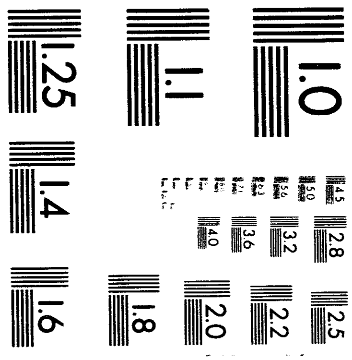
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TITLE: INTERCOMPARISON OF THEORETICAL CALCULATIONS OF IMPORTANT ACTIVATION CROSS SECTIONS FOR FUSION REACTOR TECHNOLOGY

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# Intercomparison of theoretical calculations of important activation cross sections for fusion reactor technology

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Various theoretical calculations of radionuclides in the reactions $^{94}$Mo(n,p)$^{94}$Nb, $^{109}$Ag(n,2n)$^{108m}$Ag, $^{151}$Eu(n,2n)$^{150m}$ Eu, $^{153}$Eu(n,2n)$^{152g+m2}$Eu, $^{159}$Tb(n,2n)$^{158}$Tb, $^{187}$Re(n,2n)$^{186m}$Re, $^{179}$Hf(n,2n)$^{178m2}$Hf, $^{193}$Ir(n,2n)$^{192m2}$Ir are compared. We normalize the theoretical results to the evaluated experimental data at 14.5 MeV, and take their average. This yields averaged theoretical excitation functions for the production of the various radionuclides at neutron energies ranging from threshold to 14.5 MeV. We discuss differences between the various theoretical results, and between theory and data where they exist. Our theoretical results may be used in conjunction with experimental data to produce evaluated radionuclide production cross sections for neutron energies lower than 14.5 MeV.

# I. INTRODUCTION

The International Atomic Energy Authority (IAEA) Nuclear Data Section has established a Coordinated Research Programme (CRP) on activation cross sections for the generation of long-lived radionuclides of importance in radioactive waste problems in fusion reactor technology. A number of reactions of particular importance were selected, and the CRP organized both experimental and theoretical efforts to determine production cross sections for these reactions. The first Research Coordination Meeting (RCM) was held in Vienna in November 1991 and experimental and theoretical results were presented [1]. On the basis of this first meeting, priorities for future work were established. Further measurements and calculations were presented at the second RCM of the CRP, held at Del Mar, California, April 29-30, 1993. A number of different groups have performed theoretical cross section calculations, and at the Del Mar meeting a recommendation was made to perform an intercomparison of the theoretical works. This intercomparison was performed at Lawrence Livermore National Laboratory.

A comparison of theoretical calculated cross sections for the production of radionuclides should play a number of useful roles: it identifies cases where discrepancies exist between calculations and therefore stimulates further theoretical work to understand (and hopefully remove) differences; the comparison yields spreads in theoretical calculations which can be interpreted as uncertainties in the calculations; and the averaged theoretical results can be used, with data where it exists, to provide evaluated cross sections at energies lower than 14.5 MeV.

As there is often only sparse experimental information on production cross sections of radioactive nuclides at energies lower than 14.5 MeV, theoretical calculation of the shape of the excitation functions for the production of these nuclides can be very useful. Such calculations are often normalized to the experimental value at 14.5 MeV, and then used to obtain cross sections at lower incident neutron energies. To facilitate this procedure, we compare all theoretical calculations for the excitation functions of the various reactions considered in this RCM and determine averaged theoretical excitation functions for each reaction. For some reactions there does exist experimental data at lower neutron energies. Apart from commenting on how the calculations compare with the data, we do not include this information in our work. Thus, in cases where there is data at neutron energies lower than 14.5 MeV, further evaluation work is needed before a recommended excitation function for fusion technology applications can be provided.

The various groups who have calculated radionuclide production cross sections are as follows: M.B. Chadwick and P.G. Young (GNASH code system); A.V. Ignatyuk, O.T. Grudzevich, and A. Pashchenko (STAPRE code system); Yamamuro (SINCROS-II code system); J.W Meadows (GNASH code system); and M. Gardner and D. Gardner (STAPLUS code system). All these calculations are based on Hauser-Feshbach compound nucleus theory with preequilibrium emission, and in some cases include direct reactions with a DWBA or coupled-channels approach. We refer the reader to the various contributing authors for specific details of the calculations (and see Refs. [1–6]).

