

	l=0		l=1				l=2				
J	1	2	0	1	2	3	0	1	2	3	4
A_{lJ}	.139	-.143	-.329 x10^{-1}	.630 x10^{-1}	-	.254 x10^{-1}	-	-.512 x10^{-2}	.171 x10^{-3}	.749 -10^{-1}	.139 x10^{-1}
B_{lJ}	.434 x10^{-3}	.490 x10^{-3}	.986 x10^{-3}	.679 x10^{-4}	-	.590 x10^{-4}	-	-	-	-	-

a) Analysis performed with $S_l = B_l$ and channel radius a = 4.26 f.

TABLE II

RESONANCE PARAMETERS[a)] FOR ^{40}Ca (n,n)

E_R(keV)	[b)] $_n(E_R)$(keV)	l	J	E_R(keV)	[b)] $_n(E_R)$(keV)	l	J
570.1	.2	1	3/2	924.6	.2	2	5/2
591.3	55.	0	1/2	940.5	.6	1	1/2
594.2	≤ .1	2	5/2	945.1	.5	2	(3/2)
623.5	< .1	2	(5/2)	958.8	.4	1	3/2
635.5	2.	0	1/2	970.	7.2	0	1/2
638.4	< .1	2	5/2	993.3	1.1	(2)	(3/2)
640.9	1.3	1	1/2	1003.9	11.	0	1/2
668.1	< .1	2	(5/2)	1018.7	.5	1	(3/2)
675.	2.7	0	1/2	1025.2	.3	(1)	(1/2)
694.6	.9	1	1/2	1037.4	.7	1	1/2
713.2	.1	1	3/2	1058.	.4	(1)	1/2
728.	< .1	1	3/2	1061.5	.4	(1)	1/2
738.2	3.2	0	1/2	1083.2	.7	(1)	3/2
742.8	4.4	0	1/2	1094.4	.6	2	(3/2)
747.3	.3	1	1/2	1094.9	.2	0	1/2
758.	.6	2	(3/2)	1097.7	.2	2	5/2
764.8	< .1	(2)	3/2	1126.	.5	(0)	1/2
771.5	12.	0	1/2	1129.2	.7	2	3/2
792.5	2.4	0	1/2	1160.2	.2	(2)	3/2
800.2	< .1	2	5/2	1169.	.7	1	3/2
823.	3.5	0	1/2	1189.4	3.	0	1/2
826.	.4	(1)	1/2	1202.6	4.	(2)	5/2
830.	.1	2	(5/2)	1210.8	15.	0	1/2
842.2	.9	1	3/2	1214.	1.	1	3/2
857.2	.3	2	(3/2)	1232.	1.	2	3/2
861.8	29.	0	1/2	1242.9	1.5	1	1/2
867.6	.3	1	(1/2)	1250.	.5	2	(5/2)
878.7	31.	0	1/2	1262.	.5	(2)	(3/2)
884.8	.3	1	3/2	1284.	15.	0	1/2
908.1	1.5	1	1/2				

.82 - 1 MeV	l=0	l=1		l=2	
J	1/2	1/2	3/2	3/2	5/2
A_{lJ}	.238	-.467	-.504	$.586 \times 10^{-2}$	$.345 \times 10^{-2}$
B_{lJ}	$.337 \times 10^{-4}$	$.189 \times 10^{-3}$	$.107 \times 10^{-3}$	-	-
C_{lJ}	$.250 \times 10^{-6}$	$.430 \times 10^{-6}$	$.770 \times 10^{-6}$	-	-

[a)] Analysis performed with $S_l = B_l(E)$ and channel radius a=3.59 f.

[b)] Due to the effects of resolution, the accuracy of neutron widths ≤ .5 keV is estimated to be ≈ 20 %.