In section II we describe our method of intercomparison, and in section III we present our results in both graphic and tabular form, and make some observations on them. In section IV we present our conclusions and recommendations for further work.

## II. INTERCOMPARISON METHOD

Various groups have determined the radionuclide production cross sections with differing methods, and consequently obtain differing results. We decided to combine these calculations by normalizing each calculation to the evaluated 14.5 MeV value, and determine their average. This produces an average theoretical excitation function for each of the reactions, from threshold to 14.5 MeV. One could examine the various assumptions made in the calculations (optical potentials, level densities, preequilibrium models, etc) and assess the accuracy of each calculation. This would be a useful task to perform in the future. But for the moment we have used equal weightings for all calculations when obtaining the average. Our procedure is thus:

- Normalize theoretical calculations to the 14.5 MeV evaluated values of Vonach *et al.* [7, 8].
- Produce splined fits of each set of calculated excitation functions and obtain theoretical values on a common 0.5 MeV-spaced grid
- Average the various theoretical curves on this same common grid of energy values

## III. RESULTS

In figures 1-8 we show the various theoretical calculations and the averaged theoretical value, for the production cross sections of the various radionuclides. The averaged values are shown in numerical form in Table.1.

On the basis of these comparisons we make the following observations:

1. Whilst there are some reactions for which the various theoretical calculations agree closely, in many cases agreement between calculations is poor. Calculations vary considerably for the reactions $^{109}$Ag(n,2n) $^{108m}$Ag, $^{153}$Eu(n,2n)$^{152g+m2}$Eu, $^{187}$Re(n,2n)$^{186m}$Re, $^{193}$Ir(n,2n)$^{192m2}$Ir (Figs. 2,4,6,8).

2. Experimental data below 10.7 MeV neutron energy has been recently measured at Julich/Debrecen [9], for the reactions $^{151}$Eu(n,2n)$^{150m}$Eu and $^{159}$Tb(n,2n)$^{158}$Tb. Furthermore, experimental data has recently been obtained at 10.7 MeV neutron energy for these two reactions, as well as for the reaction $^{109}$Ag(n,2n)$^{108m}$Ag by the Argonne-Los Alamos-JAERI collaboration [6]. In all

these cases the theoretical calculations consistently exceed the measurements by a factor of 2, or more.

3. It is interesting to note the very different shape of the $^{179}$Hf(n,2n)$^{178m2}$Hf compared to the other (n,2n) excitation functions. This is due to the extremely high spin (16+) of the isomer, and the calculations of Chadwick *et al.* [2] and Ignatyuk *et al.* [3] agree closely.

## IV. CONCLUSIONS

The theoretical calculations of production cross sections of the radionuclides described in this paper can be used to obtain evaluated cross sections for neutron energies below 14.5 MeV. But before this can be done, a number of inconsistencies must be addressed. Firstly, the nuclear model calculations should be compared in detail to understand why differences are obtained in certain reactions. Secondly, the large discrepancies between theory and experiment near threshold in the reactions $^{151}$Eu(n,2n)$^{150m}$Eu, $^{159}$Tb(n,2n)$^{158}$Tb, and $^{109}$Ag(n,2n)$^{108m}$Ag should be understood. We plan to report on these two tasks at the final RCM of the CRP.

## V. ACKNOWLEDGMENTS

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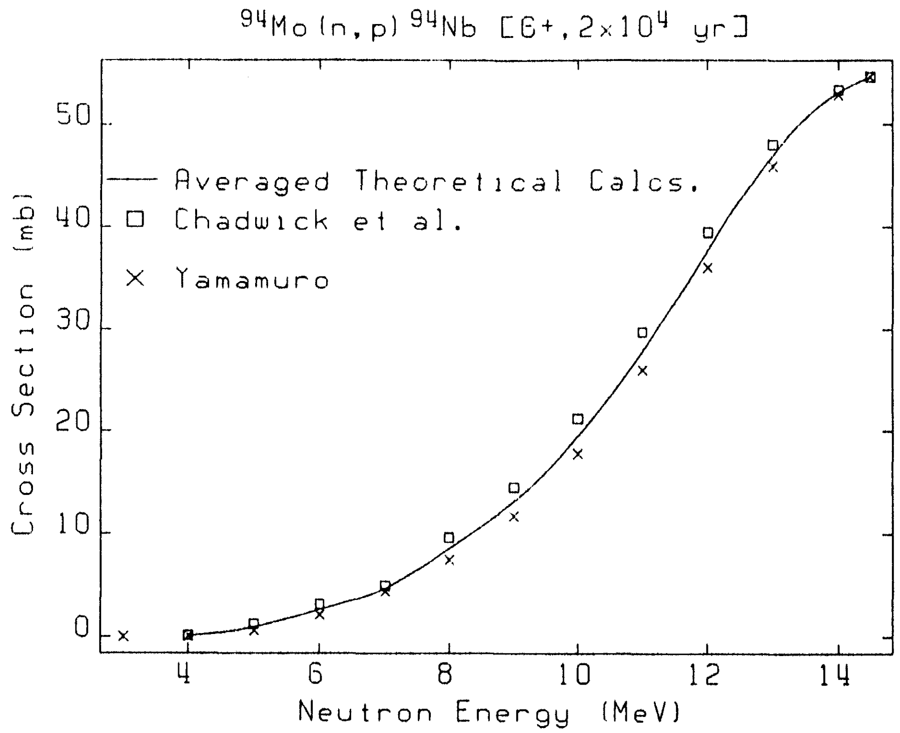


Fig. 1. Theoretical cross sections for (n,p) production of $^{93}$Nb, normalized to a value of 54.5 mb at 14.5 MeV [7].

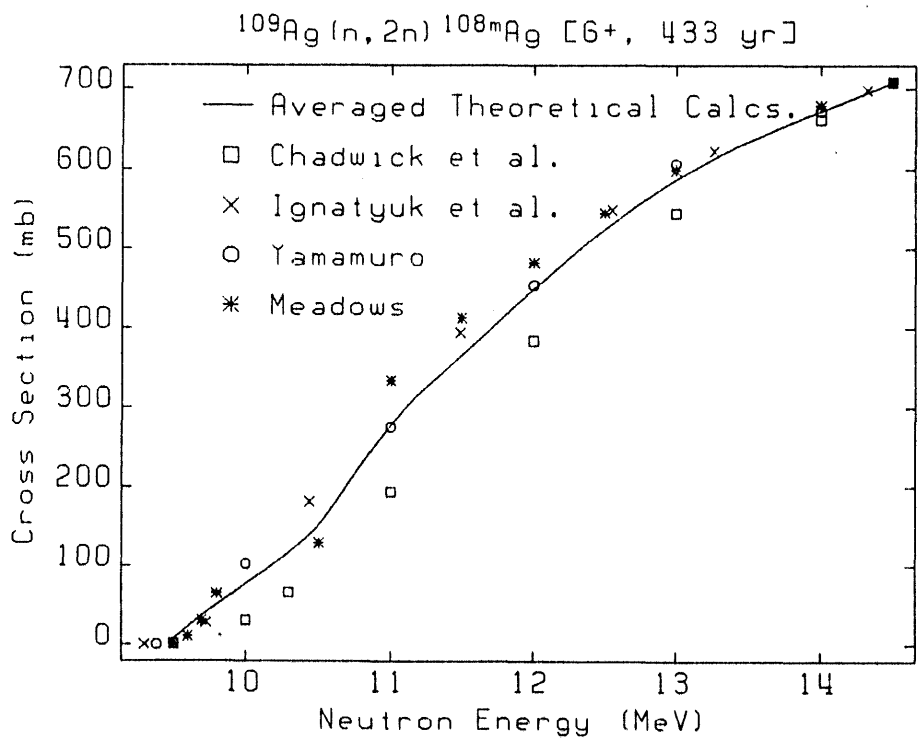


Fig. 2. Theoretical cross sections for (n,2n) production of $^{108m}$Ag, normalized to a value of 708 mb at 14.5 MeV [7].