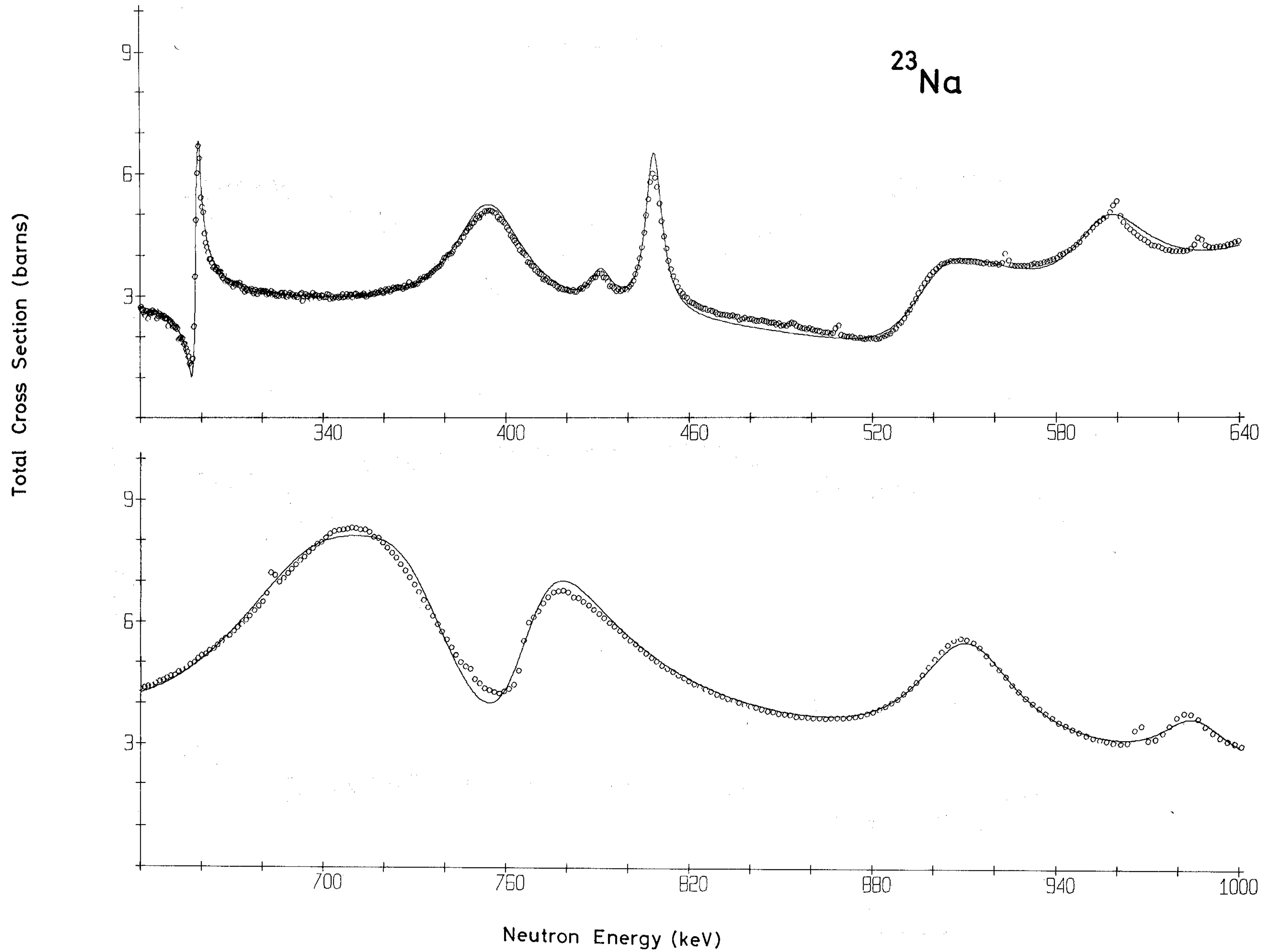
FIGURE CAPTIONS

Fig. 1 Experimental and calculated total neutron cross section of ^{23}Na from .28 to 1.02 MeV

Fig. 2 Comparison of ^{23}Na total neutron cross section data available from CCDN in the energy range from 290 to 900 keV