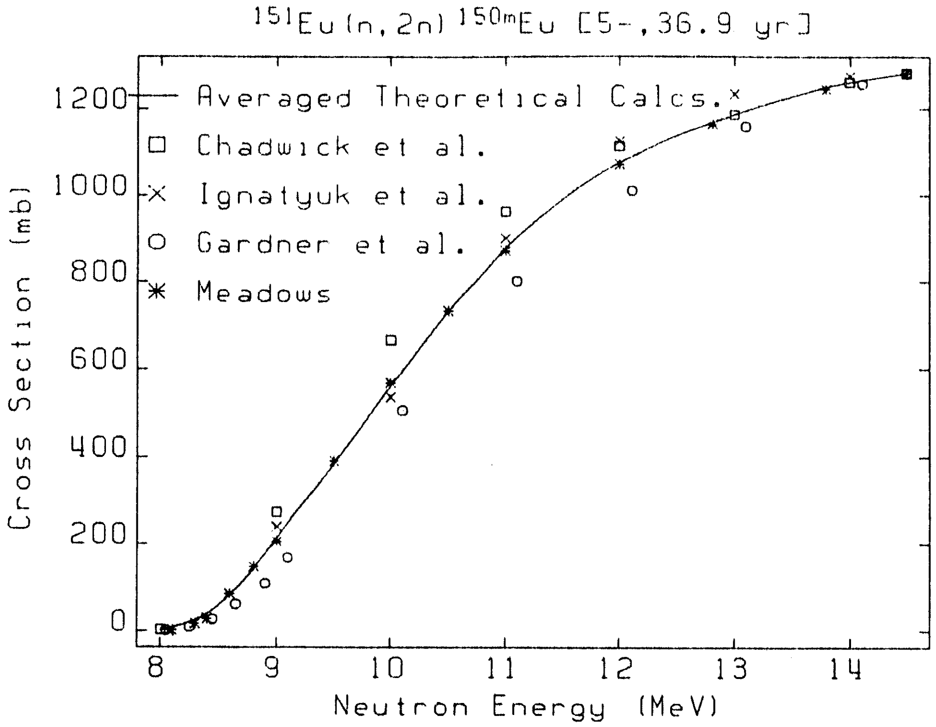


Fig. 3. Theoretical cross sections for (n,2n) production of $^{150m}$Eu, normalized to a value of 1282 mb at 14.5 MeV [7].

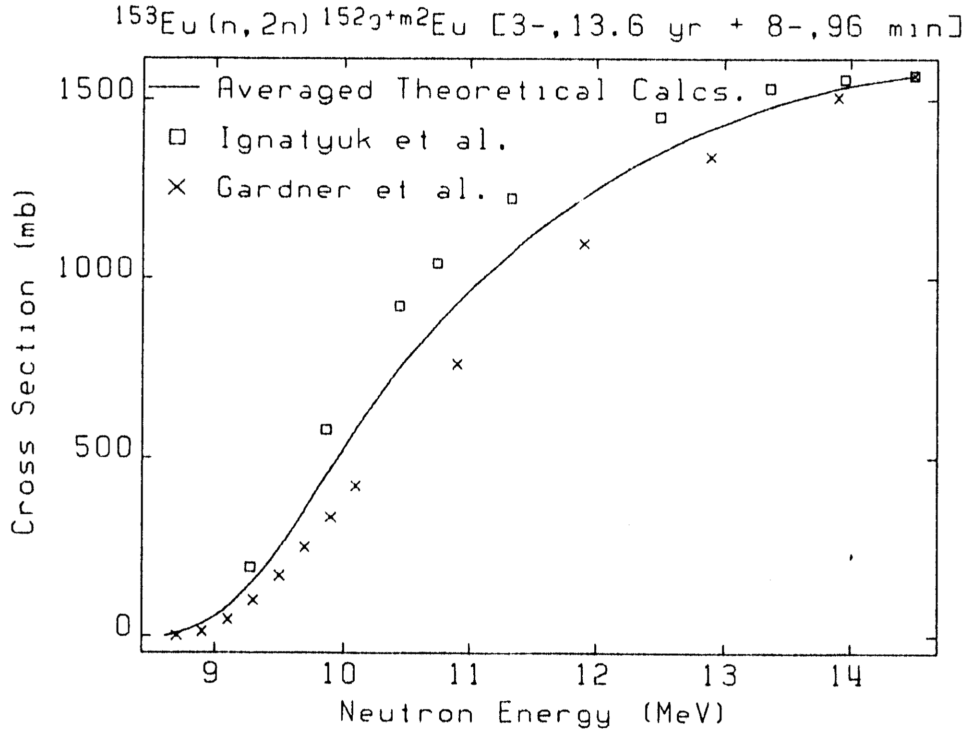


Fig. 4. Theoretical cross sections for (n,2n) production of $^{152g+m2}$Eu, normalized to a value of 1568 mb at 14.5 MeV [7].