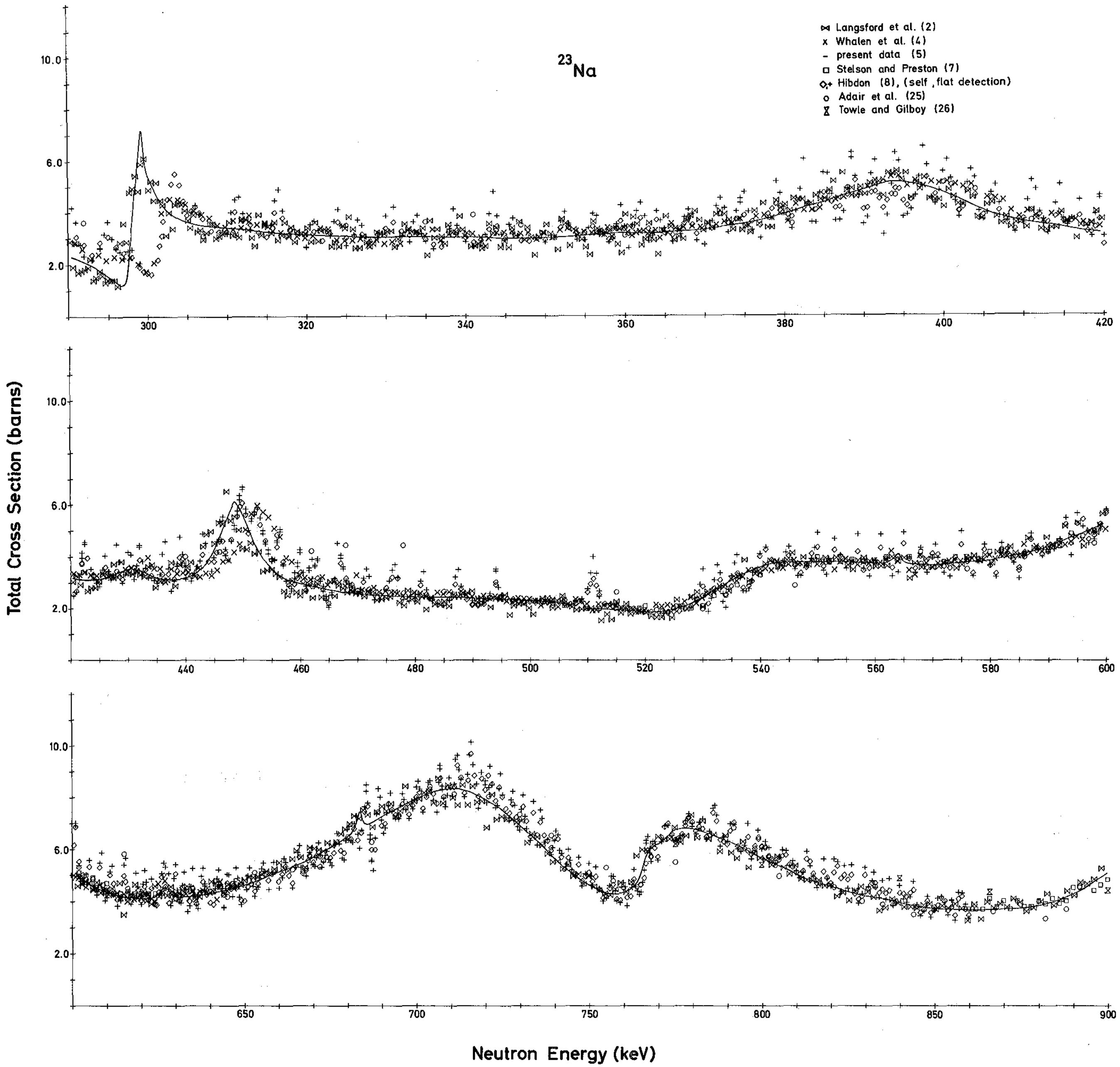
Fig. 3 Experimental and calculated total neutron cross section of Ca from 560 to 820 keV

Fig. 4 Experimental and calculated total neutron cross section of Ca from 820 to 1260 keV



23Na
Total Cross Section (barns)
9
6
3
340
400
460
520
580
640
700
760
820
880
940
1000
Neutron Energy (keV)

Fig.1



^{23}Na
⋈ Langsford et al. (2)
x Whalen et al. (4)
- present data (5)
□ Stelson and Preston (7)
◇,+ Hibdon (8), (self, flat detection)
o Adair et al. (25)
⧗ Towle and Gilboy (26)
Total Cross Section (barns)
10.0
6.0
2.0
300
320
340
360
380
400
420
440
460
480
500
520
540
560
580
600
650
700
750
800
850
900
Neutron Energy (keV)

Fig.2

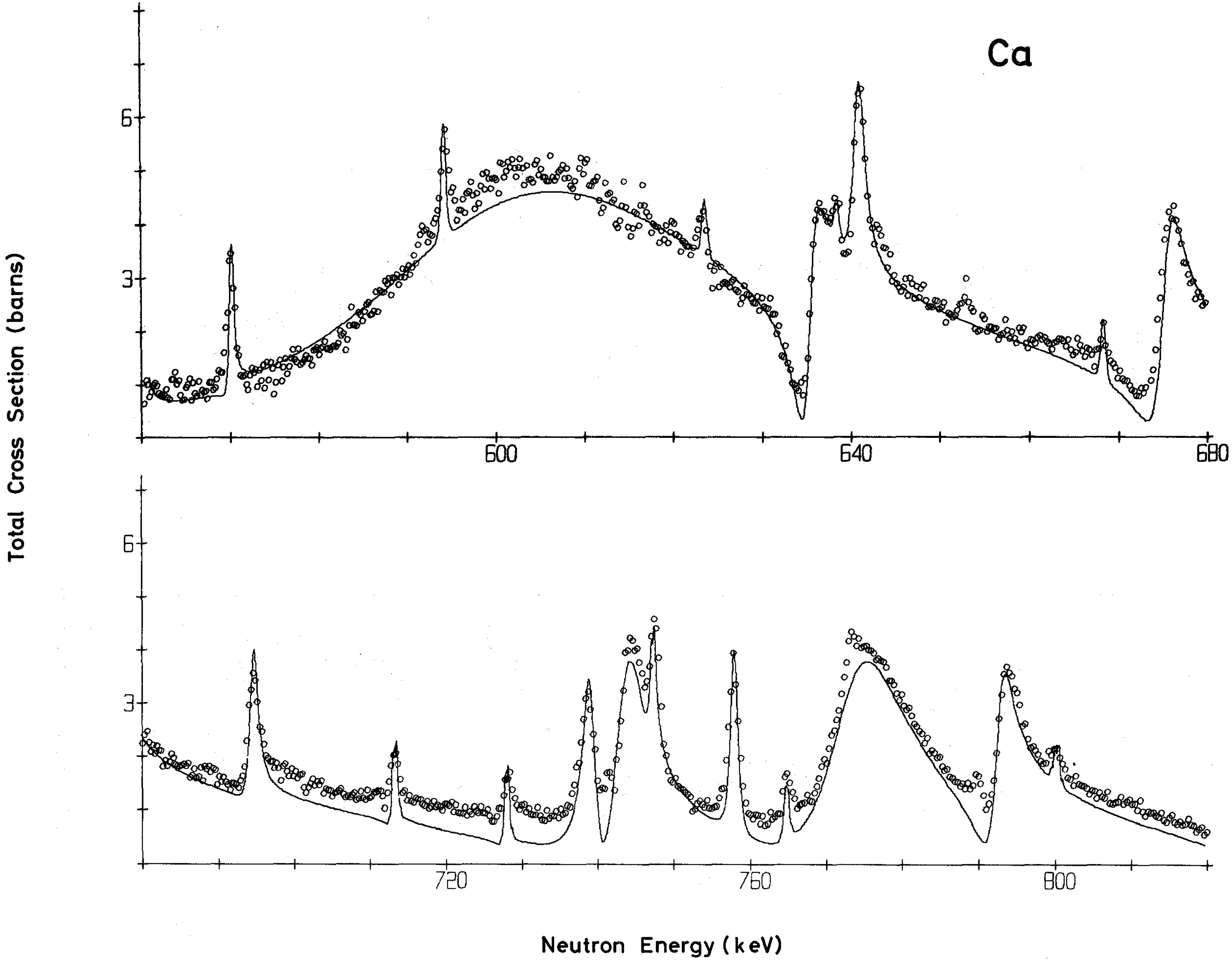

Ca
Total Cross Section (barns)
6
3
600
640
680
6
3
720
760
800
Neutron Energy (keV)