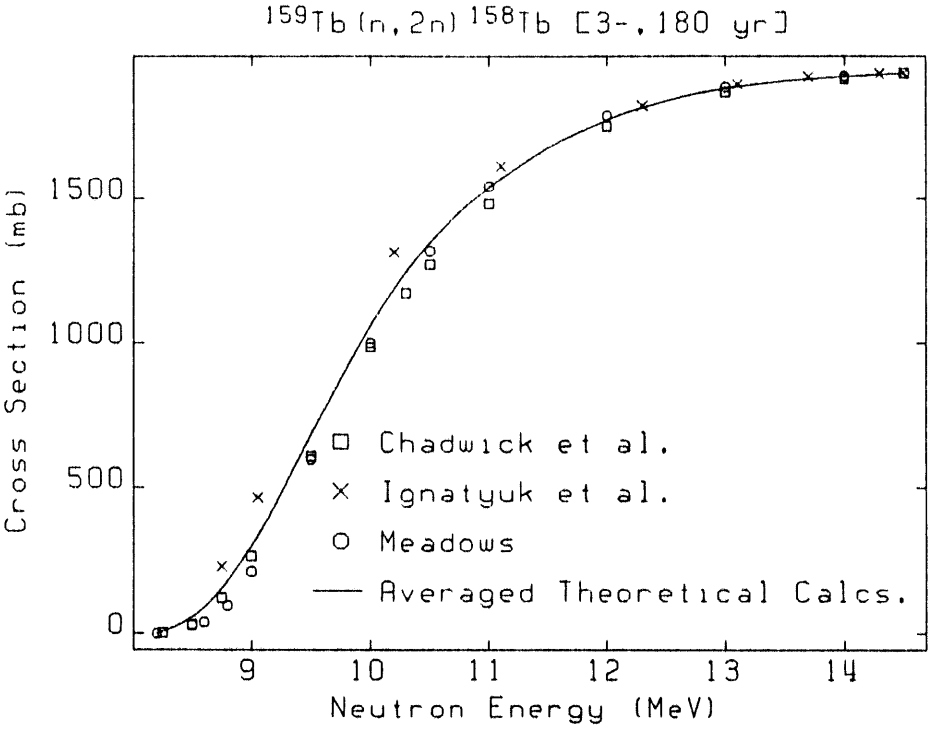


Fig. 5. Theoretical cross sections for (n,2n) production of $^{158}$Tb, normalized to a value of 1929 mb at 14.5 MeV [7].

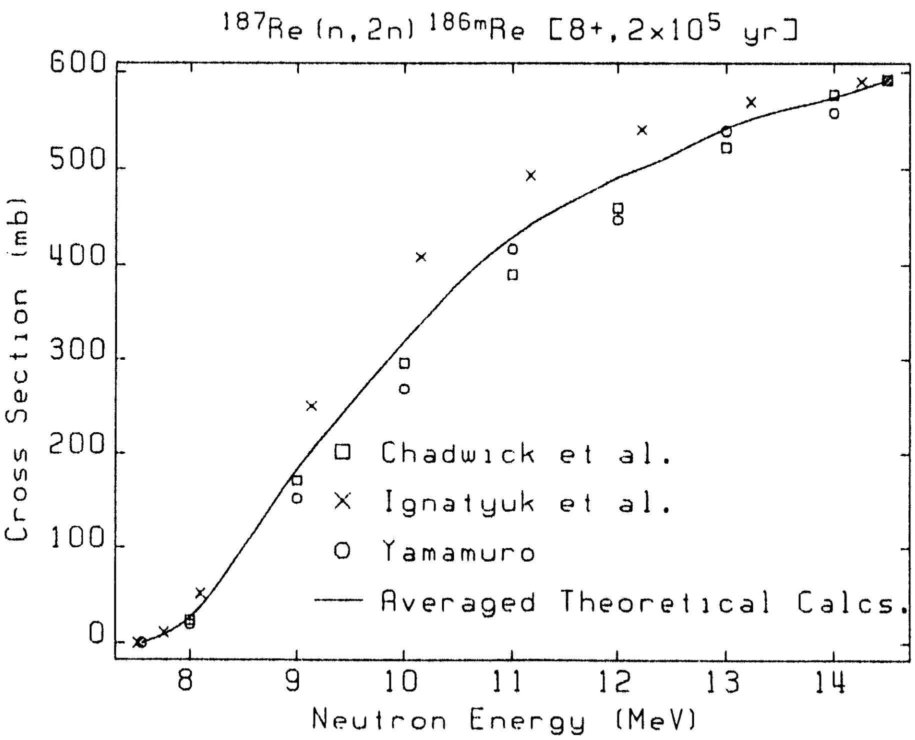


Fig. 6. Theoretical cross sections for (n,2n) production of $^{186m}$Re, normalized to a value of 592 mb at 14.5 MeV [8].