Fig. 3

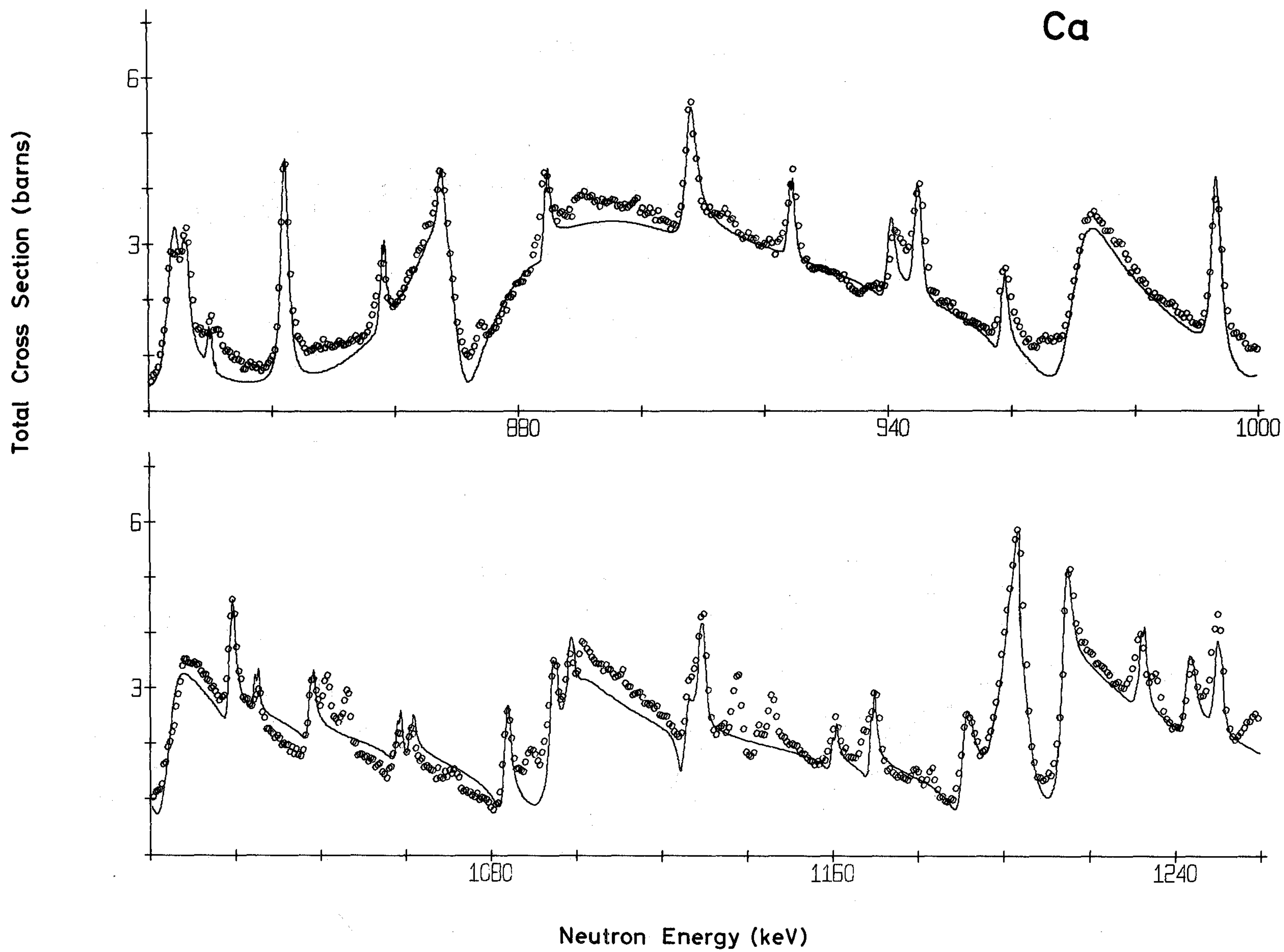

Ca
Total Cross Section (barns)
6
3
880
940
1000
6
3
1080
1160
1240
Neutron Energy (keV)

Fig. 4