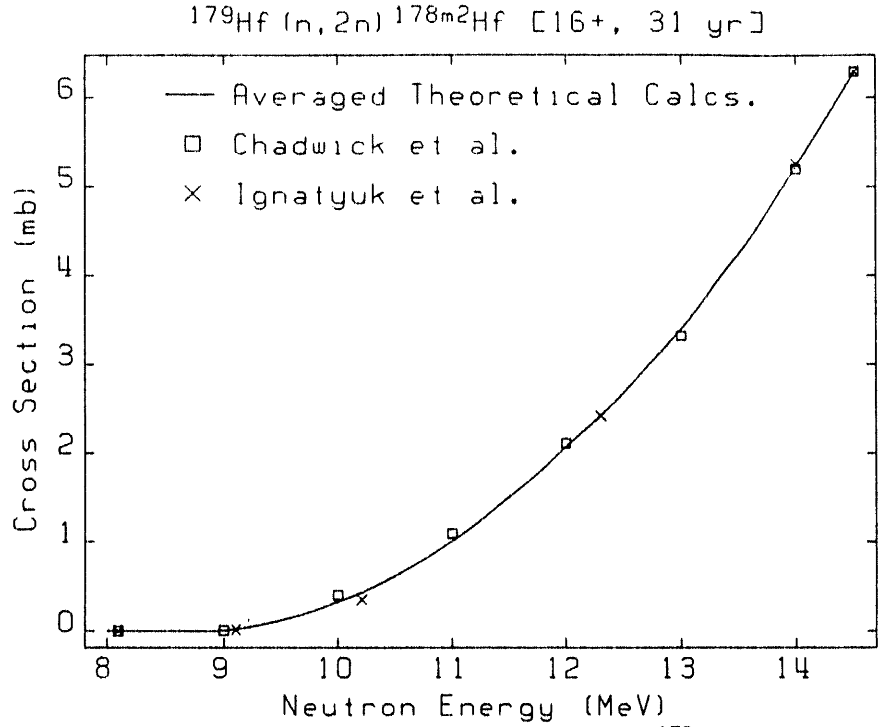


Fig. 7. Theoretical cross sections for (n,2n) production of $^{178}$Hf, normalized to a value of 6.29 mb at 14.5 MeV [7].

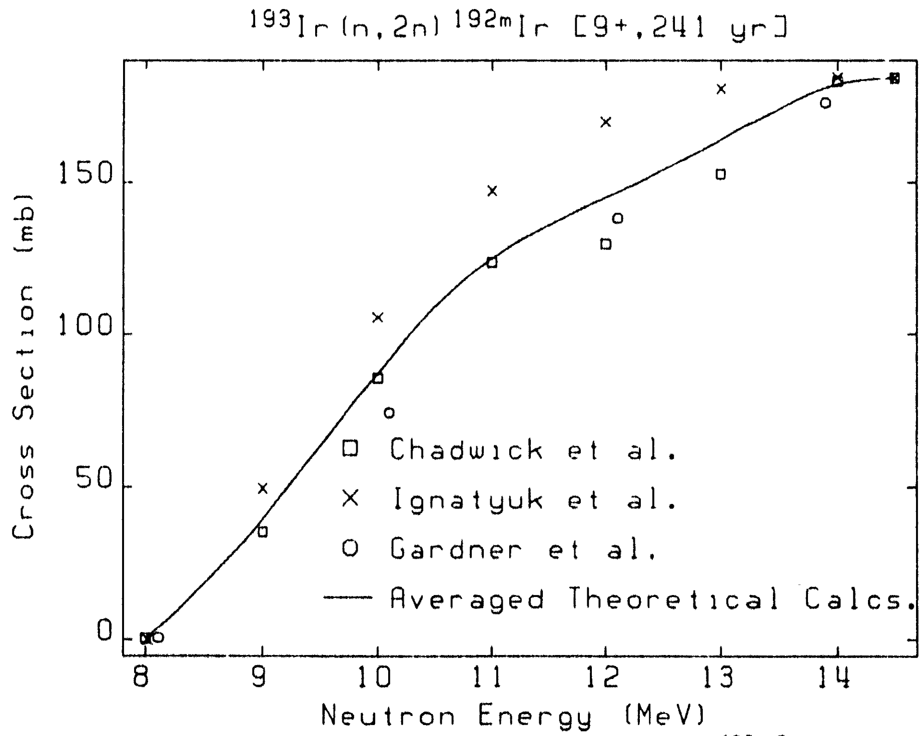


Fig. 8. Theoretical cross sections for (n,2n) production of $^{192m2}$Ir, normalized to a value of 184 mb at 14.5 MeV [8].

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[9] S. Qaim, F. Cserpak and J. Csikai, "Cross Sections for $^{151}$Eu(n,2n)$^{150m}$Eu and $^{159}$Tb(n,2n)$^{158}$Tb Reactions Near Their Thresholds", Appl. Radiat. Isot. **43**, 1065 (1992); also see S. Qaim, contributed paper in present proceedings.

Table I. Numerical values for averaged theoretical cross sections (mb).

**Table 1:**

| E (MeV) | #1 | #2 | #3 | #4 | #5 | #6 | #7 | E (MeV) | #8 |
|---|---|---|---|---|---|---|---|---|---|
| 8.0 | | 1.16 | | | 26.60 | | 3.24 | 4.0 | 0.08 |
| 8.5 | | 57.69 | | 57.87 | 100.00 | | 18.70 | 5.0 | 0.95 |
| 9.0 | | 212.81 | 55.19 | 300.93 | 183.00 | 0.01 | 39.60 | 6.0 | 2.66 |
| 9.5 | 7.50 | 384.60 | 247.74 | 680.94 | 254.00 | 0.12 | 63.50 | 7.0 | 4.71 |
| 10.0 | 77.17 | 562.80 | 525.28 | 1059.02 | 319.00 | 0.33 | 87.10 | 8.0 | 8.56 |
| 10.5 | 152.22 | 732.02 | 771.46 | 1344.51 | 380.00 | 0.62 | 109.00 | 9.0 | 13.13 |
| 11.0 | 277.54 | 876.89 | 965.89 | 1535.48 | 429.00 | 1.01 | 125.00 | 10.0 | 19.51 |
| 11.5 | 366.04 | 990.99 | 1125.82 | 1672.44 | 463.00 | 1.51 | 136.00 | 11.0 | 27.85 |
| 12.0 | 448.87 | 1075.60 | 1251.26 | 1768.89 | 491.00 | 2.07 | 145.00 | 12.0 | 37.77 |
| 12.5 | 524.63 | 1138.42 | 1354.75 | 1834.48 | 515.00 | 2.69 | 154.00 | 13.0 | 47.03 |
| 13.0 | 586.93 | 1187.13 | 1433.15 | 1876.92 | 542.00 | 3.40 | 164.00 | 14.0 | 53.03 |
| 13.5 | 634.37 | 1229.44 | 1495.87 | 1901.99 | 560.00 | 4.24 | 174.00 | 14.5 | 54.50 |
| 14.0 | 672.60 | 1261.49 | 1539.78 | 1917.43 | 574.00 | 5.23 | 182.00 | | |
| 14.5 | 708.00 | 1282.00 | 1568.00 | 1929.00 | 592.00 | 6.29 | 184.00 | | |

Reactions are labelled as follows:-

#1 $^{109}Ag(n,2n)^{108m}Ag$ (6+)

#2 $^{151}Eu(n,2n)^{150m}Eu$ (5-)

#3 $^{153}Eu(n,2n)^{152g+m2}Eu$ (3-,8-)

#4 $^{159}Tb(n,2n)^{158}Tb$ (3-)

#5 $^{187}Re(n,2n)^{186m}Re$ (8+)

#6 $^{179}Hf(n,2n)^{178m2}Hf$ (16+)

#7 $^{193}Ir(n,2n)^{192m2}Ir$ (9+)

#8 $^{94}Mo(n,p)^{94}Nb$ (6+